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Resonant nonlinear response of a nanomechanical system with broken symmetry

Dr. Gianluca Rastelli, Prof. Mark Dykman, Prof. Eva Weig, Dr. Jana Ochs, Dr. Maximilian Seitner

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

We study the response of a weakly damped vibrational mode of a nanostring resonator to a moderately strong resonant driving force. Because of the geometry of the experiment, the studied flexural vibrations lack inversion symmetry. As we show, this leads to a nontrivial dependence of the vibration amplitude on the force parameters. For a comparatively weak force, the response has the familiar Duffing form, but for a somewhat stronger force, it becomes significantly different. Concurrently there emerge vibrations at twice the drive frequency, a signature of the broken symmetry. Their amplitude and phase allow us to establish the cubic nonlinearity of the potential of the mode as the mechanism responsible for both observations. The developed theory goes beyond the standard rotating-wave approximation. It quantitatively describes the experiment and allows us to determine the nonlinearity parameters.

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Engineering the speedup of quantum tunneling in Josephson systems via dissipation

Dr. Gianluca Rastelli

MC23: Superconducting Circuits for Quantum Technologies VI, August 23, 2022, 4:30 PM - 5:30 PM

We theoretically investigate the escape rate occurring via quantum tunneling in a system affected by tailored dissipation. Specifically, we study the environmental assisted quantum tunneling of the superconducting phase in a current-biased Josephson junction. We consider Ohmic resistors inducing dissipation both in the phase and in the charge of the quantum circuit. We find that the charge dissipation leads to an enhancement of the quantum escape rate. This effect appears already in the low Ohmic regime and also occurs in the presence of phase dissipation that favors localization. Inserting realistic circuit parameters, we address the question of its experimental observability and discuss suitable parameter spaces for the observation of the enhanced rate.

D. Maile, J. Ankerhold, S. Andergassen, W. Belzig, and G. Rastelli
Phys. Rev. B 106, 045408, (2022).

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Exploiting the chemistry of liquid metallic hydrogen in mixtures with other elements

Dr Kees Van Der Beek, Professor Dr Dominik Kraus

MC38: Controlled irradiation Disorder in Model Systems: Organisation, Dynamics, and Transformations VIII, August 24, 2022, 4:30 PM - 6:00 PM

High energy densities can significantly alter the electronic structure of materials. The pressure-induced insulator-metal transition of hydrogen is a model case that has been subject of theoretical and experimental studies for many decades. Here we present evidence for the creation of liquid metallic hydrogen in C-H mixtures shock-compressed to pressures around ~150 GPa and temperatures of ~5000 K, which was probed by different in situ X-ray methods at X-ray free electron lasers. Our observations suggest new ways to study the chemical properties of this exotic state in mixture with other elements, which is highly relevant for a better understanding for the interiors of giant planets. Moreover, exploting liquid metallic hydrogen chemistry may allow to realize the synthesis of highly interesting materials such as tailored nanodiamonds with specific color centers, new ultrahard forms of carbon or hydride-based compounds possibly providing room-temperature superconductivity.

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What next for nematic liquid crystals?

Professor Helen F Gleeson

Liquid crystals allowed the development of the low-cost, lightweight, flat panel displays that underpinned the mobile revolution of our society about 20 years ago. Such devices make use of nematic liquid crystals, the simplest of a zoo of possible phases, which exhibits only long-range orientational (and no positional) order. Despite its simplicity, this genus of liquid crystals continues to offer surprises that are both intriguing in terms of their underlying physics and for the applications they could influence. This talk will describe two such systems. The responsive, shape-changing properties of nematic liquid crystal elastomers (LCEs) are the first category that the talk will address. LCEs are well-known and have inspired imaginative suggestions for applications including as artificial muscles, irises and sensors. However, the recent discovery of a family of nematic LCEs as the first synthetic molecular auxetics – with a negative Poisson's ratio - has both broadened the possibilities and provided a puzzle in understanding the physics underlying the auxetic behaviour. The second topic to be addressed is the recently-discovered polar nematic phase, which has values of spontaneous polarization that rival those of molecular crystals. These materials again offer wide-ranging and interesting applications, alongside challenges to understanding their behaviour. The talk will describe the physics of these two nematic systems, current understanding of the key parameters that control them and will speculate on some ways in which they might contribute to global challenges.

1

Levitated Electromechanics

Dr. James Millen, Dr Muddassar Rashid, Ms Katie O'Flynn, Ms Yugang Ren, Dr. Benjamin Stickler

MC17: Nanomechanical and Electromechanical Systems VIII, August 24, 2022, 4:30 PM - 6:00 PM

Nanoparticles levitated in optical fields have proven to be invaluable for studies of nanothermodynamics, fundamental quantum physics, and are amongst the most sensitive sensors of force and torque ever created. However, optical systems are challenging to miniaturize for deployment in technology.

Charged particles levitated in electrical potentials offer an exciting alternative. By coupling their motion to nearby electrodes we create an electromechanical system which circumvents the loss of quality factor with decreasing size, as seen in traditional MEMS devices.

Furthermore, we have shown that theoretically the interaction between a charged nanoparticles and nearby electrodes can be coherent, which would enable the creation of miniaturized levitated quantum electromechanical devices, for use as quantum signal transducers and for the distribution of entanglement.

4

Parity switching in a full-shell superconductor-semiconductor nanowire qubit

Deividas Sabonis

The rate of charge-parity switching in a full-shell superconductor-semiconductor nanowire qubit is measured by directly monitoring the dispersive shift of a readout resonator. At zero magnetic field, the measured switching time scale TP is on the order of 100 ms. Two-tone spectroscopy data post-selected on charge-parity is demonstrated. With increasing temperature or magnetic field,
TP is at first constant, then exponentially suppressed, consistent with a model that includes both non-equilibrium and thermally activated quasiparticles. As TP is suppressed, qubit lifetime T1 also decreases. The long TP ~ 0.1 s at zero field is promising for future development of qubits based on hybrid nanowires.

2

State Lifetime of a Synthetic Two-Level System

Gabriel Margiani, Sebastián Guerrero, Toni L. Heugel, Christian Marty, Raphael Pachlatko, Thomas Gisler, Gabrielle D. Vukasin, Hyun-Keun Kwon, James ML Miller, Nicholas E. Bousse, Thomas W. Kenny, Oded Zilberberg, Deividas Sabonis, Alexander Eichler

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

We compare the suitability of several mathematical methods to characterize the lifetime of two-level systems. The methods deal in different ways with random-walk fluctuations during a switch. Such fluctuations are not captured by a simple telegraph-noise picture and can lead to a significant overestimation of the switching rate. We show that this problem can be avoided by choosing the correct counting method. In addition to known methods relying on thresholds and the power spectral density of fluctuations, we establish that a peak in the Allan variance of fluctuations can be used to determine the lifetime. As a simple, classical test system, we utilize a nonlinear Kerr resonator driven into parametric oscillations regime, whose stable solutions mimic the physics of a single spin. We also provide an outlook of how our methods can be used to study Kramer's turnover in the synthetic quasi-potential of a parametric oscillator.

Fabrication was performed in nano@Stanford labs, which are supported by the National Science Foundation (NSF) as part of the National Nanotechnology Coordinated Infrastructure under Award No. ECCS-1542152, with support from the Defense Advanced Research Projects Agency’s Precise Robust Inertial Guidance for Munitions (PRIGM) Program, managed by Ron Polcawich and Robert Lutwak. This work was further supported by the Swiss National Science Foundation through grants (CRSII5 177198/1) and (PP00P2 163818), a DFG Heisenberg grant, and SFB 1432.

5

Turning toward the crowd: Active phase separation based on non-reciprocal torques

Jie Zhang, Ricard Alert, Jing Yan, Ned S. Wingreen, Steve Granick

Studies of active matter, from molecular assemblies to animal groups, have revealed two broad classes of behavior: alignment interactions yield orientational order and collective motion, whereas repulsive interactions lead to self-trapping and motility-induced phase separation. I will present a third class of behavior: orientational interactions that produce active phase separation. Combining theory and experiments on self-propelled Janus colloids, we show that stronger repulsion on the rear than on the front of these particles produces non-reciprocal torques that reorient particle motion towards high-density regions. Particles thus self-propel towards crowded areas, which leads to phase separation. Because this torque-based aggregation requires no self-trapping, particles in clusters retain substantial speed, and clusters remain dilute and unjammed. Overall, our work identifies a torque-based mechanism for phase separation in active fluids, and it shows that orientational interactions can yield coexisting phases with no internal orientational order.

6

An active wetting transition enables optimal collective durotaxis

Macià Esteve Pallarès, Irina Pi-Jaumà, Isabela Corina Fortunato, Valeria Grazú, Manuel Gómez-González, Pere Roca-Cusachs, Jesus M. de la Fuente, Ricard Alert, Raimon Sunyer, Jaume Casademunt, Xavier Trepat

The directed migration of cellular clusters enables morphogenesis, wound healing and collective cancer invasion. Gradients of substrate stiffness are known to direct migration of cellular clusters in a process called collective durotaxis, but underlying mechanisms remain unclear. Combining theory and experiments, we have identified a mode of collective durotaxis that emerges at the proximity of an active wetting transition. We show that clusters of cancer cells dewet soft substrates and wet stiff ones, displaying poor motility. At intermediate stiffness, close to the active wetting transition, clusters become highly motile and exhibit optimal durotaxis. Durotactic velocity increases with cluster size, stiffness gradient, and actomyosin activity. We demonstrate this behavior both on substrates coated with E-cadherin and with extracellular matrix. We develop a physical model of three-dimensional active wetting that explains this mode of collective durotaxis in terms of a balance between in-plane active traction and tissue contractility, and out-of-plane surface tension. Finally, we show that the distribution of cluster displacements has a heavy tail, with infrequent but large cellular hops that contribute to durotactic migration. Our study demonstrates a physical mechanism of collective durotaxis, through both cell-cell and cell-substrate adhesion ligands, based on the wetting properties of active droplets.

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Active elastocapillarity in soft solids with negative surface tension

Dr Jack Binysh, Dr Tom Wilks, Dr Anton Souslov

MC6: Emergent Phenomena in Driven Soft, Active and Biological Matter IV, August 23, 2022, 11:30 AM - 12:30 PM

Active solids consume energy to allow for actuation, shape change, and wave propagation not possible in equilibrium. Whereas active interfaces have been realized across many experimental systems, control of three-dimensional (3D) bulk materials remains a challenge. Here, we develop continuum theory and microscopic simulations that describe a 3D soft solid whose boundary experiences active surface stresses. The competition between active boundary and elastic bulk yields a broad range of previously unexplored phenomena, which are demonstrations of so-called active elastocapillarity. In contrast to thin shells and vesicles, we discover that bulk 3D elasticity controls snap-through transitions between different anisotropic shapes. These transitions meet at a critical point, allowing a universal classification via Landau theory. In addition, the active surface modifies elastic wave propagation to allow zero, or even negative, group velocities. These phenomena offer robust principles for programming shape change and functionality into active solids, from robotic metamaterials down to shape-shifting nanoparticles.

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Frequency comb from nonlinear damping in nanomechanical resonators

Jana Ochs, Gianluca Rastelli, Daniel Boneß, Wolfgang Belzig, Mark Dykman, Eva Weig

MC17: Nanomechanical and Electromechanical Systems VI, August 23, 2022, 4:30 PM - 6:00 PM

Since their discovery, optical frequency combs have revolutionized the field of metrology [1,2]. Consisting of many, equally spaced and narrow spectral lines, an unknown optical frequency can be measured by heterodyning it with one of the comb lines. Importantly, due to the large span of the comb its spacing and position can be determined in terms of the SI second by comparing the comb with the microwave Caesium time standard. In optical systems a frequency comb can be generated by modulating the parameters of a laser periodically, for example.

We discuss the generation of a frequency comb in a single nanomechanical mode that relies only on a single input frequency. Above a critical drive power the steady states in the rotating frame become unstable. The resonator performs self-sustained oscillations of its quadratures and a frequency comb in the power spectrum emerges (Panel A).

With increasing drive strength, the self-sustained oscillations become more and more non-sinusoidal which is reflected in the formation of more comb peaks. Both, the separation and the number of satellite peaks spanning the comb are controlled by the drive strength and detuning.

The experimental observations can be described by a model based on a nonlinear potential with a quartic (Duffing) and a cubic nonlinearity. The latter one breaks the symmetry of the system [3]. The theoretical key ingredient which ultimately leads to the generation of the frequency comb is a nonlinear and negative dissipation mechanism. By taking a negative resonantly induced friction force (RIFF) into account we can explain why the rotating coordinates start to move away from the stationary point and perform self-sustained oscillations [4]. Importantly, the RIFF reduces as the system starts to perform oscillations in the rotating frame and therefore the systems oscillation stabilizes at a fixed value of the quasienergy (Panel B). This mechanism explains the emergence of a frequency comb within a single mode.

Striving for the most simplistic model which can explain the experimental observations we assume a force-dependent linear damping coefficient. With this model at hand, we are able to reproduce the qualitative features of the experimental observations (red dots Panel A). In this talk, I will shortly present the mentioned experimental observation and focus on the theoretical aspects.

[1] Th. Udem et. al., Nature 416, 233-237 (2002)
[2] S. T. Cundiff et. al., Rev. Sci. Instrum. 72, 3749 (2001)
[3] J. S. Ochs et al., PRB 104, 155434 (2021)
[4] M. I. Dykman et al., PRL 122, 254301 (2019)

7

Quantum many-body scars have extensive multipartite entanglement

Jean-yves Desaules

MC42: Broken Ergodicity and Localisation in Quantum Many-body Systems VI, August 23, 2022, 4:15 PM - 5:30 PM

Recent experimental observation of weak ergodicity breaking in Rydberg atom quantum simulators has sparked interest in quantum many-body scars - eigenstates which evade thermalisation at finite energy densities due to novel mechanisms that do not rely on integrability or protection by a global symmetry. A salient feature of quantum many-body scars is their sub-volume bipartite entanglement entropy. In this work we demonstrate that exact many-body scars also possess extensive multipartite entanglement structure. We show this analytically, through a scaling of the quantum Fisher information density, which is found to be extensive for scarred eigenstates in contrast to generic thermal states. Furthermore, we numerically study signatures of multipartite entanglement in the PXP model of Rydberg atoms, showing that extensive quantum Fisher information can be generated dynamically by performing a global quench experiment. Our results identify a rich multipartite correlation structure of scarred states with significant potential as a resource in quantum enhanced metrology.

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A thought experiment: let’s make our upcoming trips public

Maxime Deforet

In-person scientific conferences have been interrupted during the Covid pandemic. Some were replaced by online meetings (or hybrid), with some benefits. Yet, in-person meetings are favoured over virtual ones. In parallel, scientific conferences represent a large part of academic research carbon footprint. The long-term target of the Paris Agreement is 2 tons of greenhouse gases per capita by 2050. We are now in position to decide between: going back to normal and continue to gather in international meetings, or cut back on travels for scientific conferences and return to virtual meetings.
In this context, I propose a thought experiment: let’s make our upcoming trips public. This could have three positive consequences:
- A more efficient carbon footprint: This would not reduce the carbon footprint but allow to get the most of out it, by helping organise more meetings per travel.
- Increased connectedness: People from geographically distant labs, or from distant fields, would meet more easily.
- Facilitated planning: If/when climate change becomes so severe that strong travel limitations are enforced, this system will allow to efficiently plan ahead our trips to combine visits to various institutions (similarly to what scholars were doing for long, including Marie Curie in the US in 1931 for 6 weeks).
I will discuss possible implementations in online platforms already in use by scientists.

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Multiscale analysis of colony expansion in a run-reverse motile bacteria

Maxime Deforet

MC6: Emergent Phenomena in Driven Soft, Active and Biological Matter I, August 22, 2022, 11:30 AM - 12:30 PM

A colony of motile bacteria is a good experimental example of coupling between single-cell motility behaviour and large scale colony expansion. To which extent does the behaviour of each cell control the spreading dynamics of the whole colony? An answer could lie at an intermediate scale: collective motility and long-range correlation (typically 100 µm) emerge from cell-cell interactions (typically 1 µm), and yield to colony morphogenetic patterns (typically 10 mm). I investigate this multiscale coupling in the bacterium Pseudomonas aeruginosa. Each cell can move forward or backward by spinning its single corkscrew-shaped flagellum clockwise or counterclockwise. These motile cells are so densely packed within a colony growing on an agar gel that collective migration naturally emerges. I focus on two regions: at the very edge of the colony, cells are organised as a monolayer and run-reverse swimming mode translates into a nearly jammed 2D phase. A few millimetres from the edge, the colony gets thicker (20 microns) and cells display active turbulence, with long-range nematic ordering and topological defects. I characterise cell trajectories and emergence of long-range alignement, with the aid of an innovative Deep-Learning model for segmentation and tracking, and I correlate these physical quantities to colony shapes in various motility mutants.

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Nematic superfluidity of spinor Bose-Einstein condensates

Dr. Hiromitsu Takeuchi

MC35: Collective Effects and Non-Equilibrium Phenomena in Quantum Gases and Superconductors VIII,
August 24, 2022, 4:30 PM - 6:00 PM

Recently, the terms "nematic" and "nematicity" are oftenly used in the context of some kind of magnetic properties of solid states and quantum fluids while it originates from liquid crystals that have properties between solid and fluid. The analogy is rather derived from the anisotropy of nematic liquid crystals represented by a univer vector "n" without polarity, called the director; "n" is fully equivalent to its opposite "-n". Here, we demonstrate a clear evidence of "nematicity" or "nematic superfluidity" based on the recent experiment in spinor Bose-Einstein condensate [1]. It is predicted that exotic non-equilibrium phenomena can occur toghether with the composite texture of nematic and magnetic spin orders [2,3,4].
[1] Seji Kang, Sang Won Seo, Hiromitsu Takeuchi, and Yong-il Shin, Phys. Rev. Lett. 122, 095301 (2019)
[2] Hiromitsu Takeuchi, Phys. Rev. Lett. 126, 195302 (2021)
[3] Hiromitsu Takeuchi, Phys. Rev. A 104, 013316 (2021)
[4] Hiromitsu Takeuchi,Phys. Rev. A 105, 013328 (2022)

8

Lamb shift and vacuum forces in ultrastrong coupling cavity QED

Rocío Sáez-Blázquez, Peter Rabl

MC25 : Emerging Trends in Many-Body Cavity Quantum Electrodynamics X, August 25, 2022, 2:00 PM - 3:30 PM

Over the last years there has been an increasing interest in the physics emerging from the ultrastrong light-matter interaction, where the coupling strength is comparable to the transition frequencies present in the system. Special attention has received the modification of ground-state properties under these extreme coupling conditions. Here we study the vacuum effects in a reduced cavity QED setup composed of a polar molecule interacting with the quantized field of a single-mode LC resonator. Following a rigorous microscopic description, we have been able to study the combined role of the induced charges on the metallic boundaries and the operative ultrastrong-coupling effects. Compared to large quantum chemistry simulations, our approach has also allowed us to derive analytical predictions for some regimes of interest. In particular, we have computed (non-diverging, cutoff-free) analytical estimates of the Lamb-shift corrections from all the higher electromagnetic modes and determined the modification of the interaction between a pair of molecules due to the electrostatic effects.

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EXPERIMENTAL METHODS FOR NANOFLUIDICS: FOCUS ON SEALING TECHNOLOGY FOR DELICATE NANOMATERIALS

Said Pashayev, Romain Lhermerout, Christophe Roblin, Eric Alibert, Jérôme Barbat, Rudy Desgarceaux, Rémi Jelinek, Edouard Chauveau, Clement Delacou, Saïd Tahir, Vincent Jourdain, Rasim Jabbarov, François Henn, Adrien Noury

MC7: Exploring Liquid Properties in Confined Geometry (up to mesoscopic scales) IX, August 25, 2022, 11:30 AM - 12:30 PM

Being the primordial solvent of life, water is essential to living organisms and human societies. The primordial role of water can be related to its unique physical properties particularly due to the structure of its hydrogen bond network or its dipolar moment. In extreme confinement situation, such as inside nanoscale channels, important modifications of these features are expected. Thus, many theoretical predicted that confined water in extremely small diameter pores exhibits unusual phase behavior and structure compared to bulk water. Thanks to their stiffness, hydrophobic smooth surface and high aspect ratio, Single Wall Carbon Nanotubes (SWCNT) can be considered as a model nanochannel to get insight into the confinement of water molecules. As for instance, it was calculated that the phase of confined water in SWCNT which diameter is smaller than 1.4nm, behaves as ice-like water with structures from single file water chain to pentagonal or hexagonal structure depending on the SWCNT diameter. On the other hand, it has been shown from experimental and theoretical calculations that water diffusion in SWCNT is significantly enhanced. Expanding our fundamental understanding of water properties when it is confined in SWCNTs can yield to substantial progress in desalination, drug delivery, energy harvesting, etc. applications. Although there are many numerical simulations reported on this system, only a few experimental works have been achieved and it remains a challenging task to get experimental proof on water behavior in such confined environment.

One of the main challenges to experimentally measure the properties of nanoconfined water is to be able to fabricate fully sealed microchips. Sealing is a central process for micro and nanofluidic chip fabrication, yet only a few materials can be used as they must be chemically inert, vacuum compatible, resistant to temperature change and must have no electrical effect.

In this poster, we will present a new sealing technology based on SU8 epoxy resist. We show that our bonding method is reliable and versatile for microfluidic, as it can be patterned by photolithography down to micrometric dimensions. It is thus found that a 30 μm high and 20 μm thick wall made of SU8 can sustain relatively pressures up to ~5 bars. We also measured ions permeation through the SU8 walls and found that it is similar or even better to PDMS. Electrical test shows no significant perturbation of electrical devices down to the sensitivity of our measurement set-up, i.e. pA, which makes the SU8 wall resistivity several orders of magnitude higher than that of carbon nanotubes. In addition, our sealing technology turned out to be chemically stable even at high temperature or under energy plasma. It is therefore perfectly suited for the fabrication of such as nanomaterials.

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Collective excitations of superfluid charged Fermi gases

Dr. Serghei Klimin, Prof. Dr. Jacques Tempere, Dr. Hadrien Kurkjian

MC35: Collective Effects and Non-Equilibrium Phenomena in Quantum Gases and Superconductors IV, August 23, 2022, 11:30 AM - 12:30 PM

Collective excitations of many-particle quantum systems offer experimentalists a powerful tool for testing their physical properties. This talk is a review of our recent studies of collective excitations in a superfluid state of condensed Fermi gases, with a particular attention to charged superfluids and superconductors. The talk is focused on the dispersion and damping of collective excitations at nonzero temperatures, accounting for coexistence and interaction of different branches of collective excitations: plasma oscillations, pair-breaking "Higgs" modes, and phononic-like Carlson-Goldman excitations.
In our recent works [1-6], collective excitations are investigated theoretically within the Gaussian pair fluctuation (GPF) approach and in the random phase approximation (RPA), which is equivalent to GPF. The extension of GPF to a charged superfluid is straightforward, adding a bosonic field which describes oscillations of the particle density.
The spectra of collective excitations are determined in two alternative ways. First, they are calculated through spectral weight functions for the density and pair field responses. Second, the eigenfrequencies and damping factors can be obtained in a semi-analytic way as complex poles of the fluctuation propagator analytically continued through a branch cut. Using both methods in parallel and comparing results of them, we can reliably identify collective modes.
The applied method describes collective excitations in the whole range of the coupling strength, from the weak-coupling regime of the Bardeen – Cooper – Schrieffer (BCS) pairing to the strong-coupling regime of the Bose-Einstein (BEC) condensation of molecules in real space. In the far BCS limit, we have described analytically the low-momentum quadratic dispersion of superconducting plasmons in 3D, and the resonance splitting which occurs when the eigenenergy nears the pair-breaking threshold. This work may also be applied to a superfluid state of ultracold fermions where different kind of long-range interactions can be engineered with dipolar atoms. In the BCS-BEC crossover, plasma and pair-breaking modes can interact because they are not, in general, purely amplitude or phase excitations. As a result, pair-breaking and plasma excitations show anticrossing near the continuum edge and an enhancement of the pair-breaking mode response at resonance. This resonant behavior makes pair-breaking modes promising for their experimental detection.

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Heteronanotubes with strong intertube excitonic coupling

Dr James Lloyd-Hughes

MC52: Heterostructures, Combining Organic Molecules and 2D Materials V, August 23, 2022, 2:00 PM - 3:30 PM

Heteronanotubes are a nano-scale analogue of the co-axial cable, but with added functionality: the cores and skins can be semiconductors with excitonic optical properties. Here I discuss our recent experimental and theoretical work on the ultrafast non-equilibrium properties of heteronanotubes, which highlights how excitons in the different constituents can be strongly coupled. For example, in carbon nanotube/boron nitride/molybdenum disuphide core/shell/skin heteronanotubes, excitons in the carbon nanotube cores couple quickly and efficiently to the skin, altering MoS2's excitonic features. Charge transfer across the BN tunnel barrier proceeds at slower rates, taking over 100ps. Our findings can be intuitively understood via classical analogies and by quantum models of the light–matter interaction for coupled systems.

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Unitary Fermi superfluid: Thermodynamics and Sound Modes from Elementary Excitations

Prof. Luca Salasnich, Dr. Giacomo Bighin, Dr. Alberto Cappellaro

MC35: Collective Effects and Non-Equilibrium Phenomena in Quantum Gases and Superconductors IV, August 23, 2022, 11:30 AM - 12:30 PM

We investigate the thermodynamics of the unitary Fermi gas by introducing a model based on the zero-temperature spectra of both bosonic collective modes and fermonic single-particle excitations. We calculate the Helmholtz free energy and from it we obtain the entropy, the internal energy and the chemical potential as a function of the temperature. By using these quantities and the Landau's expression for the superfluid density we determine analytically the superfluid fraction, the critical temperature, the first sound velocity and the second sound velocity. We compare recent experimental results [Science 375, 528 (2022)] of the superfluid unitary Fermi gas near the critical temperature with our model. We find very good agreement between experimental data and our theory for several quantities such as first sound, second sound, and superfluid fraction. We also show that mode mixing between first and second sound occurs. Finally, we characterize the response amplitude to a density perturbation: close to the critical temperature both first and second sound can be excited through a density perturbation, whereas at lower temperatures only the first sound mode exhibits a significant response.

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Nonlinear charge transfer in a silicate layer

Prof. Juan Archilla, Prof. Janis Bajars, Prof. Yusuke Doi, Prof. Masayuki Kimura, Prof. Yuriy Kosevich

It has been observed in fossil tracks and experiments in the layered silicate mica muscovite the transport of charge through the cation layers sandwiched between the tetrahedraoctahedra-tetrahedra layers. Lattice kinks or crowdions imply the movement of the cation in the K+ layer and therefore the transport of charge at supersonic speed. Single crowdions and double crowdions with no radiation have been found in [PRE 91 (2015) 022912, Chaos 28 (2018) 083119]. The energy of single crowdions is large, about 26 eV and could be a good candidate for primary tracks in muscovite. There are however fainter tracks, called secondary tracks, scattered from the primary tracks that should have much smaller energies of the order of tenths of eV. Moving exact breathers with such energies have also been found in [PRE 100 (2019) 022206]. However, they do not transport charge.
In this paper we present a model in which a breather can trap a hole, or a K+ looses and extra electron, becoming K++. This hole will be tight-bound to the K+ ion and our hypothesis is that it can travel from K+ to K+ when they become close enough during the breather motion. We also explore the possibility of a crowdion trapping an extra hole, becoming a super-crowdion transporting two units of charge. There is also recent evidence of negative carriers in muscovite and other silicates. In this case an electron will be attached to the K+ ion, that will become a neutral atom and as such it will not compensate the negative charge of the environment, being equal to a negative charge. We analyze both cases in the present article.

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Polarokinks and polarobreathers in a model for silicate layers

Prof. Juan Archilla, Prof. Janis Bajars, Prof. Yusuke Doi, Prof. Masayuki Kimura

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter X, August 25, 2022, 2:00 PM - 3:30 PM

It has been observed in fossil tracks and experiments in mica muscovite and other layered silicates that the transport of charge through the cation layers sandwiched between the silicate tetrahedra-octahedra-tetrahedra layers [1].

Lattice kinks or crowdions imply the movement of the cation in the K+ layer and therefore the transport of charge at supersonic speed. Single crowdions and double crowdions with no radiation have been found in [2,3]. The energy of single crowdions is large, about 26 eV and could be a good candidate for primary tracks in muscovite. There are however fainter tracks, called secondary tracks, scattered from the primary tracks that should have much smaller energies of the order of tenths of eV. Moving exact breathers with such energies have also been found in [4]. However, they do not transport charge.

If a K+ ion loses an electron, for example by beta- decay of the nuclei, or other causes, it can be described as the creation of a trapped positive hole. Within an insulator, the probability of the hole to be transferred to another ion is very low but a relatively large vibration enhances enormously the probability of transmission [5]. In this way a travelling anharmonic vibration can trap a hole and move along the lattice.

This charged vibration can be a polarokink, that is a kink or crowdion trapping an extra hole as seen in the figure.
A kink is called a crowdion because it is basically a moving interstitial, which in an ionic crystal implies a moving charge. Therefore, a polarokink transports two units of charge. It should be noted that an electric current, as measured in hyperconductivity experiments, needs this extra charge because electrons have to move through the metal contacts and wires. The anharmonic vibration can also be a breather trapping a hole, that is a polarobreather.

We study the conditions of the transfer integrals for travelling anharmonic vibrations and their properties, analyzing which are more consistent with the experimental results.

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Sideband effects and tunable frequency comb in nonlinear mechanical membrane resonators

Dr. Mengqi Fu, Dr. Fan Yang, Prof. Elke Scheer

MC17: Nanomechanical and Electromechanical Systems VI, August 23, 2022, 4:30 PM - 6:00 PM

Micro- and nanoscale mechanical resonators bear rich potential in various realms of physics. Recently, a phenomenon caused by the break of time translational symmetry in the Duffing model of mechanical systems, “quasi modes” (or “very state” in [1]) located around the drive frequency, has attracted broad interest due to its usage on easy characterization of noise squeezing by the frequency response of the fluctuations [1]. Here, we demonstrate an antiresonance effect between the quasi modes in the sideband spectra throuhg low-frequency two-tone probing measurements based on a suspended silicon nitride (Si-N) membrane (~ 500 nm thickness). We also establish a direct connection between the antiresonance frequency and the noise squeezing factor in the system, and develop a novel method of squeezing factor characterization [2].
In addition, we extend the study on the quasi modes into the flexural-mode-coupling regime [3]. In this regime , by injecting external noise sidebands of the quasi modes are excited and show that more than one pair of quasi modes exist. Moreover, a novel tunable frequency comb has been observed around the frequency of the quasi modes in the flexural-mode-coupling regime under one-tone excitation. The frequency separation between neighboring sidebands of the frequency comb is tunable and strongly depends on the damping factor, nonlinearity, vibration amplitude and the detuning frequency of the two coupled flexural modes. By systematically investigating the frequency response of the fluctuations close to the coupled flexural modes, we show that the observed frequency comb is generated when the quasi modes produced by the nonlinearity of the coupled flexural modes are crossing each other. We discuss a model accounting for this observation.

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Interlayer exciton landscape in WS2/tetracene heterostructures

Dr Joshua Thompson, Ms Victoria Lumsargis, Dr Maja Feierabend, Dr Kang Wang, Dr Leitan Dou, Prof Libai Huang, Prof Ermin Malic

MC52: Heterostructures, Combining Organic Molecules and 2D Materials VI, August 23, 2022, 4:30 PM - 6:00 PM

The vertical stacking of two-dimensional materials into heterostructures gives rise to a plethora of intriguing optoelectronic properties and presents an unprecedented potential for technological development [1]. Organic crystals, in particular represent a promising new building block in the design of novel van der Waals heterostructures [2]. Although much progress has been made combining different monolayers of transition metal dichalgonenides (TMDs), little is known about TMD-based heterostructures incorporating organic layers of molecules.

We present a joint theory-experiment study on a TMD/tetracene heterostructure demonstrating clear signatures of spatially separated interlayer excitons in low temperature photoluminescence spectra. Here, the Coulomb-bound electrons and holes are localized either in the TMD or in the molecule layer, respectively. In particular, we reveal both in theory and experiment signatures of the entire intra- and interlayer exciton landscape in the photoluminescence spectra. In particular, we find both in theory and experiment a pronounced transfer of intensity from the intralayer TMD exciton to a series of energetically lower interlayer excitons with decreasing temperature. In addition, we find signatures phonon-sidebands stemming from these interlayer exciton states. Our findings shed light on the microscopic nature of interlayer excitons in TMD/molecule heterostructures and could have important implications for technological applications of these materials.

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Topological transitions in 3D superconductor nanoarchitectures

Prof. Dr. Vladimir Fomin

MC13: Topological and Geometrical Effects in Complex Nanostructures I, August 22, 2022, 11:30 AM - 12:30 PM

Extending nanostructures into the third dimension has become a vibrant research avenue in condensed-matter physics, because of geometry- and topology-induced phenomena. Modern advances of high-tech fabrication techniques have allowed for generating geometrically and topologically nontrivial manifolds at the nanoscale, which determine novel, sometimes counterintuitive, electronic, magnetic, optical and transport properties of such objects and unprecedented potentialities for design, functionalization and integration of nanodevices due to their complex geometry and non-trivial topology [1]. Prospect directions and current challenges in the domain of superconductivity and vortex matter in curved 3D nanoarchitectures and their great potential for magnetic field sensing, bolometry, and information technology have been demonstrated [2]. A topological transition between the two types of topological defects: vortices and phase slips under a strong transport current is found in open superconductor Nb nanotubes with a submicron-scale inhomogeneity of the normal-to-the-surface component of the applied magnetic field [3]. When the magnetic field is orthogonal to the axis of the nanotube, which carries the transport current in the azimuthal direction, the phase-slip regime is characterized by the vortex/antivortex lifetime of 10 fs versus the vortex lifetime of 10 ps for vortex chains in the half-tubes, and the induced voltage shows a peak as a function of the magnetic field. The topological transition between the vortex-chain and phase-slip regimes determines the magnetic-field--voltage and current--voltage characteristics, which imply a possibility to efficiently tailor the superconducting properties of nanostructured materials by inducing a nontrivial topology of superconducting screening currents. Dynamic topological transitions in open superconductor nanotubes occur under a combined dc+ac transport current [4]. The key effect is a transition between two regimes of superconducting dynamics. The first regime is characterized by a pronounced first harmonic in the FFT spectrum of the induced voltage at the ac frequency. It is typical of two limiting cases, when the dominant area of the open tube is superconducting at relatively low magnetic fields and/or weak dc currents or normal at relatively high magnetic fields and/or strong dc currents. The second regime is represented by a rich FFT spectrum of the induced voltage with pronounced low-frequency components because of an interplay between the internal dynamics of superconducting vortices or phase slips and the dynamics driven by the ac. I acknowledge collaborations with I. Bogush, O. V. Dobrovolskiy, R. O. Rezaev, O. G. Schmidt and the financial support from the DFG (Germany) under the Project # FO 956/6-1.

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Towards a holistic model of SHI induced structural modification - Beyond the thermal spike

Dr. Jacques O'Connell, Dr. Ruslan Rymzhanov, Dr. Vladimir Skuratov, Dr. Danielle Douglas-Henry

MC38: Controlled Irradiation Disorder in Model Systems, Organisation, Dynamics, and Transformations X,
August 25, 2022, 2:00 PM - 3:30 PM

Experimental measurement of track diameters is considered important to calibrate theoretical models predicting their formation. These models are typically based on some form of thermal spike [1] with the assumption that a latent track is formed up to the maximum radius at which transient melting occurs during the spike. Track diameter data is then used to fit electron phonon coupling coefficients. For amorphizable materials this process is straightforward and produces good results. However, for non-amorphizable materials the concept of “track diameter” is not well defined. Direct observation by TEM in these materials show that ion tracks manifest as discontinuous lines of defected crystal [2] with no clear diameter. Indirect measurements of crystal disorder through techniques such as RBS in channeling geometry can be used to derive an effective damage cross section and therefrom a representative track diameter but the obtained diameter is not directly comparable with other techniques such as PL, SAXS etc. due to the probing of different defect types. Furthermore, multiply overlapped tracks in these materials lead to a steady evolution of track morphology due to accumulation of crystal defects with fluence. Molecular dynamics can follow the structural evolution of a crystal during dissipation of the ion induced excitation. However, the technique is computationally expensive and thus limited so smaller systems and short timescales, furthermore the results are completely dependent on the employed potential which again necessitates verification.
In this presentation we will present recent results in a combined TEM/MD effort towards a better understanding of the dynamics of the post-ion passage relaxation and speculate on factors responsible for the differences in amorphizable and non-amorphizable materials

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Topological superconductivity in proximitised bilayer graphene

Mr Julien Barrier, Dr Alexey Berdyugin, Dr Piranavan Kumaravadivel, Dr Na Xin, Prof Andre Geim

MC21: Bound states in hybrid superconductor nanostructures VIII, August 24, 2022, 4:15 PM - 6:00 PM

Topological insulators have been the subject of an intense research effort, as they could host excitations with non-trivial braiding statistics like Majorana fermions or non-abelian anyons, quasiparticles proposed as a basis for fault-tolerant quantum computers [1,2].
We propose that twisted bilayer graphene (tBLG) Josephson junctions can realise novel topological excitations. When the twist angle is significantly smaller than 1°, the superlattice consists of large (~µm wide) triangular domains with alternating Bernal (AB/BA) stacking order. In this system the domain boundaries allow valley-polarised 1D helical states with four gapless 1D states on each side of the triangular domains, propagating in opposite directions for valley K and K' [3,4].
In our Josephson junctions, the supercurrent persists deep into the quantum Hall regime, i.e. under magnetic fields breaking the time-reversal symmetry ensuring s-wave pairing. We observe a robust superconducting behaviour for all doping levels and magnetic fields below the critical field of the superconducting contacts, attributed to Andreev bound states propagating within narrow 1D helical channels.
Our results show that tBLG is a particularly appealing system to engineer topological superconductivity. We provide evidence of the topological nature of the domain boundaries, a decisive step towards realising exotic quasiparticles.

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Novel thermalization classes of weakly nonintegrable many-body systems

Sergej Flach

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter IX, August 25, 2022, 11:30 AM - 12:30 PM

We propose a novel framework to characterize the thermalization of many-body dynamical systems close to integrable limits using the scaling properties of the full Lyapunov spectrum. We investigate macroscopic weakly nonintegrable lattice dynamics beyond the limits set by the KAM regime. We perform our analysis in two fundamentally distinct long-range and short-range integrable limits which stem from the type of nonintegrable perturbations - weak two-body interactions (nonlinearities) versus weak lattice coupling (hopping). Long-range limits result in a single parameter scaling of the Lyapunov spectrum, with the inverse largest Lyapunov exponent being the only diverging time control parameter and the rescaled spectrum approaching an analytical function. Short-range limits result in a dramatic slowing down of thermalization which manifests through the rescaled Lyapunov spectrum approaching a non-analytic function. An additional diverging length scale controls the exponential suppression of all Lyapunov exponents relative to the largest one.

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Many Body Flat Band Localization

Sergej Flach

MC40: Strongly Disordered Insulators IV, August 23, 2022, 11:30 AM - 12:30 PM

We consider translationally invariant systems exhibiting many-body localization from all-bands-flat single-particle lattice Hamiltonians dressed with suitable short-range many-body interactions.
This phenomenon is based on symmetries of both single-particle and interaction terms in the Hamiltonian, and it holds for any interaction strength. Our generator of corresponding Hamiltonians
covers both interacting bosons and fermions for arbitrary lattice dimensions. We find two system classes - one which locks both charge and energy (heat) flows, and another one which locks only charge but not energy (heat) [1].
In the second case, we show that heat transport is completely suppressed in one dimension. In higher dimensions we establish a universal bound
on the filling fraction below which the heat transport is suppressed. The bound is based on the mapping to a classical percolation problem [2].

Finally we further relax the model constraints and start with a single-particle system which hosts both dispersive and flat bands.
Fine-tuning of the interaction results in an extensive set of local conserved
charges and a fragmentation of the Hilbert space into irreducible sectors. In each sector, the conserved charges
originate from the flatband and act as an effective disorder inducing a transition between ergodic and localized
phases upon variation of the interaction strength. Such fine-tuning is possible in arbitrary lattice dimensions and
for any many-body statistics. We present computational evidence for this transition with spinless fermions [3].

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Electron pulse compression for ultrafast LEED

Dennis Epp, Dr. Benjamin Schröder, Prof. Dr. Claus Ropers

MC51 : Ultrafast Dynamics in Magnetic and Strongly-Correlated Materials X, August 25, 2022, 2:00 PM - 3:30 PM

The properties of solid-state surface systems often differ significantly from the bulk behaviour and can exhibit complex structural and electronic phases [1]. Complexity arises from the strongly coupled electronic, lattice and spin degrees of freedom including their dynamical interaction. A powerful experiment addressing these systems is the combination of low-energy electron diffraction (LEED) with ultrafast spectroscopy. Specifically, surface phenomena are investigated with a stroboscopic pump-probe setup in which the sample is driven out of its equilibrium via a fs-laser excitation (pump) and its transient state is measured by an electron pulse (probe) with a variable delay [2]. Based on this approach, our group develops ultrafast methods in a backscattering geometry and studies structural dynamics at surfaces [3-6].

The time resolution, as the key quantity in these experiments, is limited by the dispersion-induced temporal broadening of the electron pulses during propagation towards the sample. This effect can be minimized by reducing the working distance between the electron source and the sample, while reducing the outer diameter of the electron source to facilitate the detection of backscattered electrons. Employing such miniaturized electron guns, we have recently demonstrated ULEED with a temporal resolution of 1 ps [3,4]. A promising approach to further enhance the temporal resolution of ULEED, is given by radio-frequency (rf) field compression. Here, a time-dependent electric field within a cavity is used to tailor the momentum distribution of the electron pulses in such a way that the energy distribution ΔE is inverted, i.e., the tailing electrons are accelerated while the leading ones are retarded, respectively. Subsequently, the convergence to a minimum pulse length is achieved at the temporal focus position [7-9].

In this contribution, we demonstrate temporal compression of low-energy electron pulses using rf-fields. Specifically, we combine a millimetre-sized electron gun (uncompressed pulse duration ~16 ps [4]) with a rf-cavity driven by a sinusoidal wave. A phase-locked loop synthesizer controls the timing between the incident electron pulses and the sinusoidal signal. By electron energy filtering, we measured an initial energy spread of $\Delta E \lesssim 1.5$ eV for the uncompressed pulses with mean kinetic energies in the range of 50 eV to 100 eV. Notably, using the compression cavity, we can invert ΔE and control the temporal focus position along the electron trajectory by adjusting the rf amplitude. In perspective, ULEED with sub-ps resolution will allow to directly observe the impact of electron-phonon coupling and coherent vibrational motion on the efficiencies of surface phase transitions and the resulting changes in materials functionality.

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ROOM TEMPERATURE STABILITY AND PHASE TRANSFORMATION OF SHI INDUCED TETRAGONAL TRACKS IN MONOCLINIC ZIRCONIA

Prof Michael Lee, Dr Jacques O'Connell, Dr Vladimir Skuratov

MC38: Controlled Irradiation Disorder in Model Systems: Organisation, Dynamics, and Transformations XI, August 25, 2022, 4:30 PM - 6:00 PM

Pure bulk zirconia (ZrO_2) is a polymorphic oxide that exists in three different low pressure crystal structures below its melting point namely, the high temperature phases cubic and tetragonal as well as the low temperature monoclinic phase [1]. Irradiation of bulk natural zirconia at room temperature along the monoclinic [100]m crystal axis were shown by transmission electron microscopy to produce non-continuos tetragonal latent tracks consisting of segments approximately 30 nm in length and rectangular cross sections of the order 2.5 nm. The segments were aligned along the [001]t crystal axis and approximately 9° to the [100]m axis[2]. It was suggested that the mechanism for the stabilisation of the high temperature phase could be due to the surface energy of the interface surfaces, which will determine the critical crystallite size for RT stabilization [3], or the presence of additional vacancies and interstitial oxygen atoms [4]. In this presentation we present results for irradiated bulk monoclinic zirconia to determine the influence of interfacial surfaces and hence critical size on the formation and stabilization of latent tracks.
Monoclinic ZrO_2 from the Palaborwa complex in South Africa was irradiated with 167 MeV Xe ions to a fluence of $2x10^{10}$ ions/cm² at the FLNR, JINR, Dubna. Plan view and cross sectional TEM lamellae were prepared by standard FIB lift out procedure using an FEI Helios NanoLab 650 and imaged in a JEOL ARM 200F TEM operating at 200 kV.
Individual ion tracks were found to be composed of the high temperature stable tetragonal phase. The c axis of the monoclinic and tetragonal regions was parallel with 45° relative rotation about the c axis. Discontinuities in the tetragonal phase together with a slight misalignment relative to the ion path was ascribed to the difference in a-c angle between the tetragonal and monoclinic phase.
Although stressed, the tetragonal inclusions were found to be stable at room temperature for at least several years although thermal excitation as well as excitation by high energy electrons was able to transform the tetragonal phase back into the monoclinic phase leaving behind a train of defect clusters as is typical of ion tracks in non-amorphisable crystals.
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Repeated Quantum Error Correction in a Surface Code Using Superconducting Circuits

Christopher Eichler

MC23: Superconducting Circuits for Quantum Technologies I, August 22, 2022, 11:30 AM - 12:30 PM

The ability to perform logical quantum operations fault-tolerantly by correcting unavoidable errors induced by control inaccuracies and decoherence, will be essential for building and operating large-scale quantum computers. In my talk, I present our recent demonstration of repeated quantum error correction using a surface code, which is known for it exceptionally high error threshold and its compatibility with planar qubit architectures featuring nearest-neighbor coupling. The code implemented in our experiments uses 17 physical qubits, nine of of which encode the logical information and eight of which perform repeated measurements of error syndromes. By decoding the syndrome data in post-processing we preserve initialized logical states with a low error probability of 3% per cycle. The demonstration of repeated, fast and high-performance quantum error correction supports our understanding that fault-tolerant quantum computation will eventually be realizable.

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Damping of Pseudo-Goldstone Fields in Hydrodynamics and Holography

Vaios Ziogas

Approximate symmetries abound in Nature. If these symmetries are also spontaneously broken, the would-be Goldstone modes acquire a small mass and are referred to as pseudo-Goldstones. At nonzero temperature, the effects of dissipation can be captured by hydrodynamics at sufficiently long scales compared to the local equilibrium. In this talk, we show that in the limit of weak explicit breaking, locality of hydrodynamics implies that the damping of pseudo-Goldstones is completely determined by their mass and certain diffusive transport coefficients. Additionally, we show how this result can be derived in the context of holography. Finally, we present applications to superfluids, Wigner crystal (with or without external magnetic fields) and density wave phases, and (anti-)ferromagnets.

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Ferroelectric nematic liquid crystals: material development and phase transition study

Mingjun Huang, Satoshi Aya

MC8: Complex Phases in Soft Matter II, August 22, 2022, 2:00 PM - 3:30 PM

Ferroelectric nematic liquid crystal (NF LC) has attracted considerable attention for its unique viscoelastic nature, topology and electro-optical properties. The origin of these unexpected matter state features arises due primarily to the addition of polarization field into the traditional nematics. The transitional pathway of the previous NF materials (RM734 and DIO) is mostly as Route I on cooling: isotropic liquid (Iso) – apolar nematic (N) – NF. However, the rapidly increased endeavor in the NF LC study reveals that this is not the only evolution pathway toward the NF state formation. The NF phase can appear directly from the isotropic phase, with apolar N completely suppressed (Route II). We have systematically investigated the underlying principles behind different NF LC evolution pathways. Neary a hundred of LC molecules were synthesized and analyzed. With the aid of DFT calculation and machine learing analysis of more than 160 molecules, we identified the two most critical molecular parameters dictating the NF transition pathways: the dipolar strength and mesogen shape anisotropy. During our exploration of new NF LC materials, we discover some exceptional NF molecules. These NF molecules with highly rigid rod-shape exhibit an intriguing ferroelectric-ferroelectric phase transition. The ferroelectric phase of lower temperature presents smectic like feature, with higher values of refractive anisotropy, spontaneous polarization, and flow viscosity. Especially, its polarization orientated by the electric filed performs high resistance to relaxation, being able to present ferroelectric memory effects. These new features endow the NF LC as ideal piezoelectric materials for flexible self-powered electronics.

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Nonlinear Waves in Fully Nonlinear Mass-in-Mass FPUT Chains

Professor Jonathan Wattis, Reem AlMarashi

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter XI, August 25, 2022, 4:30 PM - 6:00 PM

We present and analyse a generalised Fermi-Pasta-Ulam-Tsingou chain in which every node contains a resonator which coupled nonlinearly to the outer shell, and each outer shell is coupled nonlinearly to its two nearest neighbours. The asymptotic analysis results in four cases, depending on the form of nonlinearity of each interaction. Three cases reduce to the nonlinear Schrodinger equation, and one to a form of the Complex Ginzburg-Landau equation. We present numerical simulations of the system, showing breathers, kinks, and breather-kink combinations; we consider both stationary and moving modes. Whilst some of the predicted forms are clearly unstable, many appear to be stable, or at least extremely long-lived.

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Vertex model micro-mechanical validation in fish embryo morphogenesis

Mr. Paulo Godolphim, PhD Rodrigo Soto, PhD Leonardo Brunnet, PhD Miguel Concha, PhD Maurício Cerda

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

The vertex model is one of the most used physical models to describe confluent tissues. It is a simple model, yet one can use it to extract dynamic properties from experimental data, which is often not a simple task. Many works show the vertex model gives excellent qualitative and quantitative descriptions of different in vitro and in vivo experiments. Nevertheless, systematic validation of the model is yet barely explored. Our initial assumption is that only finding the optimal parameters that correctly describe/mimic the evolution of an (experimental) tissue is necessary but not sufficient to consider a model as an accurate description. We propose that a more restrictive condition must be matched. If a model is a good description, then the same set of parameters must be able to describe at the same time the whole tissue and also any sub-part of the tissue. We call this stricter approach Micro-mechanics, where one executes cell-by-cell independent simulations to find the optimal parameters for each cell. If the optimal parameters are homogeneous, then the model is considered valid. If not, this indicates that we need to modify the model to ensure homogeneity in the parameters alongside the tissue. Our preliminary results suggest that a simple description of the vertex model, with only perimeter and area harmonic forces, is valid in the pre-epiboly in vivo process of an Annual Killifish embryo, where the vertices' positions are compared with those obtained using fluorescent microscopy. However, large statistics is needed, increasing the number of analyzed embryos, to validate preliminary results.

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Improving Feynman's variational path-integral approach: An application to the BEC-impurity problem.

Timour Ichmoukhamedov, Jacques Tempere

MC35: Collective Effects and Non-Equilibrium Phenomena in Quantum Gases and Superconductors VII,
August 24, 2022, 2:00 PM - 3:30 PM

For many decades now, Feynman's variational path integral method has been the semi-analytic tool of choice to study various types of polaronic problems where an impurity interacting with a bosonic medium is described by a Fröhlich-like Hamiltonian. Although corrections and improvements to this approach have been previously proposed in the literature, in their applications to solid state polaron problems such corrections were found to play only a minor role and Feynman's original formulation has been widely regarded as highly accurate.

Recently, similar polaronic Hamiltonians have been emerging in the study of impurities immersed in ultracold quantum gases. Remarkably, Feynman's approach has been shown to fail for even the simplest model for such a system, the Bogoliubov-Fröhlich Hamiltonian. This has prompted the development of more advanced theoretical methods for the problem, and formed the first of numerous other difficulties in describing the Bose polaron.

In this talk, we discuss the failure of Feynman's path integral approach more closely and show how this method can be significantly improved by combining previous ideas from solid state polaron theory. In doing this we demonstrate that the variational path integral approach remains a powerful tool across many domains of polaron physics with noninteracting phonons. We also discuss the remaining theoretic problems in describing the Bose polaron that are currently also arising in solid state polaron theory.

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Vertex model characterization of active contraction pulses in epithelial cells

Rodrigo Soto

Several models have been proposed to describe the dynamics of epithelial tissues undergoing morphogenetic changes driven by apical constriction pulses, which differ in where the constriction is applied, either at the perimeter or in the medial regions. To help discriminate between these models, we analyse the impact of where constriction is applied on the final geometry of the active contracted cell, using the two-dimensional vertex model. We find that medial activity, characterized by a reduction in the reference area, generates anisotropic cell shapes, whereas isotropic cell shapes are produced when the reference perimeter is reduced. When plas- ticity is included, sufficiently slow processes of medial contractile activity, compared with the characteristic times of elasticity and plasticity, cells can achieve less elongated shapes. Similarly, for perimeter activity, the highest level of contraction is achieved. Finally, we apply the model to describe the apical contractile pulses observed within the epithelial enveloping cell layer during the pre-epiboly of the annual killifish Austrolebias nigripinnis. The analysis of the cell shape changes allowed a global fit of all parameters of the vertex model, with the pulses being quantitatively captured using perimeter activity and area plasticity.

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Silicon nitride drum resonator for phonon-cavity electromechanics

Dr. Sri Venkatachalama, Dr Alok Pokharel, Hao Xu, Dr. Eddy Collin, Dr. Xin Zhou

MC17: Nanomechanical and Electromechanical Systems X, August 25, 2022, 2:00 PM - 3:30 PM

Silicon nitride (SiN) mechanical resonators are attractive for sensing and signal processing because of their nanogram effective mass and high-quality factor, with a typical resonance frequency in the MHz range. Up to now, SiN electromechanical resonators are based on doubly-clamped beam structures, with limited space for making trade-offs among quality factors, resonance frequency, and coupling strength with external circuits.

Here, we will present our recent achievements in developing a novel electromechanical system, consisting of two capacitively-coupled distinct resonators: a SiN drum resonator and an aluminum one [1]. The whole device structure can be viewed as a parallel plate capacitor, where each plate is a membrane drum. Integrated with a versatile platform composed of microwave reflectometry and a microwave cavity, both resonators can be manipulated and detected independently. The ultra-clean fabrication process allows to have SiN drum resonators with typical resonator frequencies in ~10 MHz range and high-quality factor (Q) ~1E4 at room temperature, reaching the current state of art. In the nonlinear region, its Duffing parameter is about 10 times smaller than the theoretical estimate based on the membrane model. For the Al drum with resonance frequency ~3 MHz, we could not reach the nonlinear region with the same electrostatic driving force because its quality factor is two orders lower than that of the SiN drum, at room temperature. With this unique device structure, we investigated phonon-cavity mechanics by taking the SiN drum as a phonon cavity and performing double-tone operations, through analogue to microwave optomechanical system [2]. Here, it is quite different from conventional optomechanical systems in which the mechanical damping rate is usually much smaller than that of the coupled cavity. Electromechanically induced transparency and amplification of input signals have been demonstrated by sideband pumping the phonon-cavity. This unique coupled system gives access to observe the phonon-cavity force affecting the mechanical damping rate of both movable objects. The measurement results are in good agreement with our analytical calculations based on the electrostatic coupling model. Our results open up new possibilities in the study of phonon-cavity based signal processing in the classical and potentially in the future in the quantum regimes.

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19

Frustrated Layered Self-assembly Induced Superlattice from Two-Dimensional Nanosheets

Huanjun Lu, Yingfeng Tu

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Here we reported a hierarchical self-assembly approach towards well-defined superlattices in supramolecular liquid crystals by fullerene-based sphere-cone block molecules. The fullerenes crystallize to form monolayer nanosheets intercalated by the attached soft hydrocarbon cones. The frustration caused by cross-sectional area mismatch between the spheres and the somewhat oversize cones leads to a unique lamellar superlattice whereby each stack of six pairs of alternating sphere-cone sublayers is followed by a cone double layer. While such areal mismatch problems in soft matter are usually solved by interface curvature, the lamellar superlattice solution is best suited to systems with rigid layers. Meanwhile, formation of the superlattice significantly improves the material's transient electron conductivity, with the maximum value being among the highest for π-conjugated organic materials. The design principle of solving steric frustration by forming a superlattice opens a new avenue toward self-assembled optoelectronic materials.

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Thermal conductivity of a novel RM 734 ferroelectric nematic material at the ferroelectric-ferroelastic phase transition

Dr Dharmendra Pratap Singh, Dr Michael Depriester

MC8: Complex Phases in Soft Matter II, August 22, 2022, 2:00 PM - 3:30 PM

The development of a new liquid crystal material with novel mesogenic features is of tremendous interest. Recently, a new liquid crystalline material viz. 4-[(4-nitrophenoxy)carbonyl]phenyl2,4-dimethoxybenzoate (RM734), exhibiting ferroelectric nematic phase (NF) has been reported [1,2]. Herein, we present the temperature-dependent thermal behaviour of the RM734 compound. The thermal conductivity κ was obtained from the formula: $\kappa = e.\alpha^{a}$, where e and α are the measured thermal effusivity and thermal diffusivity, respectively, the value of a is 0.5. Both quantities were extracted via pyroelectric experiment in which the RM734 compound, placed in close contact with a pyroelectric sensor, is irradiated by a pulsed laser beam. The thermal diffusivity and effusivity were obtained under the back and front-detection configurations (Figure 1(a) and 1(b)). The thermal parameters are extracted from the pyroelectric signal at the ferroelectric-ferroelastic phase transition (Figure 1(c)).

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A case of antiferrochirality in a liquid crystal phase of counter- rotating staircases

Ya-xin Li

MC8: Complex Phases in Soft Matter IV, August 23, 2022, 11:30 AM - 12:30 PM

Helical structures continue to inspire, and there is considerable temptation to attribute helicity to columnar LCs. While short isohelical sequences are undoubtedly present, the order is only short-range, equivalent to a paramagnet without field, or with field if chiral groups or dopants are biasing the twist. However, here we report a confirmed example of a true LC phase, not a soft crystal, of achiral compounds consisting of columns, each being a long-range homochiral helix [1]. Long-range periodicity and isochirality are maintained by intercolumnar interaction. This orthorhombic LC, spacegroup Fddd, is discovered in compounds with either bent or straight rod-like pi-conjugated cores (see Fig. 1), and is subsequently found in other systems, including polymers. Interestingly, the phase forms readily in non-chiral compounds or in 1:1 racemic mixtures, but not in pure strongly chiral enantiomers. The structure is equivalent to an antiferromagnet with twist replacing spins. A theory based on interacting quadrupoles confirms this structure as energetically favoured over alternatives. Although, due to cancellation, the current Fddd phase has no overall chirality, the findings open a new approach to homochirality in achiral compounds.

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21

Relevant perturbations in a topological insulator.

Victor Kagalovsky

MC13: Topological and Geometrical Effects in Complex Nanostructures I, August 22, 2022, 11:30 AM - 12:30 PM

We study the stability of multiple conducting edge states in a topological insulator against all multiparticle perturbations allowed by time-reversal symmetry. We model a system as a multichannel Luttinger liquid, where the number of channels equals the number of Kramers doublets at the edge. We show that in a clean system with N Kramers doublets there always exist relevant perturbations (either of a superconducting or charge density wave character) which always open N − 1 gaps.
In the charge density wave regime, N − 1 edge states get localized. The single remaining gapless mode describes the sliding of a “Wigner-crystal”-like structure. Disorder introduces multiparticle backscattering processes. While single-particle backscattering turns out to be irrelevant, the two-particle process may localize this gapless mode. Our main result is that an interacting system with N Kramers doublets at the edge may be either a trivial insulator or a topological insulator for N = 1 or 2, depending on the density-density repulsion parameters, whereas any higher number N > 2 of doublets gets fully localized by disorder pinning, irrespective of the parity issue.
If N − 1 edge states are gapped by Josephson couplings and the single remaining gapless mode describes the collective motion of Cooper pairs synchronous across the channels. Disorder perturbation in this regime, allowed by the time-reversal symmetry is a simultaneous backscattering of particles in all N channels. Its relevance depends strongly on the parity if the number of channels N is not very large. Our main result is that disorder becomes irrelevant with the increase of the number of edge modes leading to the stability of the edge states' superconducting regime even for repulsive interactions.

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Compatible relevant perturbations in the strongly interacting 1D system: a variety of fractional conductances

Victor Kagalovsky

MC40: Strongly Disordered Insulators II, August 22, 2022, 2:00 PM - 3:30 PM

We consider a strongly interacting one-dimensional (1D) system with N channels. We study the conditions necessary for the coexistence of various perturbations. The most general interaction (beyond forward-scattering quadratic terms in the Lagrangian) is restricted by the neutrality requirement, meaning that each term in the Hamiltonian conserves a number of particles. To become relevant and open a gap the perturbation has to represent a new field, and new fields have to preserve the form of Lagrangian. There is another constraint (formulated by Haldane) on the type of perturbations that are allowed to coexist.
The conductance (in e2/h units) of the remaining free fields can be presented as the difference between the initial conductance of all N channels and the conductance eliminated by K compatible relevant perturbations which freeze K corresponding fields. The variety of possible combinations of the relevant perturbations provides the variety of possible fractional conductances

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Beyond the Fröhlich Hamiltonian: Large polarons in anharmonic solids

Mr. Matthew Houtput, Prof. Dr. Jacques Tempere

MC35: Collective Effects and Non-Equilibrium Phenomena in Quantum Gases and Superconductors VII,
August 24, 2022, 2:00 PM - 3:30 PM

The large polaron is a system consisting of an impurity interacting with a field and is one of the most fundamental and well-known problems of many-body physics. It finds applications in solid state physics, where the impurity is an electron and the boson field is a continuum of lattice phonons, but polaronic effects can also be observed in impurities immersed in ultracold bose gases. Large polarons are often described using the Fröhlich Hamiltonian, which assumes a linear electron-phonon interaction. However, in recent years significant interest has been raised in additional interaction terms such as the 1-electron-2-phonon interaction, both in solid state polarons and in ultracold bose polarons. In our work, Fröhlich theory is extended to include 1-electron-2-phonon interaction for the solid state polaron. Additionally, the basic properties of the resulting polaron are studied.

We derive an analytical expression for the interaction strength of an electron coupling to LO phonons. For cubic materials, the interaction strength only depends on a single scalar parameter, making it well-suited for analytical calculations. Since the resulting Hamiltonian is quadratic, we may investigate several properties using the path integral formalism: these include the energy and effective mass of the new polaron, and formation of bipolarons. It is shown that the additional term leads to significant additional trapping of the electron, broadens the bipolaron stability regime, and causes a secondary absorption peak in the optical conductivity.

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Switchable Wetting Properties in Polypyrrol-Porous Silicon Systems

Laura Gallardo, Manuel Brinker, Patrick Huber

MC7: Exploring liquid properties in confined geometry (up to mesoscopic scales) VIII, August 24, 2022, 4:30 PM - 6:00 PM

Substrates with switchable or adjustable wetting properties are desirable for actuators, smart coatings, filters or biomedical applications. On the other hand, silicon is a mainstream semiconductor widely used in the industry. In this work we explore the functionalization by electropolymerization of porous silicon with pyrrole. Polypyrrole is an electrically conductive polymer whose oxidation state can be switched by electrochemical means, thereby influencing the chemo-mechanical properties of the polymer [1, 2] and the Young contact angle of liquids deposited on its surface [3]. Here we present a study on the different oxidation states of porous silicon-polypyrrole systems using cyclic voltammetry measurements, which allow to identify transition voltages between these distinct functionalities. The switchable wettability originated at these oxidation state transitions is investigated both for bulk polymer layers and porous PPy-silicon membrane geometries.

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Mapping and manipulating ferroelectric domains in parallel stacked hexagonal boron nitride with AFM.

James Kerfoot, Vladimir Korolkov

MC18: Developments at the Frontiers of High-resolution Scanning Probe Microscopy III, August 22, 2022, 4:30 PM - 6:00 PM

By modifying the twist angle between two crystalline materials, the registry of atoms may be modified, leading to interfacial ferroelectricity in the case of parallel stacked hexagonal boron nitride (hBN) [1-3]. We provide an account of the fabrication of such parallel stacked hBN samples using a home-built transfer setup [4] and the mapping of ferroelectric domains in these samples using both electrostatic force microscopy (EFM) and Kelvin probe force microscopy (KPFM). We address the dependence of the hBN layer thickness on the morphology of ferroelectric domains, which vary in appearance between triangular domains and more distorted irregular patterns. We then go on to discuss different ways in which such domains may be mapped and manipulated using different AFM modalities. In particular, we address the measurement of these domains with different derivatives of KPFM (both amplitude modulated and sideband KPFM inside and outside of vacuum) with higher contrast extracted for sideband KPFM. We conclude by studying the manipulation of domains both electrically by applying bias via the tip and mechanically using contact mode AFM [5].

In addition to identifying new approaches to mapping and manipulating such ferroelectric domains in layered materials heterostructures using AFM, this work is also highly relevant to new devices based upon electron tunnelling between graphene layers [6] through ferroelectric hBN, with applications both to memristive devices and tunnel diodes capable of offering increased logic per chip.

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27

Quantum interference affects charge distribution in multiply- connected mesoscopic samples

Gian Paolo Papari, Vladimir M. Fomin

MC13: Topological and Geometrical Effects in Complex Nanostructures II, August 22, 2022, 2:00 PM - 4:00 PM

The experimental signature of the phase effect in multiply-connected structures is the sinusoidal magnetoresistance oscillation that was observed in a huge number of both normal [1] and superconducting [2] mesoscopic samples. Several models have been proposed so far, all ascribing the mechanism of the magnetoresistance oscillations to the oscillations of the scattered particles density. Herewith we propose a new model [3] elaborated within the Ginzburg-Landau theory, where the interference affects the spatial distribution of scattered particles while conserving their density. The measured resistance is connected to the interference mechanism inducing the change in the distribution of scattered particles getting across the ring. The new vision on the electronic interference bridges the phenomenological gap between low- and high-temperature superconductors allowing for interpreting the sinusoidal magnetoresistance oscillations in both kind of superconducting materials and in normal rings as well. We have verified the model by fitting the magnetoresistance oscillations of a YBCO sample [4] patterned with very narrow ring arms and stubs to observe a negligible parabolic background in measurements. Apart from the average radius of the ring and the value of the resistance at zero field acquired during the resistive transition, our model depends only on the voltage-sensed supercurrent. Since the sinusoidal magnetoresistance oscillation is a function of a constant Cooper pairs density, the interference is sustained without any loss of superconducting stiffness. Hence our results set a clear advance in flux-based quantum computing whose limitation relies only on the clock (commutation) frequency of the magnetic field that can be pushed up to the energy gap ranging around hundreds of GHz.

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28

Non-linear temperature dependence of dielectric response in SmC* phases

dr. sc. Dina Jukić, prof. dr. sc. Mojca Čepič

In this contribution we discuss dielectric response of ferroelectric liquid crystals. The analyses of dynamical properties of the chiral polar smectic system described by the basic theoretical model leaving the two order parameters independent leads to entirely new dynamical behaviour and provides a framework for re-examination of many existing experimental results. The approach is important for various polar systems in soft matter in particular and for analyses of dynamical systems in general.
Results of the analysis show that what is valid for stable structures cannot be straightforwardly extended to studies of system dynamics and the presented study is a clear example, what a generalisation of properties of stable structures to dynamical properties could overlook.
Already decennia ago soon after discovery of ferroelectric liquid crystals[1] a theoretical model that adequately reproduced observed properties for a system having an orthogonal higher temperature non-polar SmA phase and a lower temperature tilted polar SmC* phase was suggested[2], and dynamical properties of such systems were analysed within that model[3]. The last paper predicted two modes associated to the changes of the tilt and the polarization, and four modes in the SmC* phase, two tilt and two polarization modes.
Dielectric means were/are extensively used to analyse dynamical properties of various polar liquid crystals, and for their analysis a simplified treatment was/is used. This treatment requires the same relation between changes of the tilt and changes of polarization as is valid for stable structures, that is, polarization is proportional to the tilt and strictly perpendicular to it. Such analysis predicts only half of the modes, soft modes depend on the temperature linearly, and the relation between the mode's frequency and its dielectric response is strictly inversely proportional. However, considering the tilt and polarisation as independent the analysis reveals a non-linear dependence of soft modes, consistent with experiments. This behaviour is an indirect indication of higher frequency modes. Finally, a widely accepted inverse proportionality between the frequency and the dielectric response of the modes, is valid only close to the transition temperature. The behaviour is a direct consequence of chiral piezoelectric coupling, which influences polar properties of the relaxation modes in dependence of the temperature.

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The relation between strange-metal behavior, charge order, and superconductivity in the cuprates

Martin Greven

MC31 : The Physics of Cuprates XI, August 25, 2022, 4:30 PM - 6:00 PM

In this talk, I will review our collaborative efforts to understand the cuprate phase diagram, including x-ray measurements of charge order [1], transport results [2], as well as measurements of superconducting correlations [3] and of 'hidden' structural correlations [4]. These results point to a surprisingly simple picture of the cuprates in which inherent inhomogeneity and charge (de)localization play a central role [5].

Work funded by the US Department of Energy through the University of Minnesota Center for Quantum Materials, under grant number DE-SC-0016371.

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Disordering Mechanisms in ABO4 Metal Oxides

Mr Bryce Mullens, Dr Matilde Saura Muzquiz, Dr Frederick Marlton, Dr Zhaoming Zhang, Professor Brendan Kennedy

MC38: Controlled irradiation Disorder in Model Systems: Organisation, Dynamics, and Transformations VIII, August 24, 2022, 4:30 PM - 6:00 PM

The development of carbon-neutral energy-generation and storage is critical to combatting climate change. Various technologies are currently being developed for sustainable energy generation, such as next-generation ion conductors for solid-oxide fuel cells (SOFCs), photocatalysts for splitting water into hydrogen and oxygen gas, and materials capable of safely storing radioactive waste. ABO4 materials have become a focus for these technological advances, with LnNbO4 emerging as a potential solid electrolyte in solid-oxide fuel cells, BiVO4 as a potential photocatalyst, and CsReO4 as a potential host matrix for highly mobile nuclear fission products. Paramount to the development of these technologies is a deep understanding of their structure-functionality relationships.

In this work, different disordering mechanisms within ABO4 structures have been observed and studied. The structures of LnNbO4 oxides have been studied at temperatures corresponding to the high operational temperatures of SOFCs, revealing a quasi-first order phase transition from the monoclinic I2/a to tetragonal I41/a phase. Substitution of Nb(V) with Ta(V) is shown to decrease in the unit cell volume of the structure and stabilise the monoclinic phase over a larger temperature range. This is particularly remarkable, given that Nb(V) and Ta(V) cations have the same ionic radius despite Ta having a 5d valence shell compared to the 4d shell of Nb. Engineering such chemical substitution disorder within these structures highlights the potential of these materials to be specifically ‘tailored’ to be used for SOFCs.

These studies have been extended to various other potential functional energy materials adopting the ABO4 structure. Of interest is the metastability of the zircon polymorph of BiVO4 due to the sterically active 6s lone pair of Bi3+, and the unusual average bond lengths observed in CsReO4 due to the rotation and translation of the BO4 tetrahedra at higher temperatures.

Various ABO4 materials have been synthesised either using conventional solid-state or coprecipitation methods. Synchrotron X-ray and neutron powder diffraction methods have been used to investigate their average structures, focusing on changes in both their unit cell volumes and the temperature of their phase transitions. These studies have revealed several anomalies, revealing that different structures with differing properties can be isolated by controlling the synthesis conditions. The short-range structure has also been investigated using both neutron and X-ray pair distribution function (PDF) analysis to observe differences between the local and average structure of the materials. The experimental data has been further reinforced by ground state energy calculations performed using density functional theory. This multi-faceted approach has not been previously used for these types of oxides. These insights can be used in the development and engineering of novel and advanced energy materials using the ABO4 structure type.

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Terahertz pulse-driven collective mode in the nematic superconducting state of an iron-based superconductor

Dr. Romain Grasset, Kota Katsumi, Pierre Massat, Hai-Hu Wen, Xian-Hui Chen, Yann Gallais, Ryo Shimano

The superconducting Higgs mode [1], i.e., the collective oscillation of the amplitude of the superconducting order parameter, and other exotic collective modes such as the Bardasis-Schrieffer mode [2], i.e., fluctuations between s-wave and d-wave superconducting order parameters, are among the most fascinating, but also the most elusive, excitations in superconductors.

The superconducting Higgs mode has now been detected using intense terahertz (THz) pulses in both conventional and unconventional superconductors [1], giving rise to the emerging field of “Higgs spectroscopy”. Yet, these pioneering studies have triggered important and still unanswered questions. Among them is the possibility that even more exotic collective modes can be detected in superconductors in the presence of distinct, possibly intertwined, electronic orders.

In the present work [3] we report an out-of-equilibrium study of the superconducting collective modes in the iron-based superconductor Ba1-xKxFe2As2 in which superconductivity coexists with an electronic nematic state. Our approach is based on a THz pump-optical probe scheme (See Figure a), where collective modes are detected in the time domain as an instantaneous THz Kerr signal (See Figure b).

We reveal a striking impact of the nematic order on the nature of the superconducting collective excitations. While the Higgs mode signal is dominant in the non-nematic superconducting state, in the presence of coexisting nematicity a new signal with a striking nematic symmetry is observed which we assign to the emergence of a coupled nematic Bardasis-Schrieffer mode.

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First-Principles Investigation of the Electronic Properties of 2-D Organic-TMDC Heterostructures

Edward Black, Dr Juliana Morbec

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Two-dimensional transition metal dichalcogenides (TMDCs) are considered encouraging materials for photovoltaic applications, with differing electronic and optical properties from their bulk counterparts. Pentacene is an organic compound with high exciton mobility, and complimentary electronic properties to TMDCs. Here are investigated systems of adsorbed pentacene on to monolayers of Group-VI dichalcogenides; MoS2, MoSe2, WS2 and WSe2, for photovoltaic applications. Using ab initio methods within density functional theory, optimized atomic positions were calculated and energetically favourable adsorption sites of pentacene were determined. These sites were further investigated with a varying concentration of adsorbed pentacene, with the aim of investigating how molecule-molecule interactions affect the interaction between molecule and substrate. The electronic properties of the favourable systems were then probed and the charge balance of the systems analysed.

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Twist-Angle Control of Collinear Edelstein Effect in van der Waals Heterostructures

Alessandro Veneri, David Perkins, Csaba Péterfalvi, Aires Ferreira

MC16: Spin Control in Twisted Van Der Waals Heterostructures VI, August 23, 2022, 4:30 PM - 6:00 PM

Spin-charge conversion processes in graphene-based van der Waals (vdW) heterostrucutres have been the subject of many theoretical and experimental studies over the past decade [1,2]. The field of spintronics prides itself on uncovering the novelty of these processes with the perspectives of technology and fundamental physics in mind [3]. In recent years, the study of twisted vdW heterostructures [4], with precise relative rotation angle between the layers, has given birth to a new field known as twistronics.

In this talk, we look at the unification of spintronics with twistronics by studying the proximity-induced spin-orbit coupling (SOC) in graphene-transition metal dichalcogenide (TMD) bilayers. Previous works [5] have found that the introduction of a twist between the graphene and TMD layers allows for the tuning of the SOC strength. Twisting enables non-trivial spin textures to manifest on the Rashba-split graphene bands, such that spin and momentum are no longer locked at right-angles to one another. Using linear response theory, we show that such spin and momentum eigenstates generate a non-zero spin current response parallel to the applied electrical current at non-zero twist angles. Accounting for short-range impurities and twist-disorder, we predict the existence of a robust collinear Edelstein effect without the need for magnetic materials or skew-scattering.

*A.V. and D.P. contributed equally to the results of this research.

Acknowledgements

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Superconducting Casimir Effect: The interplay between two famous quantum effects

Minxing Xu, Mr. Robbie Elbertse, Prof. Sander Otte, Prof. Richard Norte

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

The Casimir effect describes an universal force that exists between two parallel unchanged plates placed submicron apart. This quantum phenomena plays an important role in understanding the fluctuating nature of quantum fields. It is equivalently originated either from virtual photons created by vacuum fluctuation or from the interactions between fluctuating dipoles within the nearby bodies. Meanwhile, another macroscopic quantum phenomena, superconductivity, depicts the collective quantum motion of electrons, making superconductors an excellent platform to probe the transport properties of electrons. By looking at the interplay between these two different yet related quantum phenomena, we hope to uncover a corner of science that has remained experimentally out of reach. Physicists are currently investigating whether superconducting Casimir experiments could provide a new understanding of nanoscale gravity and the underlying mechanisms of high-temperature superconductivity, or whether it solve a century-old debate on the nature of electrons. One of the biggest challenges in these experiments is stably positioning of two objects nanometers apart in cryogenic temperatures and measuring the forces between them. In order to overcome this challenge, we develop a high precision sensor to study the Casimir effect between superconductors. Using a microchip platform, we suspend a flexible superconducting membrane nanometers above another superconducting surface. A scanning tunneling microscope is used to read out the relative displacement of the suspended membrane with high precision as it is cooled into the superconducting regime. Our technique brings together the benefits microchip engineering with the precision of scanning tunneling microscopy to explore a potentially new branch of quantum physics.

The Casimir effect describes an force that exists between two parallel plates placed submicron apart. It is equivalently originated either from virtual photons created by vacuum fluctuation or from the interactions between fluctuating dipoles within the nearby bodies. Meanwhile, superconductivity depicts the collective quantum motion of electrons and can be an excellent platform to probe the transport properties of electrons. We study the interplay between these two macroscopic quantum phenomena to explore an untamed scientific corner experimentally. Investigations on the superconducting Casimir effect can provide a solution to a century-old debate on the nature of electrons, and may give a new understanding of nanoscale gravity and the underlying mechanisms of high-temperature superconductivity. Stably positioning of two parallel large objects nanometers apart in cryogenic temperatures and measuring the forces between them, is very challenging. In order to overcome this, we develop a high precision sensor to study the Casimir effect between superconductors. Using a microchip platform, we suspend a flexible superconducting membrane nanometers above another superconducting surface. A scanning tunneling microscope is used to read out the relative displacement of the suspended membrane with high precision. Our technique brings together the benefits microchip engineering with the precision of scanning tunneling microscopy to explore a potentially new branch of quantum physics.

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Crystalline order in lyotropic solution of supramolecular hollow nanotubes

Dr. Ningdong Huang, Professor Goran Ungar

MC8 : Complex Phases in Soft Matter VII, August 24, 2022, 2:00 PM - 3:30 PM

3D long-range crystalline order with 1 nanometer resolution is observed in lyotropic chromonic solutions of supramolecular nanotubes at concentrations as low as 6 wt%. The nanotubes are self-assembled from ionic star-like mesogens with three oligobenzamide branches. 100 upright-standing stars arrange side-by-side into 3 nm high supramolecular rings which in turn stack on top of each other forming long cylindrical tubes, 15 nm in diameter. These water-filled nanotubes arrange parallel to each other on an extremely highly ordered hexagonal lattice, separated by a 4-12 nm thick layer of water, depending on concentration. In spite of the thick layer of water between them, these only slightly corrugated tubes are in longitudinal register as witnessed by the presence of numerous discrete hkl Bragg X-ray reflections on higher layer lines in fiber diffraction. The existence of 3D crystalline order at such high dilution is unprecedented. We propose that the unexpected additional longitudinal register of the tubes is secured by their infinite length, high stiffness and perfect periodicity of charges and resulted by an effective cumulative long-range locking force. The emergence of structural order with concentration is also accompanied by slower dynamics of the tubes as probed by X-ray photon correlation spectroscopy. The dynamics is related to the flexibility of the tubes and the their ability to slide longitudinally, both being suppressed already at fairly low concentration by tube interlock.

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Optomechanical measurement of individual nanoparticles: towards the analysis of a single virus

Samantha Sbarra, Louis Waquier, Stephan Suffit, Aristide Lemaître, Ivan Favero

MC17: Nanomechanical and Electromechanical Systems XI, August 25, 2022, 4:30 PM - 6:00 PM

We demonstrate the effectiveness of optomechanical devices for the measurement of individual nanoparticles. A semiconductor optomechanical disk resonator is optically driven and detected under ambient conditions, as nebulized nanoparticles land on it. Multiple mechanical and optical resonant signals of the disk are tracked simultaneously, providing access to several pieces of physical information about the landing analyte in real time. Thanks to a fast camera registering the time and position of landing, these signals can be employed to weigh each nanoparticle with a sensitivity down to 30 attograms. Sources of error and deviation are discussed and modelled, indicating a path to evaluate the elasticity of the nanoparticle on top of its mere mass. The device is optimized for the future investigation of nanometric objects such as sessile nanodroplets and biological particles in the high megadalton range, including the class of large viruses.

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Polar Fluctuations Lead to Extensile Nematic Behaviour in Confluent Tissues

Andrew Killeen, Dr. Thibault Bertrand, Dr. Chiu Fan Lee

MC3: Tissue Dynamics: From In Vivo Experiments to In Silico Modelling X, August 25, 2022, 2:00 PM - 3:30 PM

Collective active nematic behaviour has been found to mediate a growing number of important biological processes, such as cell extrusion in epithelial monolayers or the formation of layers in Myxococcus xanthus colonies [1, 2]. Intriguingly, isolated epithelial cells display polar motility and generate contractile nematic stresses when elongated but exhibit extensile nematic behaviour when part of a tissue. How these cells can exhibit active nematic behaviour at the tissue level is poorly understood and deciphering the mechanisms behind this behaviour is necessary for elucidating fundamental biological processes.

Here, we resolve this cellular to tissue level disconnect with a linearized hydrodynamic theory that applies universally in the small fluctuation regime to tissues in both fluid and solid states. We show that polar fluctuations generically generate extensile stresses in confluent tissues, and so can drive extensile collective behaviour in cells that are contractile in isolation [3]. We then validate our theory by demonstrating the appearance of extensile nematic defects in both fluid and solid cell-resolution models with polar active forces. Our results also demonstrate that materials with no inherently nematic active forces can exhibit active nematic collective behaviour, and that the active nematic signatures observed in epithelial tissues can naturally emerge downstream of fundamentally polar processes.

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Superlattice Engineering of Giant Molecules: Supramolecular Soft Alloys

Professor Stephen Cheng

MC8: Complex Phases in Soft Matter I, August 22, 2022, 11:30 AM - 12:30 PM

Superlattice Engineering of Giant Molecules: Supramolecular Soft Alloys
Stephen Z. D. Cheng
School of Molecular Science and Engineering, Advanced Institute for Soft Mater Science and Technology, South China University of Technology, Guangzhou
Inverse thinking and design are critical steps in the new materials developments (materials genome approach). When we design materials with specific functional properties, we often start with independent building blocks which possess well-defined molecular functions and precise chemical structures. Using the “Molecular Lego” approach [1], we can then, in some cases with multiple steps, assemble such elemental building blocks into preferred secondary structures (or packing motifs) to construct materials possessing hierarchical superlatice structures with desired functions. In this talk, a unique approach along this research path is going to be presented. Various “giant molecules” based on the “nano-atoms” concept are designed and synthesized. “Nano-atoms” refer to shape- persistent molecular nanoparticles (MNPs) such as fullerenes, polyhedral oligomeric silsesquioxanes, polyoxometalates, folded globular proteins, and others. These “nano- atoms” possess precisely-defined chemical structures, surface functionalities and molecular shapes, which serve as elemental units for the precision synthesis of “giant molecules” via methods such as click chemistry and other efficient chemical transformations. These “giant molecules” include, but are not limited to, giant surfactants, giant shape amphiphiles, and giant polyhedral [2]. These “giant molecules” can assemble into diverse highly ordered building blocks (spherical and non-spherical) to further construct the thermodynamically stable and metastable hierarchical superlattice structures in the bulk, thin-film, and solution. Unconventional superlattice structures similar to metal alloys, such as Frank-Kasper and quasi-Frank-Kasper phases, quasicrystals with 12- and 10-fold rotational symmetries and others [3-6], can be obtained in various environments to exhibit specifically desired properties. This approach has provided a versatile platform for engineering nanostructures that are not only scientifically intriguing, but also technologically relevant.
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A quantum normal-superradiant phase transition

Jonas Larson, Axel Gagge

MC25 : Emerging Trends in Many-Body Cavity Quantum Electrodynamics X, August 25, 2022, 2:00 PM - 3:30 PM

The Dicke normal-superradiant phase transition was predicted by Hepp & Lieb, and Wang & Hioe back in '73. In '85, Hillery & Mlodinow showed that the transition survives also at T=0, i.e. the ground state becomes non-analytic at the critical coupling. Despite this non-analyticity, in the thermodynamic limit the quantum fluctuations vanish, and as such the instability is not, in a strict sense, driven by quantum fluctations. This is in contrast to some paradigm quantum critical models, like the transverse field Ising model, where the fluctuations are extensive in the system size. With this in mind, in this talk we look for a model that supports a normal-superradiant phase transition, and the quantum fluctuations are non-vanishing in the thermodynamic limit. To this end we consider a 1D Rabi-Hubbard type of model. By considering a chiral light-matter coupling we show how a very rich phase diagram results, comprising a normal, a superradiant, a charge density wave, and a `normal entangled' phase.

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Analogue model of the pre-heating and the back-reaction effect

Dr Salvatore Butera, Dr Iacopo Carusotto

MC35: Collective Effects and Non-Equilibrium Phenomena in Quantum Gases and Superconductors IX, August 25, 2022, 11:30 AM - 12:30 PM

We present an overview on our most recent results concerning the study of the back-reaction. The problem of the back-reaction plunges its roots in the field of gravity but, nevertheless, is a general concept, and relevant to a wide range of physical systems. It aims towards a self-consistent theory of the interaction between a quantum field and its background, that in the case of gravity is represented by spacetime. In other words, while at the kinematic (test field) level we observe the excitation of real particles out of the vacuum state of a field, that is driven by a background that is non-stationary (cosmological particle creation) or endowed with a non-trivial topological structure (Hawking radiation emanated from a black hole), the back-reaction problem addresses the quest of how the excited particles affect the dynamics of the background itself.

We present a recent work on the back-reaction during the Pre-Heating in the early Universe. We pursue this study by using a quantum simulator based on a Bose-Einstein condensate of ultra-cold atoms. We simulate the oscillations of the inflaton field within its potential by considering an elongated condensate that is let to oscillate in its transverse direction by exciting the corresponding (high-energy) modes. The resulting modulation of the effective longitudinal speed of sound parametrically amplifies the vacuum fluctuations in the (low-energy) longitudinal modes, that are the analogue of the matter fields in an actual cosmological scenario. At the mean-field (semi-classical) level, the back-reaction appears as an effective damping experienced by the transverse modes due to the creation of real excitations in the longitudinal modes. Beyond the semi-classical level, observable signatures of the back-reaction appears as a spatial decoherence of the transverse oscillations.

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Proliferative advantage of specific aneuploid cells drives evolution of tumor karyotypes

Ivana Ban, Lucija Tomašić, Marianna Trakala, Iva Tolić, Nenad Pavin

MC2: Self-Organisation in Living Systems VIII, August 24, 2022, 4:30 PM - 6:00 PM

Most tumors have abnormal karyotypes, which arise from healthy euploid cells and evolve through numerous complex mechanisms. In a recent mouse model with high levels of chromosome missegregation, chromosome gains dominate over losses both in pretumor and tumor tissues, whereas tumors are characterized by gains of chromosomes 14 and 15. However, the mechanisms driving clonal selection leading to tumor karyotype evolution remain unclear. Here we show, by introducing a mathematical model based on a concept of a macro-karyotype, that tumor karyotypes can be explained by proliferation-driven evolution of aneuploid cells. In pretumor cells, increased apoptosis and slower proliferation of cells with monosomies lead to predominant chromosome gains over losses. Tumor karyotypes with gain of one chromosome arise due to karyotype-dependent proliferation, while for those with two chromosomes an interplay with karyotype-dependent apoptosis is an additional possible pathway. Thus, evolution of tumor-specific karyotypes requires proliferative advantage of specific aneuploid karyotypes.

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Anderson localisation of visible light on a chip

Oliver Trojak, Tom Crane, Dr Luca Sapienza

MC40: Strongly Disordered Insulators III, August 22, 2022, 4:30 PM - 6:00 PM

Being able to control light propagation is of tremendous interest for a variety of applications including energy harvesting, sensing, drug delivery and quantum information technology.
Nowadays, technological advances allow us to control light at the nanoscale and strongly enhance the light-matter interaction in highly engineered devices, where light can be confined in small volumes for extended periods of time. However, the requirement of highly accurate fabrication techniques often limits the scalability and wide application of such devices.

We show that imperfections introduced during the fabrication can be used to efficiently confine light: we demonstrate Anderson localisation of visible light on a silicon nitride chip [1] and directly image the localised modes via a photoluminescence imaging technique.
The spectral characterisation of the localised modes reveals confinement with quality factors up to 10000, exceeding values reported for engineered two-dimensional photonic crystal cavities in the visible range. The achievement of high quality factors in the light confinement proves the potential of our devices for fundamental research in light-matter interaction, like cavity quantum electrodynamics experiments with emitters in the visible range, such as colloidal quantum dots or defect centres in diamond.
Furthemore, given that many spatially-extended photonic modes spontaneously appear along the waveguides, their mutual overlap could be used to realise quantum information networks for the propagation of quantum light, based on coupled Anderson-localised photonic modes, known as necklace states.

We then prove that our device can work as an optical sensor when a contaminant that locally changes the refractive index is introduced [2].
We measure wavelength shifts of optical resonances as large as 15.2nm, more than 100 times the spectral linewidth of 0.15nm, for a refractive index change of about 0.38. By studying the temperature dependence of the optical properties of the system, we report wavelength shifts of up to about 2nm and increases of more than a factor 2 in the quality factor of the cavity resonances, when going from room to cryogenic temperatures. Such a device can allow simultaneous sensing of both local contaminants and temperature variations, monitored by tens of optical resonances spontaneously appearing along a single photonic crystal waveguide.
Our findings demonstrate the potential of Anderson-localised light in photonic crystals for scalable and efficient optical sensors operating in the visible and near-infrared range of wavelengths.

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Superconducting devices grown by Focused Ion Beam Induced Deposition (FIBID)

Professor José María De Teresa, Dr. Pablo Orús, Mr. Fabian Sigloch, Dr. Soraya Sangiao

MC22: Nanoscale Fabrication of Superconducting Devices and Their Applications X, August 25, 2022, 2:00 PM - 3:30 PM

Focused Ion Beam Induced Deposition (FIBID) is a direct-write resist-free nanolithography technique that enables the growth of high-resolution nano- and micro-structures. FIBID relies on a gas precursor that is injected into the area of interest and decomposed by a focused ion beam. Several precursors have been reported to produce superconducting deposits, as recently reviewed by us [1], among which W(CO)6 is the most popular one. Using this precursor, high lateral resolution (in some cases reaching 10 nm) has been achieved [2], and three-dimensional helical nanowires have been grown [3]. In this contribution, we will give an overview of the superconducting devices investigated using FIBID-grown W-based deposits.
As illustrated in figure 1(a), proximity-induced superconductivity has been obtained on various nanostructures [4] [5]. As sketched in figure 2(b), in 50 nm-wide W-based nanowires superconducting-vortex transport along distances up to 10 μm has been observed [6]. Furthermore, in such nanowires the superconducting state can be suppressed by externally applying a modest lateral electric field, as illustrated in figure 1(c) [7]. Currently, we are focusing our attention towards the growth of W-based nanoSQUIDs patterned as two large pads connected by two short nanowires, as shown in figure 1(d). In these devices, the critical current oscillates as a function of the externally-applied magnetic field, which results in a large output voltage to magnetic flux change [8]. Interestingly, these nanoSQUIDs can be implemented in a cantilever, which would find applications in scanning-SQUID technology. The prospects of this technology will be discussed.
Funding by the FET-OPEN project FIBSuperProbes (grant 892427) and collaborations with the other project partners (Prof. Poggio, Prof. Koelle, Dr. Knoll) are acknowledged.

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Fig. 1. Selected applications of FIBID for the growth of superconducting nanodevices (figure reprinted from [1])

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Impact of dispersion forces on matter-wave lithography

Johannes Fiedler

MC19: Advances in the Casimir Force and Heat Transfer Phenomena III, August 22, 2022, 4:30 PM - 6:00 PM

Extreme ultraviolet lithography is the state-of-the-art tool to produce nanostructures, such as microchips. To resolve 14 nm (current limit), photons with an energy of 80 eV are required, which powerfully penetrate the substrate and result in damage. This effect causes many rejects. Further reductions in the resolution are hard a achieve because it requires high-energy photons. Current investigations to overcome these issues are performed by applying matter-wave diffraction. Due to the wave-particle duality, its theoretical resolution is in the order of a few Angstrom to nanometres. The kinetic energy of the particles dominates the transferred energy and is thus in the order of a tenth of meV. [1] However, the design of such lithography masks made of dielectric materials requires the consideration of the dispersion forces interacting between the particles and the mask. Their impacts effectively reduce the openings and imprint a spatial phase shift in the wave, bypassing the mask. [2] In this talk, we present the effective treatment of the dispersion forces and introduce the possibility of proposing mask designs to reach a wished pattern by applying a genetic algorithm approach to a neural network-based inversion. [3]

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Tabletop room temperature electron spin resonance spectrometer measurements from 30 to 600 MHz

Matthew Green, Dr Edward Laird

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

$^{15}N@C_{60}$ endohedral fullerenes possess an electron transition suitable for use as the reference frequency in an atomic clock. This transition occurs at ~38.6 MHz [1]. The clock transition of $^{15}N@C_{60}$ offers the potential for an atomic clock which can be operated at room temperature, with low power requirements and scaling down to a chip-scale device. We have developed an electron spin resonance spectrometer capable of measuring the resonances of several sample materials. This spectrometer is an improvement on that used in [1] utilising tabletop instruments, making it suitable for measuring frequencies from 600 MHz down to the clock transition, much lower than the commercial standard which targets 10 GHz and above. The improved spectrometer allows higher precision in coupling the resonator and faster measurement rates. Additionally this provides both the feedback loop for a passive atomic clock design and the opportunity to advance to a pulsed signal spectrometer. Successful measurements of DPPH and LiPc samples demonstrate the sensitivity of the spectrometer. Pulsed spectroscopy and the loop will test $^{15}N@C_{60}$ for use in an atomic clock.

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Application of soft landed nanoparticles generated using the terminated gas condensation technique to Surface Enhanced Raman

Dr Vicky Broadley, Dr Alistair Kean, Mr Srinu Saranu, Mr Dave Mason

MC9: Recent Developments in Gas Phase Synthesis of Nanoparticles and Applications X, August 25, 2022, 2:00 PM - 3:30 PM

Surface Enhanced Raman offers the promise of high sensitivity detection of trace analytes using Raman Spectroscopy, by exploiting the electric field enhancement of high radius of curvature roughened metal surfaces. Such surfaces can be prepared using a number of different techniques, including deposition of colloidal nanoparticles, magnetron sputtering and electrodeposition . Colloidal nanoparticle SERS substrates are cheap to produce but suffer from poor reproducibility due to high levels of contamination and limited process control associated with the chemical synthesis. Micropatterning techniques involving magnetron sputtering and etching offer higher reproducibility but often involve many processing steps so are expensive to produce.
Terminated gas condensation (TGC) has many advantages over other techniques for the generation of nanoparticles due to its superior control over properties, such as size, composition and purity. These characteristics make TGC nanoparticles an ideal candidate for Surface Enhanced Raman. We present results for Surface Enhanced Raman sensors fabricated using the TGC technique and demonstrate how these substrates overcome many of the barriers to the adoption of SERS for commercial use. We show how the low landing energy of gold nanoparticles generated using the TGC technique is critical to the performance of the sensors. The high mobility of the nanoparticles on the surface enables the nanoparticles to self-organise to form long chain agglomerates around the analyte. The large number of hotspots on these long chain agglomerates maximises the electromagnetic enhancement of the Raman Signal. We present results that show our novel SERS substrates offer trace molecular detection at a range of wavelengths at the ppb and ppm level. Detection levels 3 orders of magnitude higher than in-vial measurements are presented for common analytes including Caffeine and Melamine.

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Jamming transitions in biological tissues

Dr Michael Hertaeg, Assoc. Prof Dapeng Bi, Prof Suzanne Fielding

The collective motion of cells in tissues is an important feature in many biological processes, including cancer development, wound healing and morphogenesis. These processes require overall mechanical integrity and active rearrangements over long times. Recent work spanning many types of cells [1] has identified solid-like to liquid-like transitions which resemble the glass or jamming transition that is well studied in non-biological particulate systems. In tissues, however, these occur at confluence (packing fractions equal to unity), implying a different mechanism compared to simpler particulate systems. Previous experimental and theoretical work has identified the transition to be based on cell shape which is determined by the balance between cell-cell adhesion and cortical tension as well as active forces through swimming or crawling mechanisms [2].

Vertex models, where confluent cells are represented with a tiling of polygons defined by vertex positions have commonly been used in previous studies on tissue mechanics [3]. Here, we study the stress response of an active vertex model over large shear strains to elucidate the onset of rigidity transitions in living tissue. The relationship with strain rate, cell shape and activity are determined and new mechanisms responsible for observed tissue behaviour are proposed.

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Hybrid N-S Aharonov{Bohm Ring as a multifunctional thermodynamical device

Gianmichele Blasi

Thermal transport and quantum thermodynamics at the nanoscale are nowadays garnering increasing attention in the context of quantum technologies. In this work we investigate the thermoelectric performances of a quantum heat engine based on an Aharonov-Bohm interferometer connected with one metallic contact on one side and with a superconducting lead on the other. In the nonlinear regime, we demonstrate the tunability, efficiency, and heat rectification property that this mesoscopic quantum machine can achieve, confirming the exciting perspectives that this AB ring offers for developing efficient thermal machines in the fully quantum regime.

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Energy scales of the quantum electronic orders in cuprates revealed by electronic Raman spectroscopy

Professor Alain Sacuto

High-Tc cuprate superconductors are one of the iconic quantum materials. Although discovered more than 35 years ago, the complexity of their physics remains misunderstood. It calls for new concepts where the quantum electronic orders of matter are no longer independent of each other as in traditional materials. In order to understand the physics of cuprates, it is important to identify the energy scales that underlie their (T-p) phase diagram. Here, carrying out electronic Raman scattering measurements. we have succeeded in probing these energy scales. Our findings [1-5] provide important clues on the relationship between the different quantum electronic orders in cuprates that will be discussed in detail. In particular, an outstanding challenge in the field is to understand whether the charge density is related to the more exhaustively studied pseudogap and superconducting phases.

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Pattern formation and morphogenesis: veins formation in the Drosophila wing

Mr Simone Cicolini, Mr Marc De Gennes, Ms Sophie Hodara Herszterg, Mr Jean-Paul Vincent, Mr Guillaume Salbreux

MC3: Tissue Dynamics: From in Vivo Experiments to in Silico Modelling IX, August 25, 2022, 11:30 AM - 12:30 PM

How cell differentiation and morphogenesis in developing tissues during embryonic growth are regulated by mechanical and signaling interactions between cells is a key question in developmental biology. The general physical principles underlying the interplay between molecular signaling processes and mechanical changes in pattern formation are still unclear. Drosophila pupal wing is an ideal system to address these questions, because the development of the wing can be imaged in vivo at single cell resolution and because cells can acquire only two different fates: vein or intervein. A marker for the fate of intervein cells (i.e. cells which are not vein cells), DSRF, allows to follow the formation of the vein pattern. Experimental observations reveal that an initial broad, poorly defined pre-pattern (~16 hours after pupal formation) is refined into a highly precise and stereotypical venation pattern in the adult fly (~32 hours after pupal formation). Concurrently with this refinement process the wing as a whole experiences morphogenetic flows causing the tissue to shrink along the anterior-posterior axis and to elongate along the proximal-distal axis, a process known as convergent extension (see the attached image).

What is the relative role of mechanical flows and cell fate adjustments in veins refinement? Analysis of Dumpy mutant flies, flies in which the wing is prevented to undergo convergent extension, shows that the pattern is preserved (same vein width as in wild type), suggesting that the vein refinement is mainly driven by cell fate changes. Experiments indicate that the key components of the signaling system involved in fate decision are the EGFR and Dpp pathway acting to promote vein fate in nearest neighbor cell neighbors, and a Delta/Notch inhibition pathway that extends beyond nearest cell neighbors. Therefore, to explore whether signaling interactions alone can lead to vein refinement we developed a cell fate adjustment model in which the variable describing the vein/intervein state evolves according to an effective reaction-diffusion equation with short range activation and long range inhibition of vein fate. We then simulated the model onto a lattice of cells obtained by segmenting images from a wing tissue. These simulations predict a vein refinement that is in good agreement with experiments.

However, data analysis of in vivo experiments reveals a mechanical contraction due to cellular flows in the vein regions. Hence, to take into account the mechanical contribution to vein refinement we also developed a mechanochemical model. This model consists of an active fluid description of the wing in which flows and mechanical deformations are driven by cellular spontaneous active stresses and active topological transitions, where the active stress is a function of the cell fate variable obeying the equation discussed above.

In the talk, I will present data analysis of vein refinement in wild type and Dumpy flies, results of the simulations of the chemical model based only on cell fate change, and how incorporating mechanical contributions in the model can improve the accordance with experiments.

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Electric field control of domain wall network in twisted bilayers of transition metal dichalcogenides

Vladimir Enaldiev, Fabio Ferreira, Vladimir Fal'ko

MC13: Topological and Geometrical Effects in Complex Nanostructures II, August 22, 2022, 2:00 PM - 4:00 PM

For the past few years study of twisted bilayers of two-dimensional materials has become one of the hottest topics in condensed matter physics. This is mainly due to a high tunability of their transport and optoelectronic properties dictated by moiré superlattice effects [1]. At the marginal twist angles, the moiré superlattice in homobilayers undergo strong lattice relaxation accompanied by formation of domains with preferential stacking separated by a network of domain walls [2,3]. For twisted transition metal dichalcogenide (TMD) bilayers close to parallel alignment, reconstructed moiré supercell consists of two triangular domains with 3R-polytype stackings (XM and MX, see Fig. 1). Lack of mirror and inversion symmetries in the 3R domains allows them to possess out-of-plane ferroelectric polarization which is of opposite direction in the neighboring domains [5]. External out-of-plane electric field introduces an energy imbalance between the neighboring 3R domains inducing expansion of co-polarized domains by means of deformation of the triangular domain wall network. I will present a string-theory-like description of the domain wall network deformation in the electric field, demonstrating existence of universal scaling regime [6] for electric fields above a threshold field, D_\ast, determined by the moiré superlattice period, ℓ.

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Synthetic spin-orbit interaction in low dimensional conductors

Matthieu Delbecq

MC14: Beyond Charge Transport in Nanostructures and 2D Materials via Geometric Design VII, August 24, 2022, 2:00 PM - 3:30 PM

Topological phases of matter in low dimensional materials hold great promises for the exploration of new physics and as potential support for hosting topological phases. Engineering of topological phases, in particular topological superconductivity which could host non-abelian excitations such as Majorana modes, is mainly pursued by combining hybrid materials that should bring together superconductivity and strong Rashba spin-orbit interaction (RSOI) in a one dimensional conductor under a Zeeman field. Carbon nanotubes which are the closest to true one dimensional conductors and in which superconductivity can be induced by proximity could be attractive host materials but they lack an intrinsic RSOI. However spin-orbit coupling is essentially equivalent to a spatially oscillating magnetic field. It is therefore possible to induce RSOI in a low dimensional conductor by designing a local micromagnet. We realized a device made of a carbon nanotube stamped over a magnetically texture Co/Pt gate and coupled to superconducting leads. We observed subgap states in the conductance and performed a detailed investigation of their magnetic field evolution that reveals a large synthetic spin-orbit energy. The local control of the SOI at the nanoscale could turn out to be essential to build up a network of topological phases. More generally it could be used to engineer synthetic topological chains.

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Stochastic thermodynamics of a single nano-mechanical mode

Ilya Golokolenov, Xin Zhou, Arpit Ranadive, Luca Planat, Martina Esposito, Nicolas Roch, Andrew Fefferman, Eddy Collin

MC17: Nanomechanical and Electromechanical Systems VII, August 24, 2022, 2:00 PM - 3:30 PM

We report on an experimental technique that enables us to track fluctuations in a mesoscopic mechanical object cooled to millikelvin temperatures. It is based on the measurement of a mode's motion by means of a microwave cavity to which it couples. We achieve the extreme sensitivity required for these measurements using two stages of parametric amplification in series with a more conventional measurement chain. In particular, we use a quantum-limited travelling wave parametric amplifier (TWPA) preceded by built-in optomechanical gain induced by blue-sideband pumping.
We present the direct observation of a single phononic mode real-time energy fluctuations, from its statistical distribution (PDF) and power spectral density (PSD, see Figure: example at 200mK). We demonstrate that we can separate the true thermodynamics contribution from material-dependent effects, presumably linked to TLS defects (two-level systems). The latter produces a strong 1/f contribution visible in the PSD. For the former, we resolve the frequency cutoff at Γm in the PSD and the specific exponential distribution of the PDF, which are characteristic of a single mode with energy relaxation rate Γm. These stochastic thermodynamics results realised in the classical limit of the mode will be extended to the quantum regime in the future.

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Thermal bistability in local microwave heating of a superconductor

Denis Basko, Deepak Karki, Robert Whitney

MC23: Superconducting Circuits for Quantum Technologies VI, August 23, 2022, 4:30 PM - 5:30 PM

Various local probes constitute a powerful toolkit of experimental solid state physics. The well-known atomic force microscopy and scanning tunnelling microscopy (STM) are often used to probe structural and electronic properties of a material in equilibrium. Microwave impedance microscopy (MIM) enables one to probe electronic excitations without a direct contact between the probing tip and the sample. Scanning thermal microscopy, probing local changes of sample's temperature, provided a new window into dissipation in low-temperature nanoscale quantum transport. Scanning gate microscopy (SGM) is an invasive tool which successfully probes the spatial structure of inhomogeneous 2D electron gases by studying the effect of a local electrostatic perturbation due to a charged tip on the global transport properties. However, it works poorly for systems with high electron density (metals or superconductors) where electrostatic perturbation is screened at very short distances (typically, on the atomic scale). Our idea is to circumvent this difficulty by applying a local thermal perturbation.

We propose a novel probe which creates a local hot spot, a local thermal perturbation, by applying a microwave drive to a small metallic tip placed near the sample and subsequently measuring the global transport properties of the sample. Such probe would be complementary to the SGM which produces an electrostatic perturbation, and to the MIM which does not modify the sample's properties. The local heating probe might prove especially suitable for probing thin films of strongly disordered superconductors, where local heating can create a small normal region. Indeed, while single-electron STM probes the local superconducting gap and Andreev state microscopy probes the global superconducting phase coherence, a local suppression of superconductivity allows one to access the supercurrent pattern. This is especially important in view of the potential application of strongly disordered superconductors as superinductance, a key element of superconducting circuit-based quantum technology.

The spatial resolution of this probe can be significantly improved by taking advantage of a rather fundamental effect, overheating bistability. Namely, at low electron temperature and for microwave frequencies below the superconducting gap the microwave cannot produce new quasiparticles in the system, so the absorption is due to those few which are thermally activated, so the heating is weak and the low-temperature state is stabilized by an efficient phonon cooling. At the same time, at high electronic temperature the gap shrinks and microwave absorption across the gap becomes possible, which stabilizes the solution with electrons being much hotter than the phonons. For a spatially uniform microwave field such bistability was discussed in [1-3]. Here we develop the theory of this bistability in a local setting. Thanks to the bistability, the spatial resolution of the microwave tip is determined by the temperature relaxation length which can be significantly shorter (~20 nm) than the tip size (~100 nm).

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Signature of resonant modes in radiative heat current noise spectrum

Denis Basko, Jonathan Wise, Nathan Roubinowitz, Wolfgang Belzig

MC19: Advances in the Casimir Force and Heat Transfer Phenomena V, August 23, 2022, 2:00 PM - 3:30 PM

While radiative heat transfer in the far field occurs via propagating photons, the near-field heat transfer can be mediated by other excitations (e. g., surface phonons or plasmons), which are much more specific to a given structure, constituting materials, geometry, etc. As a result of extensive studies over many decades, near-field heat transfer mechanisms are understood theoretically in great detail [1]. At the same time, deducing the nature of the heat-carrying excitations directly from experiment is less straighforward: different transfer mechanisms typicallly manifest themeselves as a certain dependence of the average heat current on the temperature and the spatial distance between hot and cold bodies, which is usually a power law. To distinguish experimentally between different power laws requires a very broad range of accessible parameters, which is not always realisable.

Here, we theoretically study the noise spectrum of energy current in near-field radiative heat transfer, and show that it provides valuable information on the nature of heat-carrying excitations, absent in the average energy current. Noise is well known to contain additional useful information as compared to the average signal. This is well exploited in the field of electronic quantum transport, where the electric current noise is used to characterise conduction mechanisms and nature of charge carriers. Energy current noise is much harder to probe experimentally than that of the electric current; however, the recent measurement of electronic temperature fluctuations, directly related to heat current noise [2], suggests that such experiments are a matter of a near future.

Specifically, we calculate the noise spectrum of the energy current in two example systems where the heat is transferred by long-lived resonant modes. The first is a superconducting resonator that can be modelled by an effective quantum circuit, where the heat transfer takes place via the resonator mode [3]. The second is a macroscopic system of two-dimensional (2D) metallic layers modelled by Drude conductivity, where the heat transfer is due to strongly coupled surface plasmon modes [4]. We show that resonant modes produce a sharp feature in the radiative heat current noise spectrum, whose width is related to the lifetime of the resonant mode [5].

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Superradiant Quantum Phase transition for Landau Polaritons with Rashba and Zeeman couplings

Denis Basko, Guillaume Manzanares, Thierry Champel, Pierre Nataf

MC25: Emerging Trends in Many-Body Cavity Quantum Electrodynamics XI, August 25, 2022, 4:30 PM - 6:00 PM

We explore the possibility of the superradiant quantum phase transition (SQPT), also known as photon condensation, in a two-dimensional electron gas (2DEG) placed in a quantising magnetic field and strongly coupled to the photon field in a cavity. Then the matter excitation coupling to the photon field is represented by the cyclotron resonance transition in the 2DEG. Focusing on the coupling to the transverse photon field, we study the SQPT driven by magnetostatic interactions, whose order parameter is a spontaneously generated magnetisation.

We show that such SQPT can in principle occur through a pure in-plane Zeeman coupling to the cavity magnetic field, but it requires extremely small (unrealistic) quantum well widths or extremely fine tuning of the effective Landé factor which makes two Landau levels coincide [1]. Landau level crossings can also be induced by the Rashba spin-orbit coupling, and they favour the SQPT [2] which can be obtained for certain values of the effective Landé factor and filling factors [1].

In all cases, we find the SQPT instability to occur at rather short length scales. In order to correctly describe the matter-field coupling at these length scales, it is necessary to consider fields strongly non-uniform in space, which requires including many cavity modes [1,2].

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Kirigami Engineering of Suspended Graphene Transducers

Chunhui Dai Dai, Yoonsoo Rho, Khanh Pham, Brady McCormick, Brian Blankenship, Wenyu Zhao, Zuocheng Zhang, Matt Gilbert, Michael Crommie, Feng Wang, Costas Grigoropoulos, Alex Zettl

2D Material based electro/optomechanical systems are emerging platforms for realizing next generation technologies such as advanced sensors, actuators, and reconfigurable quantum states. Graphene has been demonstrated as an ideal resonant element for such systems due to its low mass, and high strength. Typically the membrane size dictates the operational frequency and bandwidth. However, in many cases it would be desirable to both lower the resonance frequency and increase the bandwidth, while maintaining overall membrane size. In this work, we employ focused ion beam milling or laser ablation to create kirigami-like modification of suspended pure-graphene membranes ranging in size from microns to millimeters. Kirigami engineering successfully reduces the resonant frequency, increases the displacement amplitude, and broadens the effective bandwidth of the transducer when operated in air or vacuum. Our results present a promising route to miniaturized wide-band energy transducers with enhanced operational parameter range and efficiency.

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ARPES study of normal state in high-Tc cuprates

Makoto Hashimoto

MC31: The Physics of Cuprates XII, August 26, 2022, 9:00 AM - 10:00 AM

The normal state in high-Tc cuprate superconductors have not been fully understood yet despite the extensive efforts in the field over many years. Angle-resolved photoemission spectroscopy (ARPES) has been an important tool for studying such normal state, including the pseudogap and strange metal phases [1]. With the recent instrumentation improvements, ARPES measurements in the normal state with unprecedented precision became possible, resulted in surprising findings. With a systematic doping-temperature dependence study on Bi2212 [2], we revealed that the incoherent strange metal abruptly reconstructs into a more conventional metal with quasiparticles across the putative critical doping around 19% concomitant with the collapse of the pseudogap, defining a temperature-independent vertical phase boundary. This observation is incompatible with existing pseudogap quantum critical point scenarios. By carefully studying the overdoped regime above such critical doping, we show that the normal state gap observed above 19% is due to strong superconducting fluctuations [3,4]. Combined with theoretical calculations, the result suggests that the antinodal shallow band bottom is playing an important role for the fluctuating superconductivity [3]. Furthermore, we demonstrate that ARPES-derived electronic specific heat reproduces the specific heat peak at Tc, making direct connection between ARPES spectra and thermodynamic property. Further, we reveal that this thermodynamic anomaly arises from the singular growth of in-gap spectral intensity across Tc in the overdoped Bi2212 with strong superconducting fluctuation.

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The Closeness of the Ablowitz-Ladik Lattice to non-integrable DNLS Lattices

Nikos Karachalios

While the Ablowitz-Ladik lattice is integrable, the DNLS equation, which is more significant for physical applications, is not. We prove closeness of the solutions of both systems in the sense of a “continuous dependence" on their initial data in the suitable metrics. The most striking relevance of the analytical results is that small amplitude solutions possesing the functional form of the analytical solutions of the Ablowitz-Ladik system persist in the DNLS one. It is shown that the closeness results are also valid in higher dimensional lattices as well as for generalised nonlinearities. We also discuss extensions of this approach to NLS partial differential equations and its potential applications.

(joint work with Dirk Hennig and Jesús Cuevas Maraver)

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The theoretical and experimental study of single ion magnets based on the Ho(III)-EDTA and Dy(III)-EDTA complexes in various environments: the influence of the structural changes on the spectroscopic and magnetic properties

Marek Eggen, Marek Krośnicki, Maria Korabik, Rafał Janicki, Andrzej Kędziorski

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

The rise of the interest in the Lanthanide--based SMMs (Single Molecule Magnets) and SIMs (Single Ion Magnets) can be associated with the fact that these materials show a premise of many possible applications, namely: in quantum information processing; as MRI contrast agents; as molecular spintronic and high density data storage devices. The main challenge in this field is to design a SIM or SMM material in a way that will improve its magnetic performance.
The structure surrounding the Lanthanide ion influences its magnetic anisotropy and when the anisotropy changes then the magnetic properties also change. We have explored several structure models based on Ho(III)-EDTA and Dy(III)-EDTA single ion magnets in order to investigate how the spectroscopic and magnetic properties of a cluster can be affected by the molecules of a certain solvent in the second coordination sphere and by the neighbor clusters that surround the molecule under study.
We compare our experimental results with the theoretical calculations based on the ab-initio methods. The experiments and theoretical calculations for all the structure models have been performed at many different ranges of temperatures and for diverse magnetic fields to better understand the magnetic behavior of the studied materials in various environments. We discuss the crucial role of choosing an adequate solvent in designing molecular magnets and how the solvent influences the effective energy barrier for the magnetization reversal and most of all - how the right solvent can enhance the performance of a given molecular magnet.

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Ultrafast heat and charge dynamics in graphene-based systems

Klaas-jan Tielrooij

MC51: Ultrafast Dynamics in Magnetic and Strongly-Correlated Materials XI, August 25, 2022, 4:30 PM - 6:00 PM

The special properties of electronic heat in graphene [1] provide the foundation on which several key optoelectronic device concepts are based, including photodetectors and transceivers for data communication applications [2]. It is thus crucial to understand the heating-cooling dynamics of hot carriers in graphene.

We have studied the cooling dynamics in two high-quality graphene systems which a mobility above 15,000 cm^2/Vs: WSe_2-encapsulated graphene and suspended graphene. Our ultrafast pump-probe measurements, combined with theory, indicate that the cooling time at room temperature is intrinsically limited by the coupling of electrons to optical phonons, which form an efficient heat sink even for electrons with initially insufficient kinetic energy for optical phonon emission [3].

We have also studied heat spreading of hot carriers in graphene, using a novel spatiotemporal thermoelectric microscopy technique with femtosecond temporal and nanometer spatial control [4]. When tuning to the hydrodynamic time window before the occurrence of momentum relaxation, and under Dirac-fluid conditions, we observe a giant thermal diffusivity up to 70,000 cm^2/s. Moreover, the thermal conductivity of the electron system can be larger than the already record-high thermal conductivity of the phonon system of graphene. This result is relevant for thermal management applications.

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Exceptional points and exceptional behavior in quantum metamaterials

Charles Downing, Oliver Fox

Symmetry underpins our understanding of physical law. Open systems, those in contact with their environment, can provide a platform to explore an important dual symmetry: parity-time (PT) symmetry. That is when swapping left and right, as well as the direction of time, leaves the system essentially unchanged. The condition of combined space and time reflection symmetry has immediate utility for open quantum systems, where there is balanced loss into and gain from the surrounding environment. In such circumstances, the fact that the resultant Hamiltonian is non-Hermitian may be disconcerting at first glance. While the eigenvalues of a Hermitian Hamiltonian are always real, the Hermicity condition is actually more stringent than is strictly necessary. It was shown by Bender and co-workers [1] that non-Hermitian Hamiltonians which obey parity-time PT symmetry can both admit real eigenvalues and describe physical systems. This brilliant realization has led to many recent advances [2], especially in essentially classical systems, which are intrinsically linked to topological physics [3]. However, the exploitation of PT symmetric physics in truly quantum systems is much less mature. Here
we consider a general quantum metamaterial built from qubits [4]. We discuss how the concept of PT symmetry may be generalized for quantum systems, and how this leads to a variety of flavours of exceptional point (which mark the borders between trivial and nontrivial regimes). When passing through these quantum exceptional points, we demonstrate some remarkable observable consequences, including for unconventional quantum transport throughout the metamaterial. We also suggest some experiments which should be able to tease out the differences between exceptional points in classical and quantum systems, which may be important in the development of future
quantum devices.

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Superconducting Spintronics in Curved Geometries

Sol Jacobsen

MC14: Beyond Charge Transport in Nanostructures and 2D Materials via Geometric Design VIII, August 24, 2022, 4:30 PM - 6:00 PM

Conventional singlet superconducting correlations can be converted into unequal-spin triplet pairs when interfaced with a ferromagnet. These can be rotated into equal-spin triplets when there exists a second, spin-orienting reference frame in the structure. Generation and control of such spin-polarized triplet pairs allows us to send and manipulate spin-based information with dissipationless currents. This singlet-to-spinful-triplet conversion has been governed by magnetic multilayers, conical magnets, or intrinsic spin-orbit coupling in conventional spintronics. However, it was recently shown that the conversion can be controlled by introducing curvature in the ferromagnetic wire. We show that the curvature can then be used to change the direction of the charge current in a Josephson junction (see Fig.1) [PRB 104, L060505 (2021)], and directly control the superconducting transition [arXiv:2112.12797, to appear in PRB]. In this talk, I will introduce the general framework and significance of these results, and discuss how, by taking advantage of recent developments in materials design and geometric control, this opens many possibilities for the future of superconducting spintronics.

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Charge density fluctuations and the strange-metal behavior of high-Tc superconducting cuprates

Prof. Sergio Caprara

MC31: The Physics of Cuprates IX, August 25, 2022, 11:30 AM - 12:30 PM

Besides the as yet unknown mechanism that is responsible for high-Tc superconductivity, a major unresolved issue of the cuprates is the occurrence of a strange metallic behavior above the pseudogap temperature T*. Even though such behavior has been phenomenologically described within the so-called Marginal Fermi-Liquid theory, a microscopic explanation for its occurrence is still missing. However, recent resonant X-ray scattering experiments identified a new class of overdamped charge density fluctuations characterized by low characteristic energy scales and short characteristic length scales, which are related to the well-known charge density waves. These fluctuations are present over a wide region of the temperature-vs-doping phase diagram of the cuprates and are also found well above T*. It has recently been shown that charge density fluctuations strongly affect the electron and transport properties and can explain the strange-metal phenomenology. Therefore, charge density fluctuations are likely the long-sought microscopic mechanism underlying the peculiarities of the metallic state of cuprates.

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Nonlinear localisation with machine learning methods

Dr Giorgos Tsironis

Nonlinear localisation in lattice systems can be investigated through novel machine learning techniques. We give an overview of the methods to be used and focus on classical and quantum processes that involve nonlinear modes. We show specific lattice configurations where the use of machine learning enables to optimisation of nonlinear transport properties. We use the discrete nonlinear Schroedinger equation as the basic model both in the classical and quantum domain.

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Non-equilibrium BCS-BEC crossover and effects of Fulde-Ferrell type pairing fluctuations in a driven-dissipative Fermi gas

Dr. Yoji Ohashi, Mr. Taira Kawamura, Dr. Ryo Hanai

MC35: Collective Effects and Non-Equilibrium Phenomena in Quantum Gases and Superconductors IX, August 25, 2022, 11:30 AM - 12:30 PM

We theoretically discuss how the BCS-BEC crossover phenomenon, which has extensively been discussed in thermal equilibrium ultracold Fermi gases, is altered, when the system is out of equilibrium. We consider a model driven-dissipative Fermi gas with a tunable s-wave pairing interaction, which is coupled with two reservoirs with different values of the Fermi chemical potential. To include non-equilibrium strong-coupling effects, we extend a T-matrix approximation (TMA), developed in the thermal equilibrium BCS-BEC crossover physics, to the non-equilibrium state, by using the Schwinger-Keldysh Green's function technique.

In the non-equilibrium steady state, the system-reservoir coupling naturally brings about non-zero quasi-particle lifetime, leading to the suppression of the superfluid phase transition. As another reservoir effect, we show that the two reservoirs with different values of the Fermi chemical potential imprint a two-edge structure on the momentum distribution of the Fermi gas. This structure works like a two Fermi surfaces with different sizes as in the case of the electron system under an external magnetic field, so that Fulde-Ferrell (FF)-type pairing fluctuations (which is characterized by non-zero center of mass momentum) are anomalously enhanced (although the present system has no spin imbalance). These non-equilibrium FF-type pairing fluctuations are found to be too strong to stabilize the FF-type superfluid long-range order in the present spatially isotropic system. Instead, these fluctuations lead to remarkable suppression and reentrant behavior of the BCS superfluid state in the weak-coupling BCS side. We also point out that, because the FF-type pairing fluctuations can be weakened by removing the spatial isotropy from the system, the non-equilibrium FF-type superfluid state may be stabilized, when the system is loaded on a 3D optical lattice.

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Simulation of imbibition-induced strain in oriented nanoporous silica (MCM-41) on the single pore scale

Mr. Lars Dammann, Prof. Dr. Robert H. Meißner, Prof. Dr. Patrick Huber

MC7: Exploring Liquid Properties in Confined Geometry (Up To Mesoscopic Scales) XI, August 25, 2022, 4:30 PM - 6:00 PM

Capillarity-driven flows in pores a few nanometers in diameter play an important role in many natural and technological processes, for example in clay swelling, frost heave, catalysis and transport across artificial nanostructures, bio-membranes and tissues [1]. Here we present molecular dynamics simulations modelling the capillary flow of water into oriented silica nano-pores (MCM-41) of around 3 nm diameter pore size. By providing implementations of water-water [2], water-silica [3] and silica-silica [4] forcefields we are able to simulate the spontaneous imbibition dynamics of water into the silica pores. The penetration depth of the fluid L into a cylindrical pore after time t can be described by the Lucas-Washburn equation, $L = \sqrt{v}\sqrt{t}$. v is the so-called "imbibition speed" that depends on the ratio of the fluid parameters, the fluid/wall interaction, the radius of the pore and the hydrodynamic slip-boundary condition [5]. In this work we show that during imbibition in longitudinal and radial pore direction anisotropic strains can be observed that can be classified as two distinct types of strain. At the start and the end of the imbibition process the observed strains are almost instantaneous while during the imbibition process there are continuous changes of strain that scale with the imbibition progress. As a next step we aim to develop the theoretical motivation for the observed imbibition induced strain types and their magnitudes by connecting them to the Bangham effect, that leads to continuous strains during wetting of a surface, and the acting Laplace pressure, that leads to instantaneous strains in the pores subject to capillary-flows [6]. Overall the results of the simulations should lead to better understanding of capillary-driven flows in nanoporous material and the corresponding imbibition-induced strains of the host material on a single-pore scale.

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Finite-size scaling and thermodynamic limit of a first-order dissipative phase transition in zero dimension

András Vukics, Riya Sett, András Dombi, Peter Domokos, Johannes M. Fink

MC25 : Emerging Trends in Many-Body Cavity Quantum Electrodynamics X, August 25, 2022, 2:00 PM - 3:30 PM

I present our studies over the last several years related to the photon-blockade breakdown (PBB) effect, occurring most simply in a coupled system of a bosonic mode and a two-level system. Having been identified as a first-order dissipative phase transition in a thermodynamic limit where the coupling between the subsystems goes to infinity without affecting the system size [1] (hence the designation zero-dimensional), PBB was studied in a finite-size scaling approach [2], with finite-size scaling exponents determined numerically. I describe the experimental studies: PBB was first observed in a circuit QED platform [3], and the thermodynamic limit can also be modeled with superconducting artificial atoms [4].

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Radiation effects in fluorite-related oxide structures with aliovalent substitutions.

Dr Gianguido Baldinozzi, Dr Patel Maulik, Dr Kurt Edward Sickafus

MC38: Controlled Irradiation Disorder in Model Systems: Organisation, Dynamics, and Transformations XI, August 25, 2022, 4:30 PM - 6:00 PM

Fluorite-related materials are encountered in nuclear applications as both fuel materials and for the immobilization of minor actinides. Many of these compounds display great resistance to radiation-induced amorphisation, but there seem to be differences in the detailed mechanism. We compare and contrast the observed behavior induced by ion irradiation versus the behavior at high temperatures of some systems with generic compositions close to δ-$A_4B_3O_{12}$, γ-$A_2B_5O_{13}$, and β-$A_2B_7O_{17}$ where A is a rare-earth element like Scandium and B is a tetravalent transition metal. In these structures, cation disorder and anion order compete and constitute an interesting playground for studying the separate behaviors of the two sublattices.

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Scaling Theory of Few-Particle Delocalization

Louk Rademaker

MC40: Strongly Disordered Insulators VII, August 24, 2022, 2:00 PM - 3:30 PM

We develop a scaling theory of interaction-induced delocalization of few-particle states in disordered quantum systems. In the absence of interactions, all single-particle states are localized in $d<3$, while in $d\geq 3$ there is a critical disorder below which states are delocalized. We hypothesize that such a delocalization transition occurs for n-particle bound states in d dimensions when $d+n\geq 4$. Exact calculations of disorder-averaged n-particle Greens functions support our hypothesis. In particular, we show that 3-particle states in d=1 with nearest-neighbor repulsion will delocalize with $W_c\approx 1.4t$ and with localization length critical exponent $\nu=1.5\pm 0.3$. The delocalization transition can be understood by means of a mapping onto a non-interacting problem with symplectic symmetry. We discuss the importance of this result for many-body delocalization, and how few-body delocalization can be probed in cold atom experiments.

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Fabrication and Characterization of 2D Metal-Organic Network on Weakly Interacting 2D Materials

Linghao Yan

MC12: Physics in 2D Nanoarchitectonics I, August 22, 2022, 11:30 AM - 12:30 PM

The fabrication of atomically precise structures with designer electronic properties is currently being vigorously pursued within condensed-matter physics and materials chemistry research communities [1]. Over the past two decades, low-dimensional metal-organic networks (MONs) with various atomically precise lattice structures have been fabricated on coinage metal surfaces [2]. Recently, our group has synthesized and characterized several two-dimensional (2D) MONs on the weakly interacting substrates under ultra-high vacuum (UHV) conditions using low-temperature scanning tunneling microscopy (STM) and spectroscopy (STS) [3-5]. We demonstrate a successful synthesis of a large-scale monolayer Cu-dicyanoanthracene (DCA) network that can grow across the terrace of an epitaxial graphene surface [4]. The ordered DCA3Cu2 network shows a structure combining a honeycomb lattice of Cu atoms with a kagome lattice of DCA molecules. Combing the STM/STS data with density-functional theory (DFT) results, we confirm that a kagome band structure is formed in the 2D MON near the Fermi level. We demonstrate access to multiple molecular charge states in the 2D MON using tip-induced local electric fields, which highlights the role of electron-electron interactions that are likely to give rise to exotic electronic properties. Furthermore, to realize the exciting prospect of truly designer materials, it is important to demonstrate MON synthesis on other 2D substrates. Here, I will also discuss our recent efforts of synthesizing MON on NbSe2, which extends the synthesis and electronic tunability of 2D MONs beyond the electronically less relevant metal and semiconducting surfaces to the superconducting substrates [5,6].

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Magnetotransport in 3D topological insulator nanowires

Cosimo Gorini

MC14: Beyond Charge Transport in Nanostructures and 2D Materials via Geometric Design IX, August 25, 2022, 11:30 AM - 12:45 PM

In nanostructures built out of 3D topological insulators low-temperature phase-coherent transport takes place on a 2D Dirac metal wrapped around an insulating 3D bulk. As such, it is strongly dependent on a peculiar conjunction of structural (real space) and spectral (reciprocal space) geometrical properties.

I will show that shaped topological insulator nanowires, i.e., such that their cross-section varies along the wire length, can be tuned into a number of different transport regimes when immersed in a homogeneous coaxial magnetic field. This is in contrast with widely studied tubular nanowires with constant cross section, and can be understood in terms of magnetic confinement/steering of Dirac surface carriers. Furthermore, such systems appear ideally suited for studying quantum Hall transport in (negatively) curved space.

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Metallic graphene nanoribbons with embedded spins

Rodrigo E. Menchon, Niklas Friedrich, Iago Pozo, Alessio Vegliante, Diego Peña, Jeremy Hieulle, Jose Ignacio Pascual, Daniel Sanchez-Portal, Aran Garcia-Lekue

MC12 : Physics in 2D Nanoarchitectonics II, August 22, 2022, 2:00 PM - 3:30 PM

At the moment, on-surface synthesis is a reliable method for producing atomically precise graphene nanoribbons (GNRs) and engineering their electronic properties by changing their morphology or by doping via chemical substitution. In particular, topological spin-polarized end states[1] or boron-induced magnetic boundary states[2] have been observed in recently reported GNRs. These systems, however, are neither metallic nor have a periodic array of spin states, both of which are desirable for spintronic devices.

In this work, we use Density Functional Theory simulations, Hubbard model calculations, STM, and transport measurements to gain atomic-level insight into the electronic properties and magnetic behavior of width-modulated GNRs with boron atoms in their backbones. According to our calculations, such GNRs are metallic, and spin 1/2 states form around each boron unit. Remarkably, the different symmetry of the valence band and the localized boron band protects these spin states from propagating electrons. Electronic transport measurements show low energy ballistic transport channels, and dI/dV-spectroscopy reveals spin-related fingerprints, which are consistent with the theorical findings.

The simultaneous presence of metallic character and a spin chain in a single GNR may be useful in the design of new metal-free quantum devices with a wide range of novel applications in nanoelectronics and spintronics.

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Self-imaging based logic operations

Mateusz Gołębiewski, Paweł Gruszecki, Maciej Krawczyk

MC44: New Perspectives in Magnonics, from 2D to 3D Systems II, August 22, 2022, 2:00 PM - 3:30 PM

In linear optics, self-imaging of waves, also known as the Talbot effect, is well known and has found various applications, particularly for computing scenarios in photonics. Recently, we have demonstrated this effect for spin waves using micromagnetic simulations.[1,2] Here, we decided to propose the use of spin-wave self-imaging in logic operations by simulations of interference systems that perform logic functions within thin ferromagnetic multimode waveguides. With their high programmability and scalability, we were able to design lookup tables (LUTs) and logic gates operating this way, which are particularly suitable for FPGA (field-programmable gate array)-type circuits, where multiple logic realizations can be achieved at the same time. The proposed system is composed of a wide spin-wave waveguide with 8 mono-waveguide inputs and 5 outputs (see Fig. 1) that are based on the threshold detection technique. After determining input signal phase shift $\phi = \pi/2$ as logic '1', and no shift $\phi=0$ as logic '0', we measure the spin-wave intensity at the output, and define its logic state based on the assumed threshold value. The realisation for a thin film of yttrium iron garnet and a spin-wave frequency of 40 GHz is shown in Fig. 1. Herein, I'll present selected examples of the proposed solution, bringing the attention of the magnonic community to the self-imaging effect and the potential of spin-wave diffraction and interference in logic functions. In fact, the Talbot effect is particularly suitable for designing reconfigurable magnonic logic gates, since its behaviour is affected by a wide range of static and dynamic parameters.
As the proposed layouts are feasible for experimental implementation, we believe that our numerical demonstration will attract researchers for further development and implementation. We have therefore created a physical basis for the application of the magnonic Talbot effect to signal processing.
The research has received partial funding from the NCN of Poland, project nos. 2019/35/D/ST3/03729 and 2018/30/Q/ST3/00416.

Figure 1. Design of a 2-in 5-out lookup table. In (a) there is a scheme of the symmetric SW LUT with Talbot length zT and the inputs period d marked. CI denotes control input and numbered markings I and O denote inputs and outputs, respectively. In (b) simulation results are presented, showing the operation of the lookup table based on the self-imaging (state for inputs I1=’1’, I2=’0’, CI=’0’). The upper part shows the intensity distribution on the inputs (gray columns) and their phase shift (maroon line). Below is a phase map of the functional area where the inputs are on the top edge, and the inset zooms the region where the SW self-imaging takes place. It contains normalized graphs of the dynamic magnetization intensity in 2D and the averaged one in 1D. The orange dashed line indicates the predefined threshold value.

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MAGNONIC EIGENMODES OF LATERALLY CONFINED TOPOLOGICAL SPIN-STRUCTURES IN PRESENCE OF INTERFACIAL DZYALOSHISNHKII-MORIYA INTERACTION

Prof Giovanni Carlotti

MC44: New Perspectives in Magnonics, from 2D to 3D Systems II, August 22, 2022, 2:00 PM - 3:30 PM

In the framework of chiral magnetism, there is currently a great interest towards the influence of the interfacial Dzyaloshinskii–Moriya interaction (i-DMI), provided by a heavy metal underlayer, on the propagation of spin waves (SWs) in extended films and multilayers, with emphasis given to the induced SW non-reciprocity [1]. However, the characteristics of SW eigenmodes induced by i-DMI in laterally confined spin structures, such as magnetic dots and/or magnetic skyrmions, have been less studied and there is a lack of experimental data in the relevant literature.
In this talk, after a short review of the different causes of spin-waves non-reciprocity, I will focus on the non-reciprocal behavior induced by i-DMI in artificially nanostructured systems consisting, for example, of isolated, laterally confined, magnetic nanostructures where the presence of i-DMI induces a substantial red-shift of the eigenmodes frequencies and the appearance of new peaks in BLS spectra, corresponding to odd modes that would remain invisible in the absence of DMI [2]. In addition, it will be shown how DMI strongly affects the band structure of 1D magnonic crystals consisting of either arrays of interacting Permalloy nanowires [3] or a chain of Nèel skyrmions [4]. Finally, preliminary BLS experimental data relative to arrays of dots and wuires, as well as to SW eigenmodes of skyrmions spontaneously generated in magnetic multilayers will be presented.
Financial support from the italian national project IT-SPIN (PRIN-2020LWPKH7), funded by MUR, is kindly acknowledged.

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Development of manufacturing processes for coordinate-based 3D µ-standarts

Miss Celina Hellmich, Mr Sebastian Bütefisch, Mr Thomas Weimann, Mrs Stefanie Kroker, Mr Matthias Hemmleb

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

An important contribution to the success of micro- and nanotechnologies was and is the possibility of being able to visualize and measure objects on this scale. The calibration of 3D-microscopes today requires not only the calibration of the side and height scales, but also the calibration of the flatness error of coordinate planes as well as the shear of coordinate axes. To meet these requirements, suitable standards and reference metrology are needed. The standards currently available on the market for optical microscopes are for different individual calibration steps (lateral, height steps, shape standards).
The 3D-standarts combine the properties of the commercially available standards and are therefore universally applicable. The advantage of this 3D-standards is that the calibration factors for all three axes and even the coupling factors between them can be determined in one measuring and evaluation step. Otherwise, these factors must be determined separately, e.g., with step height and 1D-/2D-grid standards, which means a multiple of measurement and evaluation effort and thus costs.
With this alternative calibration approach, geometric misalignments can be determined using 3D-reference structures with known object coordinates. The approach is based on the principle of measurement marks, as used in close-range photogrammetry, where the actual size of an object can be calculated from the comparison of the object with the measurement mark. Since the 3D-coordinates of the marks on the reference structure are known, the calibration process involves a geometric transformation of the measured object coordinates of the marks to the known object coordinates of the marks according to the calibration model.
Currently used 3D-standarts are produced with FIB . Each standard is therefore a cost-intensive custom-made product that also requires time-consuming calibration. Especially for larger structures for the calibration of optical 3D-microscopes, production using FIB is not feasible.
Therefore, wafer-based mask processes for the fabrication of 3D-standarts are to be developed so that many structures can be reproducibly fabricated and adapted to the respective device to be calibrated. The aim of the project is to provide both a validated, wafer-based manufacturing process for 3D-standarts in different sizes and a calibration strategy that ensures traceable reference measurement in verifiable accuracy levels.
First results were achieved by stepwise build-up of silicon oxide layers in combination with a dry etching process. In this way, two-level pyramid structures can be produced onto which the marker for calibration can be applied with the help of lift-off. These structures can be produced from a size range of 5µm edge length for use in the SEM, up to edge lengths of 225µm for optical 3D-microscopy.
However, the structures have a slope angle of about 80°, which works well for calibration of 3D-microscopes, but for SEM calibration the angle must be <70° to provide enough height information for height calibration. To lower the slope angle further, additional etching methods will be evaluated in the further course of the project.

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Time-resolved observation of a dynamical phase transition of atoms in a cavity

Dr Thomas Clark, Dr András Dombi, Dr Francis Williams, Dr Árpád Kurkó, Professor József Fortágh, Dr Dávid Nagy, Dr András Vukics, Dr Péter Domokos

MC25 : Emerging Trends in Many-Body Cavity Quantum Electrodynamics X, August 25, 2022, 2:00 PM - 3:30 PM

We present a dynamical, multi-level atom-cavity blockade effect and monitor its breakdown transition in time. As in the case of optical bistability, atoms initially impede transmission by detuning a cavity mode from the driving laser. The interacting system however, eventually transitions into an uncoupled state via a critical run-away process: resulting in maximum transmission. These two extremes of transmission are macroscopic reflections of well-defined atomic states, and thus are interpreted as phases of a dynamical transition. By monitoring the output of the cavity, we make time-resolved measurements of the order parameter and that of the enhanced photon number fluctuations. Considering these results for different cavity driving intensities, we establish finite-size scaling relations that suggest such a runaway effect is in fact a genuine dynamical phase transition.

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Current-induced resonance in long conductive ferromagnetic nano-wires

Mohammad Alneari

MC44: New Perspectives in Magnonics, from 2D to 3D Systems III, August 22, 2022, 4:30 PM - 6:00 PM

Conductive ferromagnetic nanostructures form important constituents in electromagnetic materials and composites for high frequency applications in communications and wave absorption [1]. They are also compatible with semiconductor fabrication methods for the development of magnonic nano-structures and devices [2]. Understanding the magnetisation dynamics and spin-wave modes of the magnetic nanostructures and their shape and size dependence enable tailoring of the magnetic and dielectric properties for targeted magnonic devices and electromagnetic systems.

Electric currents induced in conductive ferromagnetic structures (due to electrical, optical or electromagnetic coupling) lead to non-uniform electromagnetic fields with different skin depths (both non-magnetic and magnetic) that control the resonance mechanism and spin-wave modes in the magnetic nanostructures [3,4]. In this work we study the current-induced ferromagnetic resonance in long circular cobalt nano-wires, both solid and multi-layered with diameters 50 – 500 nm by solving the coupled system of the Landau-Lifshitz-Gilbert (LLG) equation and quasi-static Maxwell's equations in finite-elements using Comsol MultiphysicsÓ (see Fig. 1). We include the contributions of the magnetocrystalline anisotropy, exchange fields, magnetostatic fields and eddy currents in the solution of the coupled system. The resonance mechanisms in the nano-wires, frequencies and their size dependence will be studied by evaluating the local and integrated power dissipation spectra, and by comparison to simplified analytical models of exchange curling and thin-film modes.

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A First Principle study on structural, electronic and magnetic properties of tetragonal/hexagonal-VSe2(001)/Co heterostructure

Ms Arpita Mukherjee

MC52: Heterostructures, Combining Organic Molecules and 2D Materials V, August 23, 2022, 2:00 PM - 3:30 PM

Over the last few years, researchers have been interested in studying the various properties of Transition metal dichalcogenides(TMDs). Layered TMDs consist of one TM bonded with two chalcogen atoms forming covalent bond. Vanadium diselenide(VSe2) is a typical example whose bulk is paramagnetic and surprisingly its monolayer seems to be ferromagnetic. In bulk VSe2, Se-V-Se layers are stacked along (001) direction forming trigonal(T) phase crystal. Hence, these 2D structures can reveal distinctive properties compared to that of the bulk counterparts. Here we propose a completely new heterostructure based on VSe2 on cobalt substrate. The properties were studied using DFT and DFT+U approach considering the vanderwaals correction between the layers. Results reveal the antiferromagnetic coupling between VSe2 and Co, thereby reducing the magnetic moment of Co atom. This is a direct consequence of the presence of Co-V hybridization across the interface. Furthermore, the study was extended by varying the layers of VSe2 structure and exploring its magnetic and electronic property.
Keywords: TMDs, DFT+U, trigonal and hexagonal, magnetic property

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Thermal and electron induced relaxation of densified silica phases

Nadège Ollier

MC38: Controlled irradiation Disorder in Model Systems: Organisation, Dynamics, and Transformations IX,
August 25, 2022, 11:30 AM - 12:30 PM

Thermal and electron induced relaxation of densified silica phases
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Silica is the main constituent of the earth mantle. Silica-based glasses provide the backbone of many of nowadays rapidly expanding photonics applications, which disserve diverse fields such as optical communications, electronics, sensor technologies, medicine, and materials processing. Despite the fact that it is a simple glass and thus often used as a model vitreous system, amorphous silica presents anomalies that are still unresolved (i.e the anomalous negative pressure derivatives of elastic moduli at low P)1. Another actual open question concerns polyamorphism (different amorphous states with distinct short- and/or intermediate-range orders can be produced by thermo-mechanical path engineering) and one of the challenging questions to be addressed is the nature of the phase transformation between LDA (low density amorphous state) and HDA (High Density Amorphous, corresponding to the 2.6 g/cm3 phase obtained at 25 GPa) whereas under irradiation (neutrons, electrons, ions, ...), a maximum densification of 4-5% can be achieved2. We have shown that independently of the initial structure and density (ranging between 2.21 and 2.6 g/cm3), under a subsequent irradiation dose of 11 GGy, all silica samples relax towards a unique structure associated to a 2.26 g/cm3 density similar to metamict phase. Metamict phase was first discovered by Primak 3 in 1958 arising from quartz amorphization after a high dose of neutron irradiation of 180 x1018 neutrons/cm2. The structure of the metamict phase formed from several silica polymorphs precursors are different and no unique state is reached4. In the present talk, we report results from thermal relaxation of the metamict phase to know better about it properties and transitions between HDA and LDA. The spectroscopic method that is utilized is Raman spectroscopy. We will compare high pressure and high temperature densified silica samples obtained along different densification pathways followed by electron irradiation at 107 Gy and 11 GGy (metamict phase). Among the results of interest, we can notice that the “recovery phase” of metamict silica after a 1100°C annealing does not correspond to pristine silica. Moreover, we evidenced a sharp increase of the 4 and 3-membered rings number during the thermal relaxation corresponding to a transitory state of high dense silica phases. Several results evidenced amorphous-amorphous phase transitions between silica phases.

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Tunable Andreev-conversion of single-electron charge pulses

Pablo Burset, Benjamin Roussel, Michael Moskalets, Christian Flindt

MC21: Bound States in Hybrid Superconductor Nanostructures III, August 22, 2022, 4:30 PM - 6:00 PM

Electron quantum optics explores the coherent propagation and interference of single-electron charge pulses in electronic nano-scale circuits that are similar to table-top setups with photons [1]. So far, experiments with dynamic single-electron emitters have focused on normal-state conductors, however, the inclusion of superconducting elements [2,3] would pave the way for a wide range of applications that exploit the electron-hole degree of freedom, for example, for quantum information processing or quantum sensing. Here, we propose and analyze a tunable mechanism for the on-demand conversion of single-electron pulses into holes through Andreev processes on a superconductor [4]. To this end, we develop a Floquet--Nambu scattering formalism that allows us to describe the conversion of charge pulses on a superconductor, and we show that it is possible to generate arbitrary superpositions of electrons and holes with the degree of mixing controlled by the magnetic flux in an interferometric setup. We provide a detailed discussion of the optimal operating conditions in realistic situations and demonstrate that our proposal is feasible based on current technology.

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Design and fabrication of high kinetic inductance parametric amplifier

Mr. Cong Fu, Dr. Jharna Paul, Mr. Valentino Seferai, Dr. Sergey Danilin, Dr. George Long, Dr. Tania Hemakumara, Dr. Jonathan Williams, Prof. Martin Weides

MC23: Superconducting Circuits for Quantum Technologies V, August 23, 2022, 2:00 PM - 3:30 PM

In superconducting quantum circuits, quantum-limited travelling-wave parametric amplifiers (TWPA) exhibit promising properties -including low noise, wideband, large gain, wide dynamic range, and phase-sensitive process. The quantum-limited TWPAs play a key role in improving the readout of superconducting qubits and weak microwave signals since they add only the quantum-limit amount of noise during amplification. Conventionally, the non-linear elements of these quantum amplifiers are Josephson tunnel junctions which require sub-nanometre control of the tunnel oxide thickness. These Josephson TWPAs are very sensitive to fabrication errors due to their complexity. In this work, we present a new design strategy and fabrication process for a kinetic inductance TWPA in a three-wave mixing process, and with microstrip-based and CPW-based implementations. These two designs also present two different techniques for dispersion engineering to match the phases of two input tones. In addition, we introduced optimized periodic loadings along the waveguide to suppress higher-order harmonics and reduce the thermalisation during amplification.
We report on the experimental realisation of the high kinetic inductance parametric amplifiers. The kinetic inductance of our 15nm TiN film was determined and the design matched to realise a highly nonlinear microstrip transmission line with a 50Ω characteristic impedance. For the fabrication process, TiN films were deposited using atomic layer deposition. The electron-beam lithography along with the dry-etch technique was conducted to create the patterns varying from 500nm to 4μm widths across the 4-inch wafer. Recent results will be discussed.

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Angle-resolved photoemission spectroscopy study of P/Si(111) 6\sqrt(3)x6\sqrt(3)–R30\degree superstructure

Konstantin Shchukin, Maximilian Buchta, Yannic Falke, Dr. Giovanni di Santo, Dr. Luca Petaccia, Prof. Dr. Alexander Grüneis

The silicon - phosphorus (Si-P) system has long been a subject of surface science investigations because of its rich phase diagram with various P surface phases on Si(111) that have been studied e.g. by low energy electron diffraction (LEED). The electronic properties of this system are of technological importance because P is used as an electron donor in Si yet there are very few investigations of the electronic structure of Si-P. Systematic surface science studies by LEED of the Si-P phase diagram as a function of temperature and pressure have been carried out by van Bommel et al. [1] In a wide temperature and pressure window a P/Si(111) 6\sqrt(3)x6\sqrt(3)–R30\degree superstructure forms. In these studies the P/Si superstructure was prepared by Phosphine (PH3) adsorption on the Si(111) surface. Unfortunately, the toxicity of PH3 poses an experimental difficulty. Moreover the electronic properties of the obtained P/Si phase have not been characterized.
In the present work, we address these two shortcomings. First, we prepared the P/Si(111) 6\sqrt(3)x6\sqrt(3)–R30\degree superstructure by direct evaporation of P onto a Si(111) 7x7 reconstructed surface. We then characterized the P/Si(111) 6\sqrt(3)x6\sqrt(3)–R30\degree electronic structures by angle-resolved photoemission spectroscopy (ARPES) using synchrotron radiation. We observed that upon P adsorption to the Si(111)7x7 surface, the reconstruction and the surface state disappear and the electron energy bands with Si character are downshifted by 1eV as a result of the charge transfer from P. Finally, we present the observation of a new energy band after P adsorption that is not present for the pristine Si(111)7x7 surface.

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C_60 mono layer encapsulated in between hBN and graphene monolayers: electronic and vibrational properties

Konstantin Shchukin, Dr. Boris Senkovskiy, Niclas Edelkötter, Daniel Jansen, Yannic Falke, Reda Nabil, Dr. Marek Kopciuszyński, Dr. Alexei Barinov, Dr. Jose Avila, Dr. Pacel Dudin, Prof.Dr. Alexander Grüneis

MC12: Physics in 2D Nanoarchitectonics I, August 22, 2022, 11:30 AM - 12:30 PM

The intercalation of atoms and small molecules into layered materials has a long-standing history [1]. For example, alkali metals and FeCl_3 are frequently studied intercalants of graphite. The driving force for intercalation is a reduction of the binding energy of the ionic compound with respect to its constituents. For example, in the case of alkali metals, atoms that are evaporated onto a layered material readily intercalate in between the layers and form ionic bonds. The intercalation of large organic molecules in this way is not feasible because the energy barrier for intercalation is too high. Yet, the creation of encapsulated organic layers in between two 2D sheets is of high interest e.g. for applications in organic transistors and photovoltaics. C_60 encapsulation and subsequent C_60 doping in between monolayers comprehensive studies could lead to novel devices based on organic superconductivity. The method of choice to synthesise materials away from the thermal equilibrium is van-der-Waals assembly.

Here we combine vdW assembly [2] and molecular beam epitaxy to create a novel hBN/C_60/graphene heterostructure. For the synthesis of this sandwich compound, we evaporate C_60 onto exfoliated hBN and cap this layer with graphene. We characterize this mixed vdW/organic heterostructure by scanning photoelectron microscopy (SPEM) using synchrotron radiation. Then we investigate the samples' electronic structure by angle-resolved photoemission spectroscopy with micrometre spatial resolution (μ-ARPES)[3,4]. We measured highly dispersive graphene and hBN bands and nearly flat C_60 molecular levels. We directly demonstrate, using μ-ARPES, that the C_60 bands are only visible where the C_60 layer is encapsulated in between hBN and graphene. Accordingly, non-encapsulated C_60 on hBN disappears from the sample during the fabrication and annealing steps. Regarding the vibrational properties, we perform Raman spectroscopy and observe vibrational modes corresponding to graphene, hBN and C_60. We perform a lineshape analysis of the Raman modes of C_60 on hBN and of encapsulated C_60 in between graphene and hBN. The Raman method also demonstrates that C_60 appears only in the regions where both graphene and hBN hBN are present.
We believe that the fabrication of the mixed vdW – organic sandwiches technique is a route for the fabrication of new 2D nanoarchitectures with tailored properties.

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[3] J. Avila et al 2013 J. Phys.: Conf. Ser. 425 192023;
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Exploring novel 2D and 3D topological spin textures with advanced x-ray spectromicroscopies

Peter Fischer

MC44: New Perspectives in Magnonics, from 2D to 3D Systems III, August 22, 2022, 4:30 PM - 6:00 PM

Spin textures and their dynamics hold the key to understand and control the properties, behavior and functionalities of novel magnetic materials, which can impact the speed, size and energy efficiency of spin driven technologies. Topology, frustration, and bespoke geometries that impact spin textures have recently attracted significant scientific interest and led to intense research addressing a broad spectrum of challenging scientific and technological questions, including stability, dynamics, nucleation, and transport in novel spin textures, such as chiral bobbers, magnetic hopfions and torons, skyrmion tubes, and curvilinear magnetism [1].
Advanced characterization tools that provide magnetic sensitivity to spin textures, disentangling the role of individual components in heterogeneous material at high spatial resolution, ultimately at buried interfaces and in all three dimensions [2], and at high temporal resolution to capture the spin dynamics across scales, are required to address those questions, and are therefore of large scientific interest.
Various magnetic soft X-ray spectro-microscopies [3] using polarized soft x-rays provide unique characterization opportunities to study the statics and dynamics of spin textures in magnetic materials combining X-ray magnetic circular dichroism (X-MCD) as element specific, quantifiable magnetic contrast mechanism with spatial and temporal resolutions down to fundamental magnetic length, time, and energy scales.
In this talk, I will show our recent studies on the statics and dynamics of magnetic Hopfions, which are spin textures that can only exist in 3D. In addition to the topological winding number which are characteristic for magnetic skyrmions, they exhibit an additional topological linking number and can be viewed as twisted skyrmion tubes. Using a combination of soft x-ray magnetic microscopies we confirmed the creation of Hopfions in tailored magnetic multilayers [4], with target skyrmions [5] being precursors as predicted from theory [6]. Micromagnetic simulation using high performance computing tools on the field dependence of Hopfion structures showed characteristic dynamics including a transition to a toron state around 60mT [7].

This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division Contract No. DE-AC02-05-CH1123 in the Non-Equilibrium Magnetic Materials Program (MSMAG).

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Theory of topological Andreev states

Wolfgang Belzig

MC21: Bound States in Hybrid Superconductor Nanostructures II, August 22, 2022, 2:00 PM - 3:30 PM

Topology is ultimately unveils the roots of the perfect quantization observed in complex systems. The 2D quantum Hall effect is the celebrated archetype. Remarkably, topology can manifest itself even in higher-dimensional spaces defined by control parameters playing the role of synthetic dimensions. However, so far, a very limited number of implementations of higher-dimensional topological systems have been proposed, a notable example being the so-called 4D quantum Hall effect. In this talk I will show that mesoscopic superconducting systems can implement higher-dimensional topology and represent a formidable platform to study a quantum system with a purely nontrivial second Chern number [1]. I further demonstrate that the integrated absorption intensity in designed microwave spectroscopy [2] is quantized and the integer is directly related to the second Chern number. Finally, I discuss that these systems also possess a non-Abelian Berry phase or exotic topologies like tensor monopoles.

[1] H. Weisbrich, R.L. Klees, G. Rastelli and W. Belzig Second Chern Number and Non-Abelian Berry Phase in Superconducting Systems PRX Quantum 2, 010310 (2021)
[2] R. L. Klees, G. Rastelli, J. C. Cuevas, and W. Belzig Microwave spectroscopy reveals the quantum geometric tensor of topological Josephson matter Phys. Rev. Lett. 124, 197002 (2020)

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Robust quantum computing on qubit arrays with fixed longitudinal coupling

Nguyen Le

MC23: Superconducting Circuits for Quantum Technologies II, August 22, 2022, 2:00 PM - 3:30 PM

We propose a scheme for scalable and robust quantum computing on an arbitrarily large two-dimensional arrays of qubits with fixed longitudinal couplings. This opens the possibility for bypassing the fabrication complexity associated with tunable couplers required in conventional quantum computing hardware. Our approach is based on driving a subarray of qubits such that the total multi-qubit Hamiltonian can be decomposed into a sum of commuting few-qubit blocks, and on efficient optimization of the unitary evolution within each block. Each driving pulse can implement a target gate on the driven qubits, and at the same time implement identity gates on the neighbouring undriven qubits for cancelling any unwanted evolution due to the constant qubit-qubit interaction. We show that it is possible to realise a universal set of gates with high fidelities on the basis blocks; and by shifting the driving pattern one can realise an arbitrary quantum circuit on the array. Allowing for uncertainty in all the system's physical parameters, we obtain fidelities around 99.99% despite 1% uncertainty in the qubit-qubit and drive-qubit couplings, and a detuning uncertainty at 0.1% of the qubit-qubit coupling strength. This robust feature is crucial for scaling up as parameter uncertainty is significant in large devices.
arXiv:2110.07737

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Photon-Instanton Collider Implemented by a Superconducting Circuit: Splitting a Single Photon

Amir Burshtein, Dr. Roman Kuzmin, Prof. Vladimir E. Manucharyan, Prof. Moshe Goldstein

MC23: Superconducting Circuits for Quantum Technologies IV, August 23, 2022, 11:30 AM - 12:30 PM

How would our world look like if the fine structure constant α were of order unity? While in our small α world an atom excited to the first excited state has negligible probability of decaying to the ground state while emitting more than a single photon, such processes are important in a large α world, making photon frequency conversion effective in the single-photon regime. We show how such behavior can be realized in a superconducting circuit QED system, where a transmon, which serves as an artificial atom, is galvanically coupled to a high-impedance Josephson junction array, which acts as a waveguide for microwave photons with a high effective α. Instantons (phase slips) that occur in the transmon interact with the microwave photons, and lead to inelastic scattering probabilities which approach unity and greatly exceed the effect of the quartic anharmoncity of the Josephson potential [1]. The instanton-photon cross section is calculated using a novel formalism which allows to directly observe the dynamical properties of the instantons, and should be useful in other quantum field theoretical contexts. The calculated inelastic decay rates compare well with recent measurements from the Manucharyan group at Maryland [2]. I will also show how this effects can be used to shed a single-photon light on the Bulgadaev-Schmid superconductor-to-insulator transition in the transmon, which has been the center of a recent controversy.

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Quasi Bound-State in the continuum in a heavy fluxonium qutrit

María Hita Pérez, Pedro Orellana, Juan José García Ripoll, Manuel Pino

MC23: Superconducting Circuits for Quantum Technologies IV, August 23, 2022, 11:30 AM - 12:30 PM

Quantum excitations generally decay when coupled to a band of states with a continuous spectrum, however, there are some exceptions to those decay processes where a confined state lying at the continuum part of the spectrum lives forever. Those bound states in the continuum (BIC) were predicted long ago and have appeared on several platforms as solid-state devices or photonic devices. Some recent works have found BICs modes in typical quantum-information set-ups, such as superconducting circuits, and argue their usefulness for quantum information applications. In this case, BICs correspond to plasma excitations spatially localized in a superconducting waveguide, while a qubit is used to enforce the necessary boundary conditions.

In this talk, we show how to construct a BIC state [1], more precisely a quasi-BIC state, localized within a fluxonium device when it is capacitively coupled to a waveguide [2]. First, we introduce an effective model for the Hamiltonian, flux, and charge operators of the fluxonium qutrit, obtained via an analytical approach based on Gram-Schmidt orthogonalization and with numerical methods. Then, we analyze the capacitive coupling to a waveguide, finding that the second excited state only decays to the first excited, which is a transition that can be strongly suppressed using a large shunting capacitance for the fluxonium.

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Transport properties in the strange metal phase of cuprates: a hydrodynamical description

Dr Nadia Stegani, Dr Martina Meinero, Dr Andrea Amoretti, Dr Federico Caglieris, Dr Marina Putti, Dr Nicodemo Magnoli, Dr Luca Tomarchio, Dr Stefano Lupi, Dr Daniel K. Brattan, Dr Enrico Giannini, Dr Marco Affronte, Dr Olesia Voloshyna, Dr Silvia Seiro, Dr Andrey Maljuk, Dr Christian Hess, Dr Bernd Buechner

MC31: The Physics of Cuprates X, August 25, 2022, 2:00 PM - 3:30 PM

High-Tc cuprate superconductors (HTS) are strongly coupled systems presenting a surprising phase diagram with many intertwined phases appearing at the same time [1]. Moreover, in the normal state, the transport properties present anomalous behaviours and cannot be explained with the Fermi liquid theory.
Recently, new hydrodynamic theories have been developed in order to describe those systems in which the Fermi liquid picture fails. Indeed, hydrodynamics, which mostly relies on the symmetries of the system without referring to any specific microscopic mechanism, constitutes a promising framework to analyze these materials (see [2,3]). Moreover, it is possible to predict the dependence on temperature and magnetic field of the electric, thermal and thermoelectric transport coefficients, which turn out to depend on a fixed and limited number of hydrodynamic variables [4,5].
Within this new scenario, we measured the DC transport properties on the strange metal phase of two single crystals of optimally doped Bi-2201 and LaSrCuO. Indeed, at the optimally doping, their resistivity is linear for all the measured temperature range above Tc, which is the typical signature of the strange metal behaviour.
For both samples, we performed measurements of electrical resistivity, magnetoresistance, Hall effect, Seebeck effect, Nernst effect and thermal and optical conductivity. For each transport property we extracted and analyzed their temperature dependence, which highlights the failure of the Fermi liquid model. Moreover, the temperature dependence of the transport coefficients has been compared with the predictions of the hydrodynamical picture, in order to prove our approach.
The results on the Bi-2201 [6] perfectly agrees with the hydrodynamical predictions, providing the validity of our approach in the strange metal phase, while the analysis on LaSrCuO are still ongoing.

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Finite-time Landauer principle at strong coupling

Alberto Rolandi

MC20: Recent Advances in Quantum Thermodynamics with a Focus on Many-body Interactions IV, August 23, 2022, 11:30 AM - 12:30 PM

Landauer's principle gives a fundamental limit to the thermodynamic cost of erasing information. Its saturation requires a reversible isothermal process, and hence infinite time. We develop a finite-time version of Landauer's principle for a quantum dot strongly coupled to a fermionic bath. By solving the exact non-equilibrium dynamics, we optimize erasure processes (taking both the dot's energy and system-bath coupling as control parameters) in the slow driving regime through a geometric approach to thermodynamics. We find analytic expressions for the thermodynamic metric and geodesic equations, which can be solved numerically. Their solution yields optimal finite-time processes that allows us to characterise a fundamental finite-time correction to Landauer's bound, fully taking into account non-markovian and strong coupling effects.

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Probing BKT physics in a phase fluctuating 2D superconductor with Nernst effect

Arnab Roy, Aviad Frydman

MC40: Strongly Disordered Insulators III, August 22, 2022, 4:30 PM - 6:00 PM

The signatures of BKT transition among superconducting vortices has consistently been debated upon. In contrast to uncharged superfluid systems like liquid 4He, there appears to be several discrepancies between observations and predictions based on BKT physics of 2D-XY models. In the absence of quality numerical experiments using models like the TDGL equations, uncertainty prevails over the interpretation of experimental data. One such prediction concerns the estimation of the vortex-core energy Ec and its 'universal ratio' ~3 to the critical temperature Tc.

We have used the Nernst effect to estimate the vortex-core energy Ec in the phase-fluctuating superconductor Indium oxide. Using a thermal activation model, we have extracted Ec from Nernst effect data over an order of magnitude variation of Tc's of the disordered sample, and found a surprisingly robust constant ratio of ~10 between the two quantities. However, in line with earlier observations using other methods on widely different systems, the ratio Ec/kBTc was found to be higher than the predictions of the 2D-XY model with respect to the BKT physics. This brings out the inadequacies of the simplified XY picture in the description of disordered superconductors.

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Coordinated poleward flux of sister kinetochore fibers drives chromosome congression and alignment

Domagoj Božan, Ivan Sigmund, Agneza Bosilj, Nenad Pavin

MC2: Self-Organisation in Living Systems VIII, August 24, 2022, 4:30 PM - 6:00 PM

Chromosome alignment at the spindle equator promotes proper chromosome segregation and depends on pulling forces exerted at kinetochore fiber tips together with polar ejection forces. However, kinetochore fibers are also subjected to forces exerted by motor proteins that drive their poleward flux. Here we introduce a flux-driven centering model that relies on flux generated by forces within the overlaps of bridging and kinetochore fibers. This centering mechanism works so that the longer kinetochore fiber fluxes faster than the shorter one, moving the kinetochores towards the center. Our collaborators developed speckle microscopy in human spindles and confirmed the key prediction that kinetochore fiber flux is length-dependent. The experiments also confirmed that kinetochores are better centered when overlaps are shorter and the kinetochore fiber flux markedly slower than the bridging fiber flux. Furthermore, we extend the model to describe congression of chromosomes by considering dynamics of microtubule-kinetochore attachments and motor proteins at kinetochores and find that the length-dependent forces exerted by microtubules from farther pole can overcome the forces exerted by the greater number of microtubules from nearer pole. Thus, length-dependent sliding forces exerted by the bridging fiber onto kinetochore fibers promote chromosome congression and alignment.

Ref: Risteski et al. 2021. Coordinated poleward flux of sister kinetochore fibers drives chromosome alignment. bioRxiv doi: 10.1101/2020.12.30.424837

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Towards a dissipative cat qubit in a 3D circuit QED architecture

Desislava Atanasova, Teresa Hönigl-Decrinis, Ian Yang, Daria Gusenkova, Ioan Pop, Gerhard Kirchmair

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Quantum systems are fragile by nature and suffer from decoherence due to uncontrolled coupling to the noisy environment, creating a major obstacle to building a large-scale quantum computer. As most sources of decoherence are believed to originate from local fluctuations, storing the information non-locally would suppress the occurring errors exponentially. For this reason, this work aims to encode a quantum bit in the fundamental bosonic mode of a weakly non-linear coaxial cavity with engineered two-photon dissipation. Here, the cavity non-linearity is inherited from a fluxonium qubit, which allows us to tune the memory-ancilla interaction in situ. In contrast to the conventional transmon ancilla, this bosonic qubit possesses higher protection against ancilla-induced dephasing. Together with the engineered dissipation, the setup could be utilized as an improved building block for a fully protected logical qubit. In this poster, the progress of coupling a fluxonium qubit to a high coherence cavity is presented.

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Disorder-enhanced superconductivity in a quasi-one-dimensional strongly correlated system

Adam Lowe, Victor Kagalovsky, Igor Yurkevich

MC40: Strongly Disordered Insulators VIII, August 24, 2022, 4:30 PM - 6:00 PM

We perform an analytical and numerical study of a superconducting instability in quasi-one-dimensional (quasi-1D) disordered systems. Modeling them as an array of Luttinger liquids with Josephson-type interchain
coupling, we employed renormalization-group analysis with an extensive search for parameters that support
superconductivity enhancement. We have found that this phenomenon is possible in the parameters range that
support a latent disorder-driven phase transition between charge- and spin-density-wave phases. Our results may
explain the experimental observation of disorder-enhanced superconductivity.

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Correlating the electronic and chemical structure of defects in TMDs with atomic resolution conductive microscopy

Edward Dunn, Professor Robert Young, Dr Samuel Jarvis

MC52: Heterostructures, Combining Organic Molecules and 2D Materials V, August 23, 2022, 2:00 PM - 3:30 PM

Defects on the atomic scale lead to dramatic local changes in materials that collectively transform the macroscopic properties of the host material. The characterization of defects in 2D materials and an understanding of their formation is therefore essential. In many cases, consistent material properties and precise tuning is highly desirable, however, the chaotic formation of defects can also be exploited in order to make unclonable keys and security tags [1]. Atomic resolution imaging techniques provide unparalleled insight into 2D material defects. Scanning probe microscopy methods (SPM) [2, 3] in particular not only reveal topographic information, but also electronic properties unique to specific defect types.
Here, we show that single defects can be identified with atomic resolution using conductive atomic force microscopy (cAFM) performed in ambient conditions on monolayer flakes of transition metal dichalcogenides (TMDs). We investigate the frequency of these defects on mechanically exfoliated samples of MoS2, WSe2, and WS2, identifying preferences for specific defect types dependent on the material. By using AFM feedback for topography scans, whilst simultaneously measuring conductance, it is possible to achieve atomic resolution of defects within the bandgap of 2D material layers. Through correlation with x-ray photoelectron spectroscopy (XPS), and photoluminescence (PL) spectroscopy, it is possible to gain further insight into the role of these defects in determining optical emission, and how this can be implemented in security devices based on TMD materials.

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Simulated imaging of submolecular structure in molecules with high topographic variation

Edward Dunn, Professor Robert Young, Dr Samuel Jarvis

MC18: Developments at the Frontiers of High-resolution Scanning Probe Microscopy III, August 22, 2022, 4:30 PM - 6:00 PM

Scanning probe microscopy (SPM) has pushed the resolution of microscopes down to the atomic scale, enabling the observation of molecular structure [1-2]. Advances in the resolution of non-contact atomic force microscopy (NC-AFM) in particular, have been closely tied to the understanding of the instrument itself [3]. As greater detail on molecular structure is achieved, it becomes necessary to understand the tip-sample interactions involved in those images in order to interpret what they display. In the case of submolecular imaging, simulation of the interactions between functionalized tips [4] and molecules is essential for their interpretation.

NC-AFM typically provides sharp images of molecular features by scanning at a fixed height and measuring a frequency shift, Δf, which can be related to force gradient. Submolecular resolution is partly made possible by the strong distance dependence of Δf, particularly in the Pauli regime, and has been used with great success on planar molecular structures. However, in non-planar molecules with greater topographic variation, only the upmost atoms are observed, greatly complicating the application of NC-AFM to non-planar molecular systems.

Here we present a simulated study describing a constant force method capable of imaging 3D molecular structure. In this method we model the NC-AFM probe following contours of constant force in order to plot force iso-surfaces. We show how this method can provide submolecular detail on non-planar molecules, and provide information on the rotation of specific molecular moieties. We will describe a series of examples, including simulations of tetraphenyl porphyrins (see figure), CO adsorption iron phalocyanine, C60 fullerene, and others. Finally, we relate this simulation method to existing experimental methods that are capable of collecting force contour data.

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A fully automated wafer-scale cryogenic measurement system for superconducting quantum circuit characterization

Manognya Acharya, Dr Myunglae Jo, Dr Rais Shaikhadarov, Prof Vladimir Antonov, Dr Tobias Lindstrom

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

As superconducting quantum circuits become increasingly sophisticated, methods that allow for rapid characterization of circuits are becoming critical for the successful development of future quantum technology. Reproducibility and uniformity control of the barrier in Josephson junctions (JJs) and minimizing the variation of junction area are two key factors that directly translate to the performance and reliability of the superconducting quantum circuits [1, 2]. Improved control of these parameters allows for circuits with the optimal balance between performance of individual qubits and spectral separation.

Here we introduce a fully automated cryogenic probe station that has recently been installed at Royal Holloway University of London's SuperFab facility. The system is capable of automatically measuring the resistance of individual JJs' across a whole wafer over the full temperature range from room temperature to 4K. The system is highly versatile with capabilities including but not limited to, precision DC IV (aA), Capacitance (fF) characterization and can be used for RF measurements up to 40 GHz. We demonstrate one such capabilities by mapping the normal resistance of JJs across a wafer with varying temperatures and discuss their correlation with the critical current of JJs. This new capability enables us to optimize the quantum circuit processing techniques and provides a new platform for next-generation quantum metrology and quantum information applications.

We acknowledge the support of the UK government department for Business, Energy and Industrial Strategy through the UK national quantum technologies program.

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Exploiting non-adiabatic excitations to enhance quantum battery

Obinna Abah

MC20: Recent Advances in Quantum Thermodynamics with a Focus on Many-body Interactions V, August 23, 2022, 2:00 PM - 3:30 PM

Crossing a quantum critical point in finite time challenges the adiabatic condition due to the closing of the energy gap, which ultimately results in the formation of excitations. Such non-adiabatic excitations are typically deemed detrimental in many scenarios, and consequently several strategies have been put forward to circumvent their formation. Here, however, we show how these non-adiabatic excitations – originated from the failure to
meet the adiabatic condition due to the presence of a quantum critical point – can be controlled and thus harnessed to perform certain tasks advantageously. We focus on closed cycles reaching the quantum critical point of fully-connected models to analyze a quantum battery. Specifically, a quantum battery that is loaded by approaching a quantum critical point, whose stored and extractable work increases exponentially via repeating cycles.

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Trapping wave fields in an expulsive potential by means of linear coupling

Prof. Boris Malomed, Nir Hacker

We demonstrate the existence of confined states in one- and two-dimensional (1D and 2D) systems of two linearly-coupled components, with the confining harmonic-oscillator (HO) potential acting upon one component, and an expulsive anti-HO potential acting upon the other. The systems can be implemented in optical and BEC dual-core waveguides. In the 1D linear system, codimension-one solutions are found in an exact form for the ground state (GS) and dipole mode (DM. i.e., the first excited state). Generic solutions are produced by the variational approximation, and are found in a numerical form. Exact codimension-one solutions and generic numerical ones are obtained for the GS and vortex states in the 2D system. Both the trapped and anti-trapped components of the bound states may be dominant ones, in terms of the norm. The localized modes may be categorized as bound states in continuum, as they coexist with delocalized ones. The 1D states, as well as the GS in 2D, are weakly affected and remain stable if the self-attractive or repulsive nonlinearity is added to the system. In particular, the nonlinearity transforms the exact localized modes of the linear system into robust breathers, which keep a well-localized shape, as shown in Fig. 1. The self-attraction makes the 2D vortex states unstable against splitting, while they remain stable under the action of the self-repulsion.

Fig. 1. The evolution of two components of a breather generated in the 1D system with the self-attractive nonlinearity by an input on the form of the exact DM solution of the linear system.

Publications:
N. Hacker and B. A. Malomed, “Nonlinear dynamics of wave packets in tunnel-coupled harmonic-oscillator traps”, Symmetry 13, 372 (2021); “Trapping wave fields in an expulsive potential by means of linear coupling”, Phys. Rev. E 105, 034213(2022).

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Understanding Chemistry at Well-Defined Electrochemical Interfaces Using Nanoparticle Deposition

Dr. Grant Johnson

MC9: Recent Developments in Gas Phase Synthesis of Nanoparticles and Applications XI, August 25, 2022, 4:30 PM - 6:00 PM

Understanding and controlling complex interfacial processes occurring at operating electrodes is a grand challenge in energy storage research. Solvated cations, anions, and electrolyte make up the electrical double layer at battery electrodes where numerous insufficiently understood ion-ion, ion-solvent, and ion-metal interactions occur. Decomposition of the solvated electrolyte anion bis(trifluoromethane)sulfonimide (TFSI) is proposed to be a key reaction pathway in the formation of the solid electrolyte interface in Mg-ion batteries. Custom aliovalent metal-doped interfaces have been proposed as a potential way to reduce or prevent the decomposition of TFSI at electrodes. These passivating oxide overlayers need to allow electrochemical plating and stripping of Mg and simultaneously prevent electron transfer through the layers which causes decomposition of TFSI. Herein, we used high-power impulse magnetron sputtering (HPIMS) combined with gas aggregation to produce bare anionic aluminum nanoparticles (NPs) which were size-selected using a quadrupole mass-filter and deposited with controlled kinetic energy onto Mg electrodes. HPIMS enabled production of larger and more stable currents of anionic Al NPs than conventional direct current sputtering. Al NPs soft landed at low kinetic energy on Mg electrodes were characterized with helium ion microscopy and demonstrated to suppress the charge-transfer-induced decomposition TFSI as well as reduce the overpotential required for Mg plating. Al NPs deposited at higher kinetic energies were found, using X-ray photoelectron spectroscopy, to result in the preparation of a continuous AlO/Al overlayer on Mg. Formation of a bimetallic aliovalent-doped AlMgO interface was confirmed using atom probe tomography. Elucidating how oxide layers on surfaces may be tailored to control interphase formation is central to the design of improved electrodes for batteries.

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Role of local structures in the dynamics of sheared colloidal suspension.

Dr. Vijayakumar Chikkadi, Mr. Abhishek Kumar Gupta, Ms. Ratimanasee Sahu

MC6: Emergent Phenomena in Driven Soft, Active and Biological Matter II, August 22, 2022, 2:00 PM - 3:30 PM

Most of the materials we encounter are neither perfect solids nor simple liquids. They possess a nonzero shear modulus and flow plastically beyond a critical strain. How these yield stress materials deform and fail mechanically is a key research question in physics and engineering. While in crystalline solid the well known defects govern the flow properties, the loss of order in amorphous materials makes it difficult to locate the plasticity carriers. Knowing the precursors of mechanical failure will help us engineer amorphous materials according to the requirement. One way to approach this problem is to look at the role of microscopic structures in local rearrangements. Recent studies discovered the growth of locally favored structure as the system enters a solid phase from liquid but the significance of these local structures has not yet been explored under applied shear. Here we experimentally investigate the response of these ordered clusters of particles in a dense colloidal suspension under constant shear. Using the Topological Cluster Classification(TCC) algorithm we find that the defective icosahedra structure has the maximum population and exhibits a slower dynamics relative to the remaining system. There is a good overlap between the particles which are slow and those that belong to these structures. Furthermore, we have also looked at the changes in structural and related length scales with respect to the strain.

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Diffusion in colloidal monolayers: bridging the gap between two and three spatial dimensions

Prof. Alvaro Domínguez

MC7: Exploring Liquid Properties in Confined Geometry (Up To Mesoscopic Scales) XI, August 25, 2022, 4:30 PM - 6:00 PM

It is well established that, unlike for a three-dimensional fluid, particle interactions prevent the hydrodynamic transport coefficients from being defined for a two-dimensional fluid due to the notorious “long-time tail” feature of the velocity autocorrelation.

A colloidal monolayer formed at a fluid interface builds a bridge between these two limiting cases, and it provides insight on the transition from three down to two spatial dimensions: the positions of the colloidal particles are constrained to a plane and the colloid thus resembles a two-dimensional fluid. But the exchange of particle momentum takes place in three-dimensional space because it is mediated by the ambient fluid in the form of hydrodynamic interactions.

Here we study the behavior of the colloidal diffusivity, which is the only hydrodynamic transport coefficient for the two-dimensional colloidal fluid. The starting point is the Smoluchowski equation, i.e., the Fokker-Planck equation for the colloidal particles in the overdamped regime with due account of the hydrodynamic interactions. We then show that the diffusivity exhibits an intermediate behavior between purely two-dimensional and fully three-dimensional fluid: on the one hand, Fick’s law, which pertains to collective diffusion, breaks down altogether [1-3], as confirmed experimentally [4]. On the other hand, the coefficient of self-diffusion (or single–particle diffusion) is finite [5], but the transitional nature of the monolayer shows up in a non-analytic dependence on the colloidal packing fraction [6], at odds with the case of a fully three-dimensional colloid.

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Characterizing Scattering Parameters of Superconducting Quantum Integrated Circuits at Milli-kelvin Temperatures

Dr Manoj Stanley

MC23: Superconducting Circuits for Quantum Technologies III, August 22, 2022, 4:30 PM - 6:00 PM

Measurements of quantum integrated circuits at milli-kelvin (mK) temperatures take on new importance today because of their immediate applications in quantum simulations [1], quantum sensing [2], and quantum computing [3]. One prominent technology for constructing a quantum computer involves superconducting qubits [4] which are physically realised at the circuit level and implemented using nominally lossless capacitors, inductors, and Josephson junctions and packaged as integrated circuits [4]. Although these circuits operate only at mK temperatures inside a dilution refrigerator, all the additional supporting microwave components (directional couplers, circulators, isolators, amplifiers, attenuators, etc.) required to control and/or read out the quantum integrated circuits are often designed for use at higher temperatures (typically 10–300 K) and are merely assumed to operate normally at mK temperatures. However, when the entire setup including the microwave components is cooled to mK temperatures, the scattering parameters (S-parameters) of the components are likely to change. This makes it particularly challenging to design the whole microwave circuitry, as the successful operation of quantum circuits requires very good impedance matching and minimise reflections to achieve high fidelity [5].
In order to measure the actual S-parameters of a quantum integrated circuit at mK temperatures, a calibration scheme that shifts the reference planes of the measurement to the ends of the quantum circuit/device needs to be implemented, thus de-embedding the intervening passive and active components up to the ports of the vector network analyser (VNA) measuring instrument, operating at room temperature. Techniques to precisely characterize these circuits at low temperatures is essential to support the development of new and improved quantum and microwave circuits to create high performance quantum computing systems.
In this talk, we introduce a full 2-port calibrated S-parameter measurement setup which can characterize superconducting quantum integrated circuits and other RF integrated circuits operating at mK temperatures. The design and architecture of the measurement system consisting of in-house developed microwave calibration unit (MCU) housing the newly designed cryogenic calibration standards and the device under test (DUT) will be presented. The measurement setup is then used to demonstrate the first calibrated S-parameter measurements of an in-house developed superconducting qubit integrated circuit at mK temperature.

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Searching for Many-Body Localization in constrained models and in systems with extended symmetries

Fabien Alet

MC42: Broken Ergodicity and Localisation in Quantum Many-body Systems VIII, August 24, 2022, 4:30 PM - 6:00 PM

Many-body localization (MBL) is a unique physical phenomenon driven by interactions and disorder for which a quantum system can evade thermalisation. The existence of a many-body localized phase in one-dimensional systems is now (relatively well) established.
I will critically review the results of our numerical investigations searching for MBL in constrained systems in two dimensions as well as in models with extended symmetries.

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Anderson criticality without fine tuning

John Chalker, Sthitadhi Roy, Shivaji Sondhi

MC40: Strongly Disordered Insulators II, August 22, 2022, 2:00 PM - 3:30 PM

A remarkable recent discovery in the theory of Anderson localisation is that eigenstates of the massless Dirac equation in two dimensions with a random vector potential show spectrum-wide criticality [1]. That is, states over a wide range of energies in the spectrum are critical; more specifically, they appear to have the same statistical properties as states at the critical point of the integer quantum Hall plateau transition. The possibility of criticality over a range of energies rather than (as is usual) only at an isolated mobility edge is very striking, but it is also very surprising to find a new feature of fundamental importance in this model, which has been studied intensively for over 25 years [2]. Advances so far in this area have been based on numerical simulations [1]. Here we review these developments and present a way of understanding the results in terms of a mapping from the Dirac problem to a model for the integer quantum Hall effect.
[1] B. Sbierski, J. Karcher, and M. S. Foster, Phys. Rev. X 10, 021025 (2020).
[2] A. W. W. Ludwig, M. P. A. Fisher, R. Shankar, and G. Grinstein, Phys. Rev. B, 50, 7526 (1994).

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Many-body delocalisation as symmetry breaking

John Chalker, Sam Garratt

MC42: Broken Ergodicity and Localisation in Quantum Many-body Systems VII, August 24, 2022, 2:00 PM - 3:30 PM

We present a framework in which the transition between a many-body localised (MBL) phase and an ergodic one is symmetry breaking. We consider random Floquet spin chains, expressing their averaged spectral form factor (SFF) as a function of time in terms of a transfer matrix that acts in the space direction. The SFF is determined by the leading eigenvalues of this transfer matrix. In the MBL phase the leading eigenvalue is unique, as in a symmetry-unbroken phase, while in the ergodic phase and at late times the leading eigenvalues are asymptotically degenerate, as in a system with degenerate symmetry-breaking phases. We identify the broken symmetry of the transfer matrix, introduce a local order parameter for the transition, and show that the associated correlation functions are long-ranged only in the ergodic phase.

S. Garratt and J. T. Chalker, Phys. Rev. Lett. 127, 026802 (2021).

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Confined and buckled: Shapes of gel-encapsulated GUVs under osmotic shock

Jack Parker, Jack Panter, Natasha Rigby, Margarita Staykova, Halim Kusumaatmaja

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Buckling has increasingly been recognised as a key physical mechanism in which confined tissues generate folds. To better understand this buckling mechanism, we design a novel experimental setup in which we expose gel-encapsulated GUVs to hyperosmotic shocks. By modulating the osmotic shock and gel strengths, we can produce a range of different vesicle morphologies, from stomatocytes to cup-like shapes and tubulations, many of these reminiscent to structures commonly observed in cells and tissues. Importantly, these shapes are different from those generated by identical vesicles in a free system. Furthermore, we can replicate the experimentally observed morphologies using a computational model that accounts for volume change, membrane bending, excess area and its adhesion to the confining wall. By comparing the in-vitro and in-silico results, we gain new insights into the salient factors that determine membrane shapes under confinement.

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1D Majorana from partial supersymmetry breaking in quantum wires

Pasquale Marra, Daisuke Inotani, Muneto Nitta

Extended supersymmetry with central charges (centrally-extended SUSY) has been one of the most important notions in quantum field theory and string theory since the second string revolution in the 90s and the revolution of quantum field theory by Seiberg and Witten. Despite its great importance in formal aspects of quantum field theory and string theory, centrally-extended SUSY seems to be not directly related to reality, because the extended N=2 SUSY does not allow chiral fermions relevant for elementary particles such as quarks and leptons. In high energy phenomenology, only N=1 SUSY and its breaking are considered.

In our recent works[1,2], we provide the first experimentally accessible example of centrally-extended SUSY and partial spontaneous SUSY breaking in condensed matter. Specifically, we describe the realization of a periodic chain of partially-overlapping 0D Majorana modes in 1D Majorana nanowires, by applying periodically and spatially-modulated potentials or magnetic fields. This system realizes a dispersive 1D Majorana fermion which we identify with the Nambu-Goldstone mode (Goldstino) of the spontaneously and partially broken SUSY.
Notice that the famous Witten's no-go theorem prohibiting partial SUSY breaking can be evaded only by the presence of a central extension in the extended SUSY algebra, as realized in our model.

Despite the several proposals to realize SUSY in condensed matter, our proposal gives the first condensed-matter realization of centrally-extended SUSY. Moreover, our proposal suggests an alternative way to control the position of 0D Majorana modes in 1D Majorana nanowires, which may open the door to new braiding protocols.

[1] Marra, Inotani, Nitta, arXiv:2106.09039, accepted on Communications Physics.
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87

Control of the molecular packing in the Ia3d gyroid phase by siloxane tails and molecular core symmetry

Prof. Shoichi Kutsumizu, Ms. Yuki Kawase, Mr. Takashi Otaki, Prof. Yohei Miwa, Prof. Yasumasa Yamamura, Prof. Kazuya Saito

MC8: Complex Phases in Soft Matter I, August 22, 2022, 11:30 AM - 12:30 PM

In contrast to the elucidation of the fascinating superstructure of the Ia3d gyroid phase self-assembled by rod-like molecules in the liquid crystalline state, understanding the formation based on the chemical structure is still in an early stage. To build up rational molecular design to control the packing structure covering different assembly modes of the molecular core parts, systematic exploitation of the molecular structure is essential.

In our model system, aryloylhydrazine molecules, in this work, we focused attention on the two parts, aromatic moieties at each side of the central linkage and siloxanyl terminals at both ends because the choice directly links to the molecular symmetry and shape, profoundly influencing the formation. The first topic in the presentation is the phase behavior of a nonsymmetric core molecule with larger naphthalene and smaller benzene moieties at each side of the central linkage and the same disiloxanyl segment at the terminals, which was found to form both single-layered and double-layered core assembly modes in the Ia3d phase as a single molecule system. The second is a binary mixture of two centrosymmetric molecules having siloxanyl terminals of different sizes, remarkably stabilizing the Ia3d phase at around room temperature nearly as a thermodynamically stable phase. The interplay between the phase stability, molecular symmetry, and favorable molecular shape is discussed.

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Wetting/drying mechanisms associated with nanoconfined salt solutions: an optical reflectance study on vapour phase imbibition and adsorption

Sujeet Dutta, Hugo Bellezza, Patrick Huber, Olivier Vincent

MC7: Exploring Liquid Properties in Confined Geometry (Up To Mesoscopic Scales) XI, August 25, 2022, 4:30 PM - 6:00 PM

The wetting and drying cycles of salt solutions confined in conductive nanoporous electrodes are conceived to generate energy from low-grade waste heat by coupling the pore drying/wetting process with the charging/ discharging cycles of the electrodes. The key factor being the surface area of the electrode in contact with the adsorbing/desorbing liquid films. This objective could be realised by achieving the right set of physical conditions that allow a systematic control and manipulation of the electrically charged layers that develop
inside the porous host matrices. The first step initiated in this direction is studying the percolation of water from the vapour phase in to the nanopores through a single exposed edge of the nanoporous host matrix (Vycor®). The porous host is maintained under controlled temperature and vapour pressure (humidity), and is illuminated by a diffuse white light source. The change in the grey-scale intensity with respect to the empty state is monitored to follow the pore-filling process as a function of time. Through systematic measurements at increasing relative humidity steps, the transition from diffusive percolation to imbibition is established. Likewise, the pore-emptying phenomenon is monitored by “degassing” the system in defined pressure steps, and the imbibition/drying mechanisms are rationalised with appropriate thermodynamic and kinetic models. The focus of the next phase of such investigations shall be on the wetting/drying mechanisms of nanopores carrying salt crystals, with complementary small/wide angle x-ray scattering experiments with the objective of obtaining information on the potential thin liquid films that may form in capillary bridges in the porous host matrices upon drying, and the re-distribution of ionic clusters as a consequence of such wetting/drying cycles, both of which could lead to spurious capacitances being exhibited by the porous electrodes. The thickness and electrical conductivity of such films have been investigated on flat macroscopic surfaces with similar
surface chemistry as the pore walls of the nanoporous host with the objective of predicting the influence of such post-cursor films (left behind in the drying pores) on the electrode capacitance with respect to their dry state. In a separate set of experiments, vapour phase adsorption/desorption isotherms are obtained via optical reflectance with the objective of unravelling the influence of salt concentration on the vapour sorption characteristics, in particular playing with the contact angle of the meniscus of the adsorbed liquid film by appropriate pore- surface hydrophobization. The thermodynamic information revealed by such experiments, coupled with the imbibition characteristics will play an important role in fine tuning the pore filling and emptying kinetics in order to achieve electrodes with desirable energy storage capabilities.

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Resonant scattering of surface acoustic waves by magnetic stripe arrays

Yat-yin Au, Oliver Latcham, Andrei Shytov, Volodymyr Kruglyak

MC45: Interfaces between Magnonics and Phononics V, August 23, 2022, 2:00 PM - 3:30 PM

Scattering of bulk acoustic waves in periodic media formed by interleaving magnetic and non-magnetic layers has been predicted to demonstrate such interesting phenomena as magnetically induced transparency and Borrmann effect [1]. Here, we investigate a more practical experimental situation in which surface acoustic waves launched on a piezoelectric substrate encounter a periodic array of magnetic stripes fabricated on the substrate's surface. We will present results of numerical simulations for a series of different array designs, including single and double magnetic layer stripes or single layer magnetic stripe formed atop a continuous magnetic film with non-magnetic spacer layer in between. The choice of the magnetic material in these arrays will be discussed. We will also discuss various physical mechanisms underpinning our observations that would enable the tunability or reconfigurability of these array devices. Our results shed light on the feasibility of magnetoelastic phononics, an emerging beyond CMOS computational technology where on chip information is acoustically transmitted and magnetically stored. Figure 1 shows exemplary results on the influence of the bias magnetic field on the transmission of Love surface waves across an array of single layer nickel stripes with a blanket aluminium capping. The research leading to these results has received funding from the EPRSC of the UK (Project EP/L019876/1 and EP/T016574/1).

Figure 1 (a) Illustration of the simulation set up. Periodic boundary conditions are applied in the y direction. A transient Gaussian voltage pulse is applied to the electrode on the left to launch a Love surface acoustic wave packet propagating towards positive x direction. Transmitted amplitude of the wave pulse is recorded and Fourier transformed into frequency domain to obtain the transmission spectrum as shown in from (b) to (e), where the brown curves represent transmission for Hbias equal 100, 150, 200 and 250 Oe in positive y direction respectively. Blue curves in (b) to (e) represent the situation where Hbias is set to 3500 Oe where all magnetic dynamic responses are frozen in the frequency range of interest. The parameters lead to the above simulations results are as follows: dcap=83 nm, d=20 nm, w=233 nm, Λ=333 nm, Ndev=20. Gilbert damping factor of nickel is set to 0.01 to boost visibility of the magnetic resonance dip.

1 "Hybrid magnetoacoustic metamaterials for ultrasound control", O. S. Latcham, Y. I. Gusieva, A. V. Shytov, O. Y. Gorobets, and V. V. Kruglyak, Appl. Phys. Lett. 117, 102402 (2020).

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Influence of the magnetic field configuration of a magnetron on the cluster growth mechanism in a gas aggregation source

Joao Coroa, Giuseppe Sanzone, Hailin Sun, Ewald Janssens, Jinlong Yin

MC9: Recent Developments in Gas Phase Synthesis of Nanoparticles and Applications IX, August 25, 2022, 11:30 AM - 12:30 PM

Cluster production using physical methods provides several advantages compared with chemical routes, such as better control of the size distribution and the minimised impact on the environment. On the other hand, their slow deposition rate has inhibited the physical approaches from being used more widely.
To address this issue, we have systematically studied the influence of aerodynamics on the efficiency of cluster transportation in a cluster source [1]. Another important factor that needs to be considered is the influence of magnetic field configuration on the magnetron sputtering device.

In the 1980s, it was found that by tuning the unbalance degree of the magnetic field configuration, one can significantly increase the number of electrons escaping from the plasma sputtering region, increase the ion flux and the associated high ion bombardment on the substrate and thus produce very dense thin films [2]. Subsequently, simulations have been carried out to better understand how the unbalanced magnetic field influences the sputtering parameters [3].

Although significant progress has been made in the understanding of how the magnetic field influences the magnetron sputtering process, there are very few reports about its influence on cluster formation. An exception is a recent work by Vaidulych et al [4], where it is argued that a decrease in the magnetic field-assisted with an increase in the flow of the carrier gas greatly improves the deposition rate of the nanoparticles. However, in this approach, the sputtering
rates across experiments were not strictly maintained, which might influence the results in an unexpected way.

In this poster, we will present the plans and preliminary simulation results on the influence of the magnetic field and its impact on cluster growth. The electromagnetic modelling software package OPERA will be used to optimise the magnetic field configuration, and several magnetrons will be built to validate the simulation results. The objective is to reveal the physical mechanism of the impact of a varying magnetic field on cluster growth.

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Water in nano-confinement

Dr Dhanadeep Dutta

MC7: Exploring Liquid Properties in Confined Geometry (Up To Mesoscopic Scales) VII, August 24, 2022, 2:00 PM - 3:30 PM

Water confined in nano-pores has attracted significant interest due to its relevance in wide range of fields stretching from geology to medicine and biology. It is observed that water under nano-confinement remains in supercooled liquid state far below its bulk freezing temperature. The curtailed hydrogen bonding network of water inside the nano-confinement plays crucial role in the phase transition of liquid water into ice. The structure of ice in nano-pore has been observed anomalously different from the structure of bulk ice formed in the ambiance. The geometry and the size of the nano-pores play important role on the structure of nano-confined ice. Also the structure of ice nano crystal highly depends on the level of pore filling. Hydrogen bonding network gets perturbed by the variation of hydration level of pores, which in turn modifies the evolved ice structure. We have observed in MCM-41 nanopores (pore size ~2.5nm) using synchrotron based xrd that crystalline ice phase is creeping outside the cylindrical pore below 240K, where as a short-range ice is evolved inside the pore below 220K. The crystalline structure is composed of mixture of hexagonal and cubic phases, whereas the short-range ice is observed to be a cubic rich phase with a small fraction of hexagonal stacking planes. On the other hand, inside the uniform nano-pores of MIL-101(Cr) framework (pore size ~1nm) more than 94% of ice is of cubic phase which is a record high number of the cubicity of ice crystal so far. We further observed through neutron diffraction that the confined cubic ice is thermodynamically stable against the transition to hexagonal ice up to the temperature 240K. This confirms that the cubic ice formed inside the uniform nano-pores MIL-101(Cr) framework have minimum stacking faults. Our finding will be helpful in opening up the possibility of the formation of cubic ice having 100% cubicity which is of current interest in understanding the ice clouds in polar stratosphere.

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Universal distributed quantum gates in microwave links

Guillermo Peñas

MC23: Superconducting Circuits for Quantum Technologies II, August 22, 2022, 2:00 PM - 3:30 PM

We propose a realistic setup, inspired by already existing experiments, within which we develop a general formalism for the implementation of distributed quantum gates. Mediated by a quantum link that establishes a bidirectional quantum channel between distant nodes, our proposal works both for inter- and intra node communication and handles scenarios ranging from the few to the many modes limit of the quantum link. We are able to design fast and reliable state transfer protocols in every regime of operation, which, together with a detailed description of the scattering process, allows us to engineer two sets of deterministic universal distributed quantum gates. Gates whose implementation in quantum networks does not need entanglement distribution nor measurements. By employing a realistic description of the physical setup we identify the most relevant imperfections in the quantum links as well as optimal points of operation in which we achieve very competing fidelities for two-qubit distributed gates.

arXiv:2110.02092

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Fabrication of Hierarchical Porous Silicon and Fused Silica by Means of Silver Nanoparticle-Catalyzed Chemical Etching

Ms. Stella Gries

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Many biological tissues and materials exhibit a multiscale porosity with small, often nanoscale pores as well as large, macroscopic pores or capillaries in order to achieve simultaneously large inner surfaces for effective vascularization in combination with an optimized mass transport capability. Achieving such a hierarchical porosity in artificial porous media is an active research field. We focus on porous silicon structures, especially on hybrid materials with a porous silicon matrix and a soft matter filling, like polymers, electrolytes and water. We want to achieve tailored properties which can be adapted to a broad application field including sensor technology, photonics, energy conversion as well as storage, and biomedicine.
Here we present a novel approach based on metal-assisted chemical etching (MACE) of electrochemically fabricated macroporous silicon for the synthesis of wafer-scale, single-crystalline silicon with a bimodal pore size distribution.
The MACE process is mainly guided by a silver-catalyzed redox-reaction at the silicon surface in which an oxidizing agent, in this case hydrogen peroxide, is reduced and induces holes into the silicon which is locally oxidized. The additional presence of hydrofluoric acid allows the dissolution of the oxidized silicon surface in contact with the silver nanoparticles. By adjusting silver nanoparticle and oxidizing agent concentration macroporous silicon membranes can be porosified on wafer scale into hierarchical porous silicon (hp-Si). The resulting semiconducting material offers good hydraulic permeabilities and simultaneously a large inner surface for potential applications in energy harvesting
or conversion or for on-chip sensorics and actuorics. The structure shows anisotropic macropores in the range of a few micrometers which are interconnected by isotropic sponge-like meso-scaled pores with diameters below 100 nm.
Finally, the hp-Si membrane can be transformed by thermal oxidation at temperatures above 800°C into hierarchical porous fused silica (hp-SiO2). This material could be of particular interest for opto-fluidic and photonic applications in the visible range of light. The overall volume expansion during this transformation can be up to 10 %, which is less than for bulk-silicon; it is observed to be up to 50 %. The decreased expansion comes from a densification process, so the porosity and the pore sizes decrease during the incorporation of oxygen but the macropores remain connected by the smaller fabricated pores.

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Bound states in normal-insulator-superconductor van der Waals heterostructures

Dr. Paritosh Karnatak, Zarina Mingazheva, Kenji Watanabe, Takashi Taniguchi, Helmuth Berger, László Forró, Christian Schönenberger

MC21: Bound states in hybrid superconductor nanostructures VIII, August 24, 2022, 4:15 PM - 6:00 PM

The effects of dimensionality, crystal symmetries, and strong spin orbit coupling impart fundamentally novel properties to superconducting van der Waals materials, such as NbSe2 and TaS2. In their monolayer or few-layer forms these superconductors display novel phenomena, such as the survival of superconductivity up to tens of Teslas of applied in-plane magnetic field, layer dependent superconducting properties and competition with other phases.
In this work we perform tunnel spectroscopy on NbSe2 by utilizing MoS2 or hexagonal Boron Nitride (hBN) as a tunnel barrier. We observe subgap excitations and probe their origin by systematically studying various heterostructure designs. We highlight two types of Andreev bound states one arising at the edge of NbSe2 and others from defects in MoS2. We reveal the nature of latter type by studying the subgap excitations in applied in-plane magnetic fields up to 9 T. Their magnetic nature highlights that singlet ground states are the most typical ones but occasionally doublet type ground states are formed or in rare cases we observe accidental degeneracy between the two. Finally, we discuss the role of spin orbit coupling in the system, based on our observations of subgap excitations that anti-cross as well as the ones with a nearly vanishing g-factor.

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Quantum embedding approaches for materials simulations on quantum computers

Dr Francois Jamet, Abhishek Agarwal, Dr Ivan Rungger

MC36: Integrating Quantum Computers in Condensed Matter Physics Simulations VI, August 23, 2022, 4:30 PM - 6:00 PM

Quantum embedding approaches for materials simulations, such as the dynamical mean-field theory (DMFT), provide corrections to first-principles calculations for strongly correlated electrons, which are poorly described at lower levels of theory. These embedding methods are computationally demanding on classical computing architectures and hence remain restricted to small systems, limiting the scope of their applicability. Quantum computers have the potential to overcome this limitation. We present a method to compute the Green's function in a continued fraction representation using a Krylov basis. We consider two methods to construct the Krylov basis. The first is based on the Krylov variational quantum algorithm (KVQA, arXiv:2105.13298), while the second method uses the quantum subspace diagonalization for the Green's function (QSD-G).

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Developing a SLUG Microwave Amplifier for Axion Detection

Dr Gemma Chapman, Dr Jamie Potter, Dr Kewen Pan, Dr George Long, Mr Laith Meti, Dr John Gallop, Dr Bhaswati Chakraborty, Dr Ed Romans, Prof Ling Hao

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Ultra-low noise amplifiers are a key requirement in haloscope axion search experiments, making it possible to search the large potential low-power frequency space. Radio-frequency amplifiers incorporating superconducting quantum interference devices (SQUIDS) are unique in that they can achieve noise performances approaching the quantum limit. As part of the UK's Quantum Sensors for the Hidden Sector consortium, we are looking to implement a variant of the dc SQUID rf amplifier – the superconducting low-inductance undulatory galvanometer (SLUG) previously investigated as a quantum-limited amplifier for quantum technologies [1]. The SLUG is preferred to conventional dc SQUID amplifiers, which have intrinsic upper frequency limits, as the rf signal is injected directly into the SLUG loop, allowing extension to the gigahertz range. Our single-layer amplifier incorporates a dc SQUID into a tuneable superconducting co-planar waveguide resonator. The Josephson junctions are formed by nanobridges fabricated by focused ion beam lithography, which have been previously shown to have noise limits of sub-μΦ0/(Hz)1/2 [2] and demonstrate Josephson supercurrent performance up to 50 GHz [3].
We present characterisation measurements of prototype SLUG devices demonstrating non-hysteretic I(V) behaviour for large critical currents approaching Ic = 1.5 mA, and a large flux-to-voltage transfer function greater than 300 μV/Φ0. These results, in tandem with numerical modelling, indicate that an 8 GHz SLUG will be able to exceed 20 dB gain with an instantaneous bandwidth of approximately 1 GHz, and noise performance approaching the standard quantum limit.

Acknowledgment: This work was supported in part by the UK Research and Innovation (UKRI) under Grants for projects (QSHS and QTNM), UK STFC and the UK National Measurement System.

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Direct coherent control of an Andreev spin-orbit qubit

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MC21: Bound States in Hybrid Superconductor Nanostructures V, August 23, 2022, 2:00 PM - 3:30 PM

Andreev qubits based on spin-orbit doublet states are a promising platform both as a spin-based quantum memory and for coherently coupling macroscopic electromagnetic modes of superconducting qubits to spinful semiconducting states. Previous implementations of these qubits in Al-InAs/Al-based Josephson junctions required the encoding of qubit states into an excited state manifold that could only be accessed via incoherent parity switches of the superconductor. Such a scheme requires initialization of the qubit via either post-selection or Raman driving. Here, we exploit the charging energy of a gate-defined quantum dot Josephson junction to build a system where the doublet states become the ground and first excited states of the system. Direct spin-flip spectroscopy enabled by applying a microwave tone to the central quantum dot gate reveals a transition between the two doublet states, which can be tuned over a range of 12 GHz by applying a magnetic field. We demonstrate coherent single qubit manipulation over the whole frequency range. Integrating this quantum dot junction as the Josephson element of a transmon qubit, we observe coherent coupling between the transmon and Andreev spin-orbit qubit transitions. This suggests a pathway to a hybrid architecture that combines the beneficial aspects of both types of qubit platforms.

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Complete absorption of topologically protected waves

Guido Baardink, Gino Cassella, Luke Neville, Paul A. Milewski, Anton Souslov

MC6: Emergent Phenomena in Driven Soft, Active and Biological Matter III, August 22, 2022, 4:30 PM - 6:00 PM

Chiral edge states can transmit energy along imperfect interfaces in a topologically robust and unidirectional manner when protected by bulk-boundary correspondence. However, in continuum systems, the number of states at an interface can depend on boundary conditions. Here we design interfaces that host a net flux of the number of modes into a region, trapping incoming energy. As a realization, we present a model system of two topological fluids composed of counter-spinning particles, which are separated by a boundary that transitions from a fluid-fluid interface into a no-slip wall. In these fluids, chiral edge states disappear, which implies non-Hermiticity and leads to a novel interplay between topology and energy dissipation. Solving the fluid equations of motion, we find explicit expressions for the disappearing modes. We then conclude that energy dissipation is sped up by mode trapping. Instead of making efficient waveguides, our work shows how topology can be exploited for applications towards acoustic absorption, shielding, and soundproofing.

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Polariton Luminescence of Molecular Systems in a Cavity: Non-Markovian Fano Resonances, Motional Narrowing and Intermolecular Correlation

Professor Boris Fainberg, Dr. Vladimir Osipov

MC25: Emerging Trends in Many-Body Cavity Quantum Electrodynamics XI, August 25, 2022, 4:30 PM - 6:00 PM

In the last time Frenkel exciton polaritons (EPs) in organic materials and biological structures attracted considerable interest in relation to their Bose-Einstein condensation, low threshold polariton lasing, and polariton chemistry in microcavity. The concept of EPs suggests strong light-matter interaction that is supported by a considerably larger oscillator strength of organic systems compared to inorganic semiconductors. Polariton absorption of electron-vibrational systems was considered in nanofibers of organic dyes using a realistic non-Markovian model of molecular vibrations [1], and in a single-mode cavity in the presence of Brownian dissipation [2]. Theoretical description of EP luminescence in molecular systems is a challenge since in this case both the interaction with radiation field and electron-vibrational interaction are strong. Elastic cavity emission of polaritons in a single-mode microcavity in the presence of Brownian dissipation from molecular vibrations was considered in Ref.[2] for a specific case when polariton linewidth is the mean of cavity and molecular linewidth, although only at resonance when the cavity frequency is equal to that of a molecular resonance. Meanwhile, the interaction of the polariton with molecular vibrations should depend on exciton contribution to EP. In this work using a realistic non-Markovian theory for the description of the polariton-molecular vibrations interaction we calculate polariton luminescence in the polariton basis. Since the proper description of the Stokes shift is very important for the correct theory of luminescence, we adopt here a realistic model, according to which each member of the progression with respect to a high-frequency optically active molecular vibration in the absorption and luminescence molecular spectra is broadened due to the presence of the low-frequency optically active vibrations. The point is that the Stokes shift in dyes is mainly due to the presence of the low-frequency optically active vibrations. We show that the frequency shift and broadening of polariton luminescence spectra strongly depend on the exciton contribution to the exciton polariton that is a function of frequency.

Further we considered a single-mode microcavity. It is usually believed that polariton states are formed when splitting of the upper and lower polariton branches is much larger than broadening of molecular resonances. In contrast, our non-Markovian theory demonstrates the main characteristic features of the Fano resonance in the polariton luminescence associated with the characteristic "zero" frequency, at which luminescence intensity is equal to zero, and a peculiar asymmetric and ultra-sharp line shape for splitting of the upper and lower polariton branches of the same order of magnitude as inhomogeneous broadening of the molecular spectra. In other words, we predict non-Markovian Fano resonance in the polariton luminescence due to interference contributions from the upper and lower polariton branches [3]. In addition, we predict motional narrowing of the EP luminescence spectrum in the microcavity. Our theory also enables us to consider a non-equilibrium (hot) EP luminescence.

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Elasto-plastic properties and self-organization of tissues probed with biomimetic emulsion

Quentin Guigue

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Biological tissues remodelling occurs through bio-chemical signalling and mechanical processes. In such complex biological systems, unravelling the contribution of a given parameter, for instance cell-cell adhesion regulation, therefore represents a huge challenge. In order to work in a simplified framework, we use adhesive emulsions as a biomimetic system of adhesive tissues, where each oil droplet mimics a cell in the tissue and droplets can adhere to each other through specific (DNA bond) or non-specific (Biotin-Streptavidin bond) interactions to mimic cell-cell adhesion.
We focus on how this intercellular adhesion modulates the response of tissues under mechanical perturbations such as those encountered during development. We thus study the elastoplastic response of the emulsion as a function of the tuneable binding energy, interaction hierarchy, and applied stress, both in static and dynamical settings.
We statically correlate the deformation of the droplet with the binding energy given by the length of the strand in the case of DNA bond aiming to characterize the inter-droplet adhesion under minimal constraint (only buoyancy) in a diluted regime.
Secondly, we flow dense emulsions in a microfluidic constriction where the geometry of the channel determines the stress field applied to the system. In particular, we try to uncover the influence of this geometry over the rearrangements that occur in the packing and the possible formation of structures such as force chains or arches that are common in granular media.

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Controlling Piezoelectric Love Waves in Magnetoacoustic Devices

Oliver Latcham, Yat-Yin Au, Andrey Shytov, Simon Horsley, Volodymyr Kruglyak

MC45: Interfaces between Magnonics and Phononics V, August 23, 2022, 2:00 PM - 3:30 PM

We study the scattering of piezoelectric Love waves from isolated magnetic stripes and arrays of those. Typically these surface acoustic waves have long lifetimes and can be coupled – via magnetostrictive effects - to the magnetization dynamics within a thin magnetic stripe. The coupling is enhanced in the vicinity of the Kittel resonance of the stripe, which can be tuned via the externally applied magnetic field. We analyze the reflection, transmission and losses, including radiation into the bulk, for Love waves propagating through the stripe-substrate interface. The scattering coefficents spectra exhibit asymmetric (Fano) lineshapes (reflection) and Lorentzian (transmission, absorption) near the magnetoelastic anti-crossing. We identify that, for waves emitted from the coupled interface, the emitted power has a dominant contribution from the bulk inelastic decay channel. This contributes heavily to the suppression of resonant magnetoelastic signatures in the scattering, playing a similar role to Gilbert damping. When the stripes are arranged into periodic arrays the magnetoelastic signatures are resonantly enhanced due to Bragg scattering, which also result in magnetoelastic Borrmann and induced transparency effects. We identify a non-leaky branch at the first phononic band gap that is protected from Brekhovskikh attenuation. This is reflected in the scattering coefficients, where an increase in attenuation can be observed above the first phononic band gap.

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Bose-Einstein condensation of Efimovian triples in the unitary Bose gas

Silvia Musolino, Hadrien Kurkjian, Mathias Van Regemortel, Michiel Wouters, Servaas J. J. M. F. Kokkelmans, Victor E. Colussi

MC35: Collective Effects and Non-Equilibrium Phenomena in Quantum Gases and Superconductors VIII,
August 24, 2022, 4:30 PM - 6:00 PM

In an atomic Bose-Einstein condensate quenched to the unitary regime, we predict the sequential formation of a significant fraction of condensed pairs and triples. At short distances, we demonstrate the two-body and Efimovian character of the condensed pairs and triples, respectively. As the system evolves, their size becomes comparable to the interparticle distance, such that many-body effects become significant. The structure of the condensed triples depends on the size of Efimov states compared with density scales. Unexpectedly, we find universal condensed triples in the limit where these scales are well-separated. Our findings provide a new framework for understanding dynamics in the unitary regime as the Bose-Einstein condensation of few-body composites.

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Layered topological semimetal GaGeTe and its high-pressure behaviour

Prof. Francisco Javier Manjón, Mr. Samuel Gallego-Parra, Dr. Enrico Bandiello, Mr. Akun Liang, Dr. Estelina Lora Da Silva, Prof. Placida Rodriguez-Hernandez, Prof. Alfonso Muñoz, Prof. Aldo Humberto Romero, Dr. Vanesa Cuenca-Gotor, Prof. Juan Ángel Sans, Prof. Rosario Vilaplana, Dr. Catalin Popescu, Dr. Frederico Alabarse, Prof. Carlos Rudamas, Prof. Daniel Errandonea, Prof. Alfredo Segura, Mr. Daniel Díaz-Anichtchenko, Prof. Cestmir Drasar

MC46: Structure, Dynamics and States in Matter Under High Pressure IV, August 23, 2022, 11:30 AM - 12:30 PM

Topological Dirac semimetals can be driven into a topological Weyl semimetal or a topological insulator by symmetry breaking or increasing spin-orbit coupling, respectively. In these topological semimetals Dirac and Weyl fermions can be found almost 100 years after their theoretical predictions [1]. Topological semimetals have unusual electronic properties, like extremely high mobility, chiral effects, negative magnetoresistance, anomalous Hall effect, and low lattice thermal conductivity. These extraordinary effects promise to be useful for many devices and applications, like optical detectors, catalysis, spintronics, valleytronics, straintronics, and highly efficient thermoelectrics [2].
GaGeTe is a layered material composed of germanene and GaTe sublayers that has been recently predicted to be a basic Z2 topological Dirac semimetal [3]. Only one polytype of GaGeTe (alpha phase) is known and has a trigonal centrosymmetric structure (space group R-3m, No. 166, Fig. 1) [4,5]. Its vibrational properties were also reported almost 40 years ago [6]. In this work, we show that as-grown samples of GaGeTe show traces of at least another polytype (beta phase) with an hexagonal non-centro-symmetric structure (space group P63mc, No. 186). Moreover, we suggest that another hexagonal polytype (gamma phase, space group P-3m1, No. 164) could also be found at room conditions.

Figure 1. Crystal structure of alpha-GaGeTe (left), beta-GaGeTe (center), and gamma-GaGeTe (right) at room conditions.

Both alpha and beta polytypes have been identified in as-grown samples and characterized by means of X-ray diffraction and Raman scattering measurements at room temperature both at room and high pressure with the help of ab initio calculations. It has been found that the already reported Raman-active modes of alpha-GaGeTe in [6] correspond in fact to beta-GaGeTe. Both alpha and beta polytypes undergo phase transitions above 6 GPa that will be commented.

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The (2×1) reconstruction of calcite(104)

Philipp Rahe

MC18: Developments at the Frontiers of High-resolution Scanning Probe Microscopy III, August 22, 2022, 4:30 PM - 6:00 PM

Calcite, the most stable polymorph of calcium carbonate ($CaCO_3$), is not only an abundant mineral in the Earth's crust, but furthermore forms a central constituent in biominerals in living organisms such as shells, teeth, or micro lenses [1]. Calcite is broadly used as a construction material, is employed in agricultural soil and water treatment, has applications in pharmaceuticals, and is currently investigated as a capture material for CO_2 with the aim to offset greenhouse emissions [2]. Despite intensive studies of the pristine and hydrated calcite(104) surfaces, surprisingly, there is still serious ambiguity regarding the properties of this surface: effects such as a row-pairing [3] or a (2 × 1) reconstruction [4] have been reported, yet so far with conflictive conclusions and without structural explanation.

Here, we apply a combination of high-resolution non-contact atomic force microcopy (NC-AFM) with functionalized tips at 5K, density functional theory calculations with state-of-the-art dispersion corrections, and NC-AFM image calculations to clarify the microscopic geometry of the calcite(104) surface. A (2 × 1) reconstruction is consistently found in the experimental data and is explained by the ab-initio derived geometry (see panel (a)), where an alternating row structure with a rotation of every second carbonate group is found. NC-AFM image calculations (see panel (b)) are in excellent agreement with high-resolution NC-AFM data (see panel (c)). Furthermore, we developed an algorithmic symmetry test to assess the symmetry properties of the surface. When using symmetric CO tips, excellent agreement is found with an assignment of calcite(104) to the planar space group pg, thus rendering the row-pairing to be a tip artefact. In conclusion, our study confirms the presence and determines the microscopic geometry of the (2 × 1) reconstruction of calcite(104) and assigns the surface to the planar space group pg. These findings are most critical for future studies where physical processes on calcite(104) – (2 × 1)pg are influenced by the surface microscopic structure.

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Mitigating parasitic interactions in superconducting circuits

Xuexin Xu, Mohammad Ansari

Implementation of high-performance two-qubit gates is a key factor for scalable quantum computation. However, the state-of-the-art superconducting two-qubit gates are yet far from being perfect due to the parasitic ZZ coupling. In this talk, we introduce a general theory to evaluate the “static” ZZ interaction between seemingly idle qubits as well as the “dynamic” ZZ interaction between driving entangled qubits, and find the characteristics of both static and dynamic ZZ freedoms. Moreover, by combining the two freedoms we propose a new parasitic free gate which can zero ZZ before, during and after entanglement.

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Qubit as a quantum probe of control distortions and temperature

Arkady Fedorov

MC23: Superconducting Circuits for Quantum Technologies III, August 22, 2022, 4:30 PM - 6:00 PM

Control lines distortions lead to gate infidelities while non-zero effective temperature leads to improper initialization of qubits' states. Characterising these imperfections and distortions becomes imperative to progress towards real-world applications and breaking the error-correcting threshold for current noisy intermediate-scale quantum processors. In this talk, I am going to present a set of tools we have developed to employ a qubit itself as a probe of transfer functions of control lines, effective temperature, setup stability and how to use the results to improve the fidelity of entangling gates. I will also present the application of on-the-fly data processing with neural networks to state classification in a single-shot quantum measurement.

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Uniaxial strain-tuning of the surface electronic structure of Sr2RuO4

Edgar Abarca Morales, Gesa Siemann, Andela Zivanovic, Igor Markovic, Chris Hooley, Dmitry Sokolov, Naoki Kikugawa, Cephise Cacho, Matthew Watson, Clifford Hicks, Andrew Mackenzie, Phil King

MC50: Fermi Surface Topological Transitions - Effects of Interactions VII, August 24, 2022, 2:00 PM - 3:30 PM

Ruthenates are well known for their rich phase diagrams and distinct correlated electron states that are accessible via small changes in structure or composition [1]. Much of this richness can be attributed to the presence of van Hove singularities (vHS) in their electronic structure, which are located in close proximity to the Fermi level. In the unconventional superconductor Sr2RuO4 one such vHS is at sufficiently low energy that it can be driven through the Fermi level using uniaxial strain, which has been found to more than double the superconducting Tc and to stabilize a non-Fermi liquid state [2,3,4]. In the bilayer sister compound Sr3Ru2O7, in-plane rotations of the RuO6 octahedra and the corresponding doubling of the in-plane unit cell turn the vHS into higher (4th) order [5]. Tuning this vHS to the Fermi level with large magnetic fields is thought to drive an exotic nematic state to emerge, which exhibits signatures of quantum criticality [6,7]. Interestingly, the octahedra rotations that characterize Sr3Ru2O7 are also found for the surface layer of Sr2RuO4, potentially making such states accessible also at the surface of the single-layer compound [8]. Here, we report the evolution of the electronic structure at the surface layer of Sr2RuO4 under large in-plane uniaxial strains of $\varepsilon_{xx}-\varepsilon_{yy}=-0.8\pm0.1\%$. From angle-resolved photoemission, we show how the induced strain drives a sequence of Lifshitz transitions, fundamentally reshaping the low-energy electronic structure and the rich spectrum of van Hove singularities that the surface layer of Sr2RuO4 hosts. From comparison of tight-binding modelling to our measured dispersions, we show that, surprisingly, the uniaxial strain is accommodated predominantly by bond-length changes rather than modifications of the octahedral tilt and rotation angles. Our study thus sheds new light on the nature of structural distortions at oxide surfaces, and how targeted control of these can be used to tune density of states singularities to the Fermi level, in turn paving the way to the possible realisation of quantum criticality.

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Nanopatterning of YBa2Cu3O7-x by gallium focused ion beam

Dominik Hanisch, Max Pröpper, Paul Julius Ritter, Marco Tollkühn, Meinhard Schilling, Benedikt Hampel

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

The nanopatterning of high-Tc superconducting yttrium barium copper oxide (YBa2Cu3O7-x) thin films is a challenging task. A reproducible manufacturing process with controlled Josephson junction parameters is crucial for the fabrication of large Josephson junction arrays for applications like voltage standards. An adaptive manufacturing process using a gallium focused ion beam process (Ga-FIB) allows modifications of the Josephson junction geometry directly. This enables a versatile parameter modification of individual Josephson junctions. Consequently, arrays with homogeneous Josephson junctions or precisely tuned Josephson junctions for the detection of THz radiation can be manufactured.

The superconducting thin films are deposited by pulsed laser deposition on strontium titanate (SrTiO3), lanthanum aluminate (LaAlO3) or lanthanum aluminate - strontium aluminum tantalate (LSAT) bicrystal substrates. The Josephson junctions form at the grain boundary of the substrates, as the lattice defect of the grain boundary is adopted by the superconducting thin film during its epitaxial growth as a non-superconducting tunneling barrier. A lithography process together with an optimized argon ion beam etch process is used to obtain micrometer wide bridges. A gentle etch process is crucial to achieve structures with steep edges while maintaining a high oxygen content in the thin film. However, a reliable fabrication of nanometer wide bridges with this process is difficult to achieve. The modification of micrometer wide bridges with a Ga-FIB is able to achieve nanometer resolution due to its very small focus with a diameter of a few nanometers and nearly no defects outside the interaction volume of the gallium ions in the film. The Ga-FIB suppresses superconductivity in the irradiated thin film through disorder of the crystal structure and implantation of gallium ions into the thin film lattice. The gallium ion beam can be deflected to write well-defined insulating barriers into the film, which can be used to individually alter the widths of Josephson junctions.

In this work, we optimize a Ga-FIB-based patterning process to fabricate superconducting nanobridges made from the high-Tc superconductor YBa2Cu3O7-x. The patterning process is used to modify the widths of Josephson junctions. We present measurements of their electrical properties including the critical current Ic and the normal state resistance Rn in comparison to non-modified Josephson junctions. The promising results demonstrate the use of a Ga-FIB as a precise tool for the optimization of high-Tc Josephson junctions.

We gratefully acknowledge the support by the Braunschweig International Graduate School of Metrology - B-IGSM, by the DFG Research Training Group GrK 1952/2 “Metrology for Complex Nanosystems,” by the Laboratory for Emerging Nanometrology - LENA, by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany’s Excellence Strategy - EXC-2123 QuantumFrontiers - 390837967, by the Quantum Valley Lower Saxony – QVLS, and by the MWK, Federal State of Lower Saxony, Germany within the project "QuanTec".

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Magneto-acoustic waves: Surface acoustic waves for magnonics

Prof. Dr. Mathias Weiler

MC45: Interfaces Between Magnonics and Phononics IV, August 23, 2022, 11:30 AM - 12:30 PM

Spin waves form the basis for the field of magnonics, where they are used for information transport and processing [1]. Acoustic waves, in particular surface acoustic waves (SAWs), are widely employed as frequency filters in mobile communication technology. SAWs have group velocities comparable to that of spin waves and consequently can be generated with magnon-compatible wavelengths and frequencies. In magnetic media, spin waves can interact with SAWs which defines the field of magnetoacoustics. Magneto-acoustic phenomena can be used to excite and detect magnetization dynamics acoustically and control SAW propagation magnetically. Because of the ellipticity of the magneto-acoustic driving fields, as well as the spin-wave non-reciprocity due to dipolar coupling and the Dzyaloshinskii-Moriya interactions [2,3], magneto-acoustic waves are thereby generally chiral and non-reciprocal.

I will introduce the fundamentals of magnetoacoustics and give a brief overview of selected key results in the field. After the introduction, I will focus on the symmetry and non-reciprocity of magneto-acoustic waves in magnetically ordered thin films and heterostructures [4-6]. We quantitatively model the SAW-spin wave interaction based on the Kalinikos-Slavin equation and spin wave excitation by elliptically polarized coherent phonons to reveal that the magnon-phonon coupling is driven not only by magneto-elastic interactions [7] but also by magneto-rotation [4,8]. The efficient coupling of SAWs and spin waves can also be used to explore non-linear magneto-acoustic dynamics [9]. Non-linear and non-reciprocal magneto-acoustic waves may be useful for the implementation of miniaturized on-chip microwave components.

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A Fourier-free approach to k-space: Can single-point tunnel spectra measure dispersion?

Yi-Ying Sung, Filipe Junqueira, Brian Kiraly, Philip Moriarty

MC18: Developments at the Frontiers of High-resolution Scanning Probe Microscopy III, August 22, 2022, 4:30 PM - 6:00 PM

From the earliest days of scanning tunnelling microscopy [1], it was recognised that, in principle, tunnelling spectroscopy can yield k-space information via the dependence of the transmission coefficient, T(ϵ,V,z) on k_par, the wavevector parallel to the surface:

$$T(\epsilon,V,z)=\exp\left(-(2\sqrt{2m})/\hbar\ \sqrt{((\varphi + eV/2-\epsilon)+k\_par^2}\ \right)$$

where ϵ is the energy of the state, V is the applied bias, and φ is the mean tip-sample work function. Typically, however, it is assumed that tunnelling spectra are dominated primarily by states at the Γ point and the dependence of T on k_par is ignored. Recently, Feenstra et al. [2], among others, have used this dependence to associate spectroscopic features with specific high symmetry points in the Bouillon zone of 2D semiconductors.

Although Fourier transformation of real space dI/dV maps is now routinely used to probe dispersion of the Shockley surface state at noble metal surfaces [3], our focus here is on the extent to which single-point tunnelling spectroscopy alone can yield information on band structure. We use triangular electron resonators [4], of the type shown in Fig. 1, to provide a highly structured sample density of states that can be readily simulated via a combination of suitably broadened Lorentzians [5] (see inset to Fig. 1(C)). Moreover, step edges quench the surface state and provide a powerful means of characterising the tip LDOS (Fig. 1(C)).

Fig. 1(D) shows a simple illustrative example of the key influence of k_par on the background of a tunnelling spectra. This type of modification of the spectral background was recognised some time ago by Hofer and Garcia-Lekue [6], but has yet to be explored, or exploited, experimentally. We shall discuss the extent to which the k_par dependence can be extracted from dI/dV spectra measured for a variety of electron resonators on noble metals.

Fig. 1(A). A triangular electron resonator, side length ~ 12 nm, formed on a Au(111) surface via tip indentation. The island is a single atomic step high. (B) Constant current dI/dV map measured at -300 mV. The red and white dots superimposed on the image highlight the locations of dI/dV spectra. (C) Open (blue) circles, red circles: dI/dV spectra measured at positions shown in (B). The inset shows a fit to the experimental data comprising a set of broadened Lorenztian functions. (D) Influence of k_par on tunnelling spectra. Simulated spectra (using WKB trapezoidal approximation) without (full line) and with (dashed line) inclusion of k_par in the expression for the transmission coefficient.

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Correlation between superfluid stiffness and condensation energy in the Yukawa-SYK model on a lattice

Davide Valentinis, Gian Andrea Inkof, Joerg Schmalian

MC31: The Physics of Cuprates XII, August 26, 2022, 9:00 AM - 10:00 AM

Primary examples of high-temperature superconductors, such as cuprates, are characterized by a non-Fermi liquid (NFL) normal state, in which the electronic spectrum is devoid of sharp quasiparticle excitations [1-3]. One striking feature of the superconducting state in cuprates is the observed strong correlation among the coherence-peak spectral weight, the superfluid stiffness, and the condensation energy, as a function of temperature and doping [4,5].
We reproduce and analyze the correlation between the phase stiffness and the condensation energy across the Fermi-liquid (FL) to NFL crossover in a Yukawa-SYK model on a lattice.
The Sachdev-Ye-Kitaev (SYK) approach for complex fermions [6,7], based on all-to-all random interactions among N fermion flavors in a zero-dimensional dot, has been shown to capture aspects of strange-metal physics, like an extended regime of resistivity proportional to temperature. This dot can be employed as a building block for lattices, with sites connected by hopping [8-12]. A superconducting instability in the single dot emerges by coupling to an Einstein phonon (the Yukawa-SYK model [13-15]), which is at once responsible for Cooper pairing and for the incoherent nature of the normal state [16,17].
In this work, we generalize the Yukawa-SYK model to a lattice with random hopping parameters. We exactly solve the model in the large-N limit at particle-hole symmetry, we construct the phase diagram, and we characterize the FL to NFL crossovers both numerically and analytically, in the normal and superconducting states.
In the FL regime, we find that increasing hopping exponentially decreases the critical temperature, which is maximal in the single-dot NFL limit at given coupling. However, the phase stiffness and the condensation energy display a correlated, non-monotonic behavior as a function of coupling: they are maximal precisely at the NFL/FL crossover. Our results offer an analytically controlled scenario to study the interplay between NFL and FL phases, the thermodynamics, and the electromagnetic response in unconventional and quantum-critical superconductors.

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Ultrafast magnetization reversal by resonant excitation of optical phonons

Andrei Kirilyuk

MC51: Ultrafast Dynamics in Magnetic and Strongly-Correlated Materials IX, August 25, 2022, 11:30 AM - 12:45 PM

Identifying an efficient pathway to change the order parameter via a subtle excitation of the coupled high-frequency mode is the ultimate goal of the field of ultrafast phase transitions [1,2]. This is an especially interesting research direction in magnetism, where the coupling between spin and lattice excitations is required for magnetization reversal [3]. Despite several attempts [4,5] however, the switching between magnetic states via resonant pumping of phonon modes has not yet been demonstrated.
To provide resonant excitation of the phonon modes, we use pulses from FELIX (Free Electron Lasers for Infrared eXperiments, Nijmegen, The Netherlands). The IR/THz light with photon energy ranging between 25 meV and 124 meV (wavelength 10-50 μm) is typically used.
And thus we show how an ultrafast resonant excitation of the longitudinal optical phonon modes in magnetic garnet films switches magnetization into a peculiar quadrupolar magnetic domain pattern, unambiguously revealing the magneto-elastic mechanism of the switching [7]. In contrast, the excitation of strongly absorbing transverse phonon modes results in thermal demagnetization effect only. The mechanism appears to be very universal, and is shown to work in samples with very different crystallographic symmetry and magnetic properties, including weak ferromagnets and antiferromagnets [8].

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Coexistence of localization and transport in many-body two-dimensional Aubry-André models

Dr Antonio Strkalj, Dr. Elmer V. H. Doggen, Prof. Claudio Castelnovo

MC42: Broken Ergodicity and Localisation in Quantum Many-body Systems VII, August 24, 2022, 2:00 PM - 3:30 PM

Many-body localization (MBL) provides a mechanism to avoid thermalization in interacting systems. It is well understood that the MBL phase can exist in closed one-dimensional systems subjected to random disorder, quasiperiodic modulations, or homogeneous electric fields. However, the fate of MBL in higher dimensions remains unclear. Although some experiments on randomly disordered two-dimensional (2D) systems observe a stable MBL phase on intermediate time scales, recent theoretical works show that the phenomenon cannot persist forever and in a thermodynamic limit due to the rare regions and the avalanche instability. On the other hand, quasiperiodic systems do not host rare regions, and the avalanche instability is avoided; yet, the existence of an MBL phase in these systems remains to date largely unexplored. Using the numerical method of time-dependent variational principle, we investigate the localization properties of the many-body 2D Aubry-André quasiperiodic model by studying its out-of-equilibrium dynamics. We show that a stable MBL phase exists in the thermodynamic limit, in contrast to random disorder. Furthermore, we show that deterministic lines of weak potential, which appear in this model, support transport while keeping the localized parts of the system unchanged.

A Štrkalj, EVH Doggen, C Castelnovo, arXiv:2204.05198 (2022)

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Effective Temperature Pulses in Open Quantum Systems

Pedro Vinicius De Castro Portugal, Fredrik Brange, Christian Flindt

Controlling the temperature of nano-scale quantum systems is becoming increasingly important in the efforts to develop thermal devices such as quantum heat valves, heat engines, and refrigerators, and to explore fundamental concepts in quantum thermodynamics. In practice, however, it is challenging to generate arbitrary time-dependent temperatures, similarly to what has been achieved for electronic voltage pulses. To overcome this problem, we here propose a fully quantum mechanical scheme to control the time-dependent environment temperature of an open quantum system. To this end, we consider a collection of quantum harmonic oscillators that mediate the interactions between the quantum system and a thermal reservoir, and we show how an effective time-dependent temperature can be realized by modulating the oscillator frequencies in time. By doing so, we can apply effective temperature pulses to the quantum system, and it can be cooled below the temperature of the environment. Surprisingly, the scheme can be realized using only a few oscillators, and our proposal thereby paves the way for controlling the temperature of open quantum systems.

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Multi-Scale, Non-Equilibrium Molecular Dynamics Simulations in the Adaptive Resolution Method

Mauricio Sevilla, Luis A. Baptista, Kurt Kremer, Robin Cortes-huerto

MC7: Exploring Liquid Properties in Confined Geometry (up to mesoscopic scales) X, August 25, 2022, 2:00 PM - 3:30 PM

We discuss a multi-scale, open-boundary method to perform non-equilibrium molecular dynamics simulations [1]. Initially, the system of interest, described in atomistic resolution, is embedded in an infinite reservoir of noninteracting particles at a constant temperature, volume, and chemical potential [2]. We use the Hamiltonian adaptive resolution method to enforce these coexistence conditions. A system/reservoir interface is defined via a switching field that smoothly connects atomistic and ideal gas Hamiltonians. An external potential, applied only to particles instantaneously present at the interface, balances the excess chemical potential of the system [3]. Finally, to ensure that the size of the reservoir is infinite, a particle insertion/deletion algorithm controls the density in the ideal gas region.

We show that it is possible to study non-equilibrium phenomena with this open-boundary setup. To this aim, we consider a prototypical confined liquid under an external constant density gradient. The resulting pressure-driven flow across the atomistic system exhibits a velocity profile consistent with the corresponding solution of the Navier–Stokes equation. This method conserves, on average, linear momentum and closely resembles experimental conditions. Finally, we present examples illustrating our approach's capabilities to study various direct and indirect out-of-equilibrium conditions in complex molecular systems.

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Dynamic clustering of colloidal particles in an active bath of bacteria

Pragya Kushwaha, Mr. Sayan Maity, Mr. Vivek Semwal, Dr. Vijayakumar Chikkadi, Dr. Shradha Mishra

MC6: Emergent Phenomena in Driven Soft, Active and Biological Matter III, August 22, 2022, 4:30 PM - 6:00 PM

The fluctuations of micron sized colloidal particles in a Brownian solvent and their phase behavior have been investigated since the time of Einstein and Onsager. However, the phase behavior of colloids in an active bath has received attention only in the recent few years. In this talk, I will present experimental results on dynamic clustering and phase behavior of colloidal particles that are suspended in an active bath of bacteria. The clusters of colloidal particles in an active bath form and break rapidly, which is reminiscent of dynamic cluster formation found in purely active systems. Further, the average size of the clusters are observed to grow with increasing size ratio of colloidal particles to bacteria. We will discuss the role of entrainment and scattering process between a bacteria and a single colloidal particle to provide insight into the physics of growing clusters. Our experimental results would be complemented with simulation results that shed new light on this phenomenon.

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Oxygen sublattice organization in the pseudo-binary system Nd2O3-CeO2

Henry Charlton, Gianguido Baldinozzi, Karl Whittle, Maulik Patel

MC38: Controlled Irradiation Disorder in Model Systems: Organisation, Dynamics, and Transformations XI,
August 25, 2022, 4:30 PM - 6:00 PM

Aliovalent cation substitutions in MO2 drive the formation of oxygen vacancies as a charge compensation mechanism. There is evidence for systematic ordering of vacancies in non-stoichiometric MO2-x systems (M = Pr, Ce, and Tb) leading to the formation of several intermediate fluorite-related phases. In pseudo-binary oxide systems of the family Ln2O3:MO2 with Ln3+= La, Nd, Gd, …, oxygen vacancies are also formed to maintain charge neutrality. The existing literature about these mixed systems reports a perfect solubility of the aliovalent cations and postulates a random distribution of the anion vacancies suggesting an ideal solid-solution behaviour and a monotonic increase of their concentration over the whole range of compositions: a smooth change between the α-type structure (fluorite) and the A-type or C-type Ln2O3 structure is usually assumed. Nevertheless, the average lattice parameter of this description seems to display some departure from the expected linear behaviour. Indeed, by analogy with the intermediate phases of the PrO2-x system, a cornucopia of phases would be expected to form also in a pseudo-binary system. However, the cation mobility and their capacity to rearrange at various temperatures decreases rapidly with temperature and this changes the extent of the problem as kinetic considerations become a relevant feature. Chemical homogeneity and charge ordering of the cation sublattice of these systems would require high temperature, prolonged annealing that are only effective just above the charge-ordering transition temperature. Moreover, these annealing should occur over a time span dictated by the chemical diffusion coefficient: achieving these two conditions (ordering occurring only when the cation inter-diffusion is sluggish) can be practically impossible in samples produced by powder metallurgy techniques. In order to achieve chemical homogeneity without relying on cation diffusion and, at the same time to minimize non-equilibrium processes, various compositions of NdxCe1-xO2-x/2 were fabricated at low temperature as nanocrystalline powders using a freeze-drying method. The structures of these compounds were studied by x-ray diffraction and selected area electron diffraction. In these homogeneous systems, we observe a departure from the random oxygen-deficient fluorite structural model. A set of structures derived from the fluorite were used to model the effect of the vacancy order upon the diffracted intensities. While the average fluorite structure remains present at moderate doping levels, a phase change occurs in the region 0.36 < Ndx < 0.48, marked by the appearance of low intensity superstructure peaks in the diffraction patterns. The powder diffraction data is best described by a monoclinic Ln6O11-type structure (SG P21/c), often referred to as “β phase” in PrO2-x. These findings question the equilibrium character of the current phase diagrams and require a possible critical reassessment of several of these pseudo-binary systems. This work was funded by EPSRC through the Next Generation Nuclear Centre for Doctoral Training (NGN-CDT) programme.

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Time-frequency representation of dynamical Andreev conversions

Benjamin Roussel, Pablo Burset, Christian Flindt

MC21: Bound States in Hybrid Superconductor Nanostructures III, August 22, 2022, 4:30 PM - 6:00 PM

Coherent control of electronic excitations is now possible down to the single-electron level. This has enabled the emergence of a new field of condensed matter known as electron quantum optics [1], where electrons can be emitted, controlled and measured one by one, drawing a parallel with the quantum theory of light. A new perspective on the field is shed by the addition of superconductors [2]. In presence of superconductors, quantum correlations between different charge sectors are allowed. Those correlations, which vanish when only normal metals are present, offer a new playground for electron quantum optics.

However, this calls for an overhaul of the theoretical concepts in electron quantum optics, taking into account the superconducting correlations. In normal-state conductors, one is interested in the first-order coherence [3], which encodes the single-electron wavefunctions that are present in the system. In the superconducting case, we must also take into account the superconducting correlations via the pair amplitudes (or the anomalous part of the Green function).

The simplest process that can generate these anomalous correlations is the Andreev conversion [4]: an electron going through a superconducting interface is transformed into a quantum superposition of an electron and a hole. Because this process is dynamical (the charge pulse is of finite duration) but also frequency dependent (there is a different behavior above and below the gap), it is natural to consider time-frequency representations to understand the Andreev conversion of an electronic pulse.

In this work [5], we introduce the general formalism adapted to treat the case of superconducting correlations. This allows us to analyze the response of a typical superconductor, when a pulse of unit charge is sent onto it. We use time-frequency representations to analyze and understand the Andreev conversion of an incoming electron in various regimes. In particular, we show that for a pulse containing only small frequencies compared to the gap, the pulse keeps the same shape and is retarded by a delay in the inverse of the gap.

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Atomistic Simulations of the Nucleation & Growth of Nanoparticles from the Gas Phase

Panagiotis Grammatikopoulos

MC9: Recent Developments in Gas Phase Synthesis of Nanoparticles and Applications IX, August 25, 2022, 11:30 AM - 12:30 PM

As Richard Feynman famously put it, “equilibrium occurs when all the fast things have happened but the slow things have not”; and gas-phase synthesis is quite well-known to comprise very fast, out-of-equilibrium processes.

Yet, controlled synthesis of far-from-equilibrium nanoparticles is key to exploiting potentially unique physical and chemical properties. For example, shape determines the type of surfaces of a nanoparticle, which, in turn, can dictate function (e.g., the ways atoms are arranged on the surface of a nanocatalyst can be decisive for an electrochemical reaction). Further, even though the fabrication of nanoalloys by gas-phase synthesis has been technically possible for some time now, co-deposition of many elements is complicated, due the non-equilibrium processes it entails, with kinetic factors often playing a more important role than energetics.

The main thesis of this talk is that atomistic computer simulations are pertinent to address this challenge, since they can explain the often counter-intuitive kinetics of nanoparticle nucleation & growth, which typically involve temporal and spatial scales beyond the resolution capabilities of experimental characterization techniques. A single, method-independent narrative will be used that describes the nucleation & growth of e.g., metallic nanocubes or partial core-shell (ukidama) nanoparticles in a coherent manner. More interestingly, new, yet unpublished theoretical findings will inform experimental recipes for the consistent growth of high-purity tailored nanoparticle samples by gas-phase synthesis.

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Disentangling coupled degrees of freedom in correlated materials using resonant x-ray diffraction

Laurenz Rettig

MC47: X-ray Free Electron Lasers for Condensed Matter & Materials Physics (XFELs for CMMP) II, August 22, 2022, 2:00 PM - 4:00 PM

Correlated materials are characterized by a variety of couplings between the elementary degrees of freedom, leading to novel ground states with broken symmetries and often intriguing properties. Yet the quantification of those interactions and their relevance for the formation of broken-symmetry ground states and phase transitions remains a major challenge. In particular, in thermal equilibrium the various degrees of freedom are often strongly tied together by the interactions, and show similar behavior, making it difficult to assess the strength of the couplings and the driving force behind a symmetry-breaking phase transition. Studying such systems in the time domain after ultrafast optical excitation promises a way to break this link and to disentangle the contributions of the individual degrees of freedom by their intrinsically different dynamics.

Resonant x-ray diffraction (RXD) has proven to be a versatile tool to study ordered states in various complex materials. In particular, the energy dependence of the resonant diffraction signal near transition metal K- and L-edges, and Lanthanide L- and M-edges encodes a wealth of information about the atomic and orbital states involved in the ordered states. Combining this technique with the tunable, bright and narrow-band femtosecond x-ray pulses nowadays available at x-ray free-electron laser sources, provides great opportunities to separate the dynamics of intimately coupled degrees of freedom.

In my talk, I will address two examples where such an approach has been successfully applied. First, in antiferromagnetic Ho, time-resolved RXD tuned around the Ho L3 edge allows addressing both a magnetic dipole and quadrupole transition separately. Thereby we can separate the dynamics of itinerant Ho 5d/6s and localized Ho 4f electrons, and reveal a strong intra-atomic exchange coupling of the two magnetic subsystems [1]. In addition, I will discuss the photoinduced melting of charge and orbital order in the mixed-valence manganite Pr0.5Ca0.5MnO3 (PCMO) [2]. Combining time-resolved RXD data below and at the Mn K-edge resonance allows separating the dynamics of charge ordering from structural motions. These results give strong evidence for the charge order as the main driving force of the coupled electronic and structural phase transition in PCMO [3].

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Quantum machine learning using high-quality superconducting qutrits

Weixi Zhang, Shuxiang Cao, Deep Lall, Dr Peter Leek, Dr Ivan Rungger

MC23: Superconducting Circuits for Quantum Technologies I, August 22, 2022, 11:30 AM - 12:30 PM

Qutrits are three-level quantum systems that can be used for quantum computation. Compared to qubits, the advantage of increasing the dimension beyond two is that equivalent quantum circuits can potentially be built using fewer qutrits and gates, which can be of advantage for quantum machine learning (QML). We have built and benchmarked a qutrit based on a superconducting coaxmon, and find high fidelities and long coherence times. We use gate-set tomography (GST) to rigorously characterize the performance of quantum logical gates on the superconducting qutrits. In comparison to the process tomography protocol, GST can eliminate the measurement and state preparation (SPAM) error. We propose an efficient measurement basis to implement qutrit tomography with only 4 measurement axes. We compare the GST data with the qutrit Clifford randomized benchmarking results and find good agreement.
We propose a practical application of the high-fidelity superconducting qutrit with newly developed parameterized qutrit circuits to perform QML classification on classical data. Our quantum machine learning approach is a special case of a general variational quantum algorithm (VQA). We first apply the quantum circuits on an emulator to perform classical-quantum classification on the Iris dataset and the palmer-penguins dataset. We show that the additional dimensions provided by qutrits allow to encode more classical data into qutrits than qubits. This allows qutrit classifiers to reach similar classification accuracy compared to qubit classifiers, but with fewer qutrits and fewer gates. If the number of used qutrits is equal to the number of qubits, the classification accuracy is significantly higher.
Our runs on a superconducting qutrit achieve the same classification accuracies as predicted by the noiseless emulators. This firstly confirms the high quality of the superconducting qutrits, and secondly provides a proof of concept that the proposed QML algorithm can run on existing hardware. Our results show that using more than two states in the superconducting coaxmons may improve performance of variational quantum algorithms.

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Antimicrobial and aging properties of Ag cluster-doped amorphous carbon coatings

Giuseppe Sanzone, Susan Field, David Lee, Jingzhou Liu, Pengfei Ju, Minshi Wang, Parnia Navabpour, Hailin Sun, Jinlong Yin, Peter Lievens

MC9: Recent Developments in Gas Phase Synthesis of Nanoparticles and Applications XI, August 25, 2022, 4:30 PM - 6:00 PM

Giuseppe Sanzone1, 2, Sue Field1, David Lee3, Jingzhou Liu4, Pengfei Ju4, Minshi Wang5, Parnia Navabpour1, Hailin Sun1, Jinlong Yin1, (*), Peter Lievens2

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Inside a spacecraft, the temperature and humidity, suitable for the human crew onboard, also creates an ideal breeding environment for the proliferation of bacteria and fungi; this can present a hazard to human health, and create issues for the safe running of equipment. To address this issue, wear-resistant antimicrobial thin films prepared by magnetron sputtering were developed, with the aim to coat key internal components within spacecrafts. Silver and copper are among the most studied active bactericidal materials, thus this work investigated the antibacterial properties of amorphous carbon coatings, doped with either silver, silver and copper, or with silver clusters. The longevity of these antimicrobial coatings, which is heavily influenced by metal diffusion within the coating, was also investigated. With a conventional approach, amorphous carbon coatings were prepared by co-sputtering, to generate coatings that contained a range of silver and copper concentrations. In addition, coatings containing silver clusters were prepared using a separate cluster source to better control the metal particle size distribution in the amorphous carbon matrix. Antibacterial tests were performed under both terrestrial gravity and microgravity conditions, to simulate the condition in space. Results show that although silver doped coatings possess extremely high levels of antimicrobial activity, silver cluster doped coatings are equally effective, whilst being more long-lived, despite containing a lower absolute silver concentration.

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Radiation effects in Gd2Ce2O7: role of anion sublattice in disordering and limitations of Gibbons model for damage evolution in disordered systems.

Dr. Maulik Patel, Dr. Jeffery Aguiar, Dr Kurt Sickafus, Dr. Gianguido Baldinozzi

MC38: Controlled Irradiation Disorder in Model Systems: Organisation, Dynamics, and Transformations XI, August 25, 2022, 4:30 PM - 6:00 PM

Disordering in ternary oxide systems derived from the parent fluorite structure have attracted significant attention with particular interest in correlating the crystal chemistry and ordering of metal cations and oxygen anions to their radiation tolerance, ionic and thermal conductivity. Radiation effects in these systems have been mainly focussed on the role of cations in the disordering and amorphization while the role of anion sublattice is not well understood due to the unavailability of model system which allow to deconvolute the effect of both cation and anion sublattices. The current work will discuss the role of anions in a specific system (Gd2Ce2O7) when subjected to Swift Heavy Ion irradiations and characterised using quantitative X-ray diffraction analysis. Our results show that the topological disorder on the anion sub-lattice grows faster than that on the cation sub-lattice. In addition, radiation damage descriptions are usually binary, in that they model damage evolution as a transition from an initial, pristine unirradiated structure to a new, final irradiated structure, this final state is often an amorphous phase: these models track the relative proportions of the two phases i.e. amorphous or crystalline, at any time during irradiation, as well as the rate of the transformation from the initial state to the final state. Here, we develop a different approach wherein we describe at the atomic scale the homogeneous and coherent materials' response to irradiation before amorphization takes place. Material response can then be understood with greater mechanistic insight, compared to the conventional, binary response where the latter approach simply addresses the question, "Does the material amorphize or not?".

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Exploring fundamental aspects of the structural organization in weberite-type tantalate oxides

Igor Gussev, Dr. Gianguido Baldinozzi, Dr. Eric O'Quinn, Dr. Jörg Neuefeind, Dr. Maik Lang

The design of advanced energy-related materials that are specifically engineered to maintain structural stability in a variety of harsh operating conditions, such as high pressure, temperature, and radiation fields, requires the development of specific experimental techniques and analyses that address the organization of complex materials over length scales that range from the interatomic distances to several hundreds of nanometers. Such structural characterization is important as compositional and structural disorder forms as a consequence of exposure to extremes that impact thermal, mechanical, and chemical properties. Weberite-type tantalate oxides (A3TaO7) are promising candidates for many energy-related applications, but there is only a limited understanding of how their atomic-scale structure changes as a result of exposure to extremes (e.g., high temperature and ion irradiation). We performed state-of-the-art neutron total scattering experiments across a compositional range of weberite-type tantalate oxides and analyzed the real space, short-range pair correlation functions to establish evidence that their local atomic arrangements adopt an organization different from their well-known 'average' structure across longer length scales. This finding appears to be a general phenomenon for a range of weberite-type oxides structures, spanning from fully ordered (orthorhombic Pr3TaO7) to fully disordered (cubic Yb3TaO7). Comparing short- and long-range structural behaviors across the compositional series have revealed a complex organization of structural correlations across different length scales: the short-range analysis suggests a strong dependence of the ionic radius of the A-site cation and the distortion of a local structural motif that monotonically increases across the compositional series, while the long-range analysis confirmed the existence of three distinct structure types. This behavior is explained by the incompatibility of tilt systems in the long-range structure due to the increasing local distortions.

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Exploring fundamental aspects of the structural organization in weberite-type tantalate oxides

Igor Gussev, Dr. Gianguido Baldinozzi, Dr. Eric O'Quinn, Dr. Jörg Neuefeind, Dr. Maik Lang

MC38: Controlled irradiation Disorder in Model Systems: Organisation, Dynamics, and Transformations VIII, August 24, 2022, 4:30 PM - 6:00 PM

The design of advanced energy-related materials that are specifically engineered to maintain structural stability in a variety of harsh operating conditions, such as high pressure, temperature, and radiation fields, requires the development of specific experimental techniques and analyses that address the organization of complex materials over length scales that range from the interatomic distances to several hundreds of nanometers. Such structural characterization is important as compositional and structural disorder forms as a consequence of exposure to extremes and impact thermal, mechanical, and chemical properties. Weberite-type tantalate oxides (A3TaO7) are promising candidates for many energy-related applications, but there is only a limited understanding of how their atomic-scale structure changes as a result of exposure to extremes (e.g., high temperature and ion irradiation). We performed state-of-the-art neutron total scattering experiments across a compositional range of weberite-type tantalate oxides and analyzed the real space, short-range pair correlation functions to establish evidence that their local atomic arrangements adopt an organization different from their well-known 'average' structure across longer length scales. This finding appears to be a general phenomenon for a range of weberite-type oxides structures, spanning from fully ordered (orthorhombic Pr3TaO7) to fully disordered (cubic Yb3TaO7). Comparing short- and long-range structural behaviors across the compositional series have revealed a complex organization of structural correlations across different length scales: the short-range analysis suggests a strong dependence of the ionic radius of the A-site cation and the distortion of a local structural motif that monotonically increases across the compositional series, while the long-range analysis confirmed the existence of three distinct structure types. This behavior is explained by the incompatibility of tilt systems in the long-range structure due to the increasing local distortions.

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Study of the edge spin-waves in the crescent-shape ferromagnetic nanorods in dependence on the bias magnetic field orientation

Hanna Reshetniak, Mateusz Gołębiewski, Maciej Krawczyk

MC44: New Perspectives in Magnonics, from 2D to 3D Systems II, August 22, 2022, 2:00 PM - 3:30 PM

The magnetic field is the primary stimulus used to control magnetism and spin-wave dynamics. Thus, the study of the influence of the magnetic field on ferromagnetic nanostructures in different geometries is extremely relevant for research in the field of modern technologies, especially for the development of 3D magnonic circuits. The influence of the external magnetic field on the spectrum of spin waves in magnetic nanowires is now quite well understood [1, 2]. Recently, it has been experimentally demonstrated that the 3D network formed from the crescent-shape nanorods is promising for development of 3D ferromagnetic systems for various applications, including magnonic circuits [3, 4]. However, the crescent-shape of nanorods (see Fig. 1) impact on spin waves and their manipulation with the magnitude and magnetic field orientation has not yet investigated. Our analysis of the external magnetic field rotation reveals untypical results, which makes this research interesting and important for future investigations. In particular, we show that the edge localized spin-wave modes decouple when the external magnetic field rotates. As a consequence, the two edges can behave as two separate channels for spin-wave guiding with their frequencies controlled by the magnitude and orientation of the field. Such crescent-shaped nanorods can be used as two-channel spin-wave waveguides that support different frequencies on both sides of the nanorod, after breaking the symmetry by the field rotation. We therefore believe that crescent nanorods provides an opportunity to develop 3D magnonic circuits in deep nanoscale.

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The research leading to these results has received founding from the National Science Centre of Poland, project no 2020/39/I/ST3/02413.

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Gate-based parametric single-qubit operations and coherence for the Majorana transmon model

Elena Lupo, Eytan Grosfeld, Eran Ginossar

MC23: Superconducting Circuits for Quantum Technologies II, August 22, 2022, 2:00 PM - 3:30 PM

The strong results shown by superconducting circuit-based qubits, coupled to the need to improve coherence and precise control, lead to new hybrid designs with embedded non-superconducting device elements. In particular, one-dimensional semiconductors hosting topologically protected Majorana Zero Modes (MZMs) could lead to new hybrid platforms with increased controllability and reduced sensitivity to various decoherence mechanisms. Among these newly proposed hybrid qubits, the Majorana transmon exploits the hybridisation between two MZMs through a Josephson junction and encodes the quantum information in the resulting basis of fermion parity states [1]. Within a circuit QED architecture, the Majorana transmon has been presented as a potential tool either for qubit manipulation and readout [2] or in general for a reliable detection method of the Majorana modes [3]. Here [4] I theoretically study the Majorana transmon dynamics under parametric modulation of the off-set charge of the system, which can be straightforwardly implemented via an external time-dependent voltage bias. The notional reduction of the MZMs topological protection due to this additional hybridisation is potentially countervailed by properties which make it an attractive qubit compared to state-of-the-art transmons. One property is a much higher anharmonicity of the energy spectrum. The second is the suppression of the dipole coupling between the two lowest energy levels, making the potential qubit protected from radiative decay. I will show how this modulation can be used for implementing multiple single-qubit gates and how the effect of wide-band 1/f charge noise affects both the free and driven evolution. I will show estimates of coherence times and loss of fidelity using analytical and numerical methods.
For this work we acknowledge funding from the European Commission project HiTIMe.
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Quantifying the diffusion of porphyrins on Au(111):

A temperature-dependent STM study

Matthew Edmondson, Alex Saywell

MC18: Developments at the Frontiers of High-resolution Scanning Probe Microscopy II, August 22, 2022, 2:00 PM - 3:30 PM

The diffusion of surface-confined molecules is a fundamental step within the formation of self-assembled structures and on-surface reactions. Scanning probe microscopies (SPM) provide a route to characterising the diffusion pathways of these molecules and allow a quantitative analysis of energetic barriers via Arrhenius-type rate analysis.[1] In particular, SPM allows the relationship between atomic-scale surface structures and molecular diffusion to be explored; a potential method for influencing on-surface reactivity.[2]
The Au(111) surface, frequently used as a substrate for on-surface coupling reactions [3], exhibits the well-known 'herringbone' reconstruction which may influence the diffusion of molecule species. In this work, we report on the diffusion of individual 2H-TPP on the Au(111) surface; characterising the diffusion rate via variable-temperature scanning tunnelling microscopy within specific regions of the reconstructed surface. The energy barrier to diffusion (obtained via Arrhenius analysis) was found to differ between the FCC and HCP regions of the herringbone reconstruction, indicating that local geometric/electronic surface-features play a role in on-surface diffusion.

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Spider-web nanomechanical resonators by Bayesian optimization with ultralow dissipation

Andrea Cupertino, Dongil Shin, Matthijs de Jonge, Peter Steeneken, Miguel Bessa, Richard Norte

MC17: Nanomechanical and Electromechanical Systems VIII, August 24, 2022, 4:30 PM - 6:00 PM

Nanomechanical resonators are highly demanded in ultra-sensitive detectors, cavity optomechanics and quantum technologies thanks to their exceptionally low dissipation. High-tensile materials and in particular silicon nitride have emerged as a prominent platform for such resonators operating at room temperature due to their remarkable isolation from ambient thermal noise. The amount of mechanical isolation is characterized by a resonator's mechanical quality factor, thus a high quality factor is a desirable property which can greatly enhance a resonator's sensitivity. Different strategies have been developed to manipulate the stress, bending, and mode shape in those resonators to increase the quality factor. However until now, design process has remained driven by human intuition and trial-and-error experimentation.

Here we develop a spiderweb nanomechanical resonator inspired by nature and optimized by machine learning. Spiderweb are lightweight micro-mechanical structures with an extraordinary strength-to-weight ratio. Their unique geometries are designed to be most sensitive to vibrations emanating from the web, resulting in a good isolation from surrounding vibrations. Those remarkable properties makes them a promising starting point for machine-learning algorithms to discover new strategies to increase the quality factor of nanomechanical resonators.

The obtained resonator exhibits vibration modes which eliminate clamping losses via a novel "torsional soft-clamping" mechanism discovered by Bayesian optimization. The bio-inspired resonator is then fabricate in silicon nitride and measured with an optically interferometer, experimentally demonstrating a new class of nanomechanical resonators with quality factor surpassing 1 billion at room temperature. Contrary to state-of-the-art designs, our result is achieved with a compact design and without any sub-micron features to be fully compatible with optical lithography and allow an easy and low-cost manufacture at large scales. This result demonstrates the ability of machine learning to work in tandem with human intuition to augment creative possibilities and uncover new strategies in computing and nanotechnology.

Shin, D., Cupertino, A., de, M. H. J., Steeneken, P. G., Bessa, M. A., Norte, R. A., Spiderweb Nanomechanical Resonators via Bayesian Optimization: Inspired by Nature and Guided by Machine Learning. Adv. Mater. 2022, 34, 2106248.

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Cryogen-free Scanning Gate Microscope for the interrogation of coherence limiting defects in superconducting quantum circuits at millikelvin temperatures

Marius Hegedus, V. N. Antonov, S. E. Kubatkin, A. V. Danilov, S. E. de Graaf

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

The performance of superconducting quantum devices is hindered by decoherence and low frequency 1/f noise. This is widely attributed to the existence of material defects, which behave as two-level quantum systems (TLS) coupled in large numbers to superconducting devices through their electric dipole moments. In order to find improved materials and fabricate more coherent circuits we need to gain a better understanding of TLS and their microscopic nature. A tool capable of probing an individual TLS and revealing their location is needed. Global electrostatic gate tuning is an effective technique for identifying individual TLS present somewhere in superconducting qubits and resonators [1, 2]. To reveal the precise locations of TLS, we have built a cryogenic Scanning Gate Microscope (SGM) which enables the interrogation and localisation of individual TLS using a nanoscale tip as an electrostatic gate electrode. To provide a Scanning Probe Microscopy (SPM) environment suitable for quantum devices, mK temperatures must be reached inside a well shielded, vibration and noise-free SPM platform. We constructed the microscope based on the near-field microwave microscope operating in the single photon regime [3]. We describe the operation of our SGM inside a cryogen-free dilution refrigerator at ~10 mK, with a SPM platform designed to host long coherence time qubit samples and discuss its performance towards detecting TLS. We aim to locate and image individual TLS in a Transmon qubit circuit utilising our SGM.

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Nonmonotonic quantum phase gathering in curved spintronic circuits

Eusebio J. Rodríguez, Diego Frustaglia

MC14: Beyond Charge Transport in Nanostructures and 2D Materials via Geometric Design VIII, August 24, 2022, 4:30 PM - 6:00 PM

Spin carriers propagating along quantum circuits gather quantum spin phases depending on the circuit's size, shape, and spin-orbit coupling (SOC) strength. These phases typically grow monotonically with the SOC strength, as found in Rashba quantum wires and rings. In this work we show that the spin-phase gathering can be engineered by geometric means, viz. by the geometric curvature of the circuits, to be non-monotonic. We demonstrate this peculiar property by using one-dimensional polygonal models where flat segments alternate with highly curved vertices. The complex interplay between dynamic and geometric spin-phase components -- triggered by a series of emergent spin degeneracy points -- leads to bounded, global spin phases. Moreover, we show that the particulars of the spin-phase gathering have observable consequences in the Aharonov-Casher conductance of Rashba loops, a connection that passed unnoticed in previous works.

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Final state bias in adiabatic quantum computing

Dr John Samson

MC40: Strongly Disordered Insulators VI, August 23, 2022, 4:30 PM - 6:00 PM

Adiabatic quantum computing encodes an optimisation problem in a Hamiltonian H_p whose eigenvalues represent the cost function to be minimised. The system Hamiltonian H(t) is interpolated from a simple initial Hamiltonian (H_i) at time t=0 to this problem Hamiltonian Hp at t=T: H(t) = (1-t/T)H_i + (t/T)H_p in the case of linear interpolation. If the system is initially in the (assumed easily prepared) ground state of Hi and the gap to the first excited state does not vanish, then for sufficiently large T there is a large overlap of the final state with a ground state. If there are degenerate ground states, the algorithm is known to give a biassed distribution, fully suppressing some solutions in the adiabatic limit [1].

Here we test this against an n-qubit Sherrington-Kirkpatrick Ising spin glass Hp, with random pairwise interactions J_{ij} = ±1; H_i is a transverse field. The state space is a hypercube, with the edges representing H_i and the potential at the vertices specified by H_p. An exhaustive list of all inequivalent cases for small numbers of qubits indicates a number of scenarios, simulated with our previously developed Taylor-series based algorithm [2]. We relate the probability of a given ground state to the connectivity of the subgraph of the hypercube representing the ground state space.

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Curvature control of the superconducting proximity effect in diffusive SFS Josephson junctions and ferromagnetic nanowires

Tancredi Salamone, Henning G. Hugdal, Morten Amundsen, Sol H. Jacobsen

MC14: Beyond Charge Transport in Nanostructures and 2D Materials via Geometric Design VII, August 24, 2022, 2:00 PM - 3:30 PM

There is currently great interest in the inclusion of superconducting components in spintronic devices, because they can provide dissipationless currents, greatly enhancing device performances for spin-based data processing. Coupling a conventional s-wave superconductor to a ferromagnet allows, via the proximity effect, to generate superconducting triplet correlations. A long-ranged proximity effect is typically achieved by generating long-range triplet correlations via magnetic inhomogeneities or intrinsic spin-orbit coupling (SOC).

We reported (Phys. Rev. B 104, L060505 (2021)) that spin supercurrents can be induced in diffusive SFS Josephson junctions without any magnetic misalignment or intrinsic SOC. Instead, the pathway to spin-triplet generation is provided via geometric curvature, and results in a long-range Josephson effect. In addition, the curvature can induce a dynamically tunable 0-π transition in the junction. This switching of current direction is therefore testable in a single sample.

The generation of triplet correlations can be employed to achieve a superconducting triplet spin-valve effect in superconductor-ferromagnet (SF) hybrid structures, for example by switching the magnetizations of the ferromagnets between parallel and antiparallel configurations in F1SF2 and SF1F2 trilayers, or in SF bilayers with both Rashba and Dresselhaus SOC. In our most recent work (Phys. Rev. B 105, 134511 (2022)) we exploit the curvature control of the superconducting triplet correlations to show that the superconducting critical temperature of an SF hybrid structure can be tuned by varying the curvature of the ferromagnetic wire alone, with no need of another ferromagnet or SOC. Furthermore, we show that the variation of the critical temperature as a function of the curvature can be exploited to obtain a robust, curvature-controlled, superconducting triplet spin-valve effect.

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How accurate is Density Functional Theory to describe work extraction?

Krissia Zawadzki, Amy Skelt, Irene D'Amico

MC20: Recent Advances in Quantum Thermodynamics with a Focus on Many-body Interactions IV, August 23, 2022, 11:30 AM - 12:30 PM

Very recently, the quantum thermodynamics community started to explore work extraction in many-body interacting systems. At the same time, this is an essential issue in envisioning quantum devices and using them in applications such as quantum heat engines, modeling them is a very challenging task. The need to deal with non-integrable Hamiltonians and consider out-of-equilibrium dynamics from the sudden quench to adiabatic brings an urge to develop approximations for quantum thermodynamics.
In the present study, we show that Density Functional Theory (DFT) offers an elegant toolkit to construct these approximations by mapping the unitary into a non-interacting effective Kohn-Sham Hamiltonian. We define two levels of approximation: a `simple' one that uses the same approximation for the initial state and unitary, and a `hybrid' one, in which the initial state is as accurate as of the exact one. We discuss the performance of our DFT-inspired approximations to evaluate the work extraction in Hubbard chains submitted to a finite-time ramp that drives the system from a metallic phase to the Mott- and band-insulator. Our results indicate that simply correcting the initial state by means of the `hybrid' approximation allows for very accurate results in the case in which the external driving does not enhance many-body interactions.

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Quantum Friction in the Presence of a Perfectly Conducting Plate

Xin Guo, Kim A. Milton

MC19: Advances in the Casimir Force and Heat Transfer Phenomena II, August 22, 2022, 2:00 PM - 3:30 PM

A neutral but polarizable particle sitting near a perfectly conducting plate feels a force normal to the surface of the plate, which tends to pull the particle closer to the plate. This is the well-known Casimir-Polder force, which has long been theoretically proposed and experimentally observed. Will a force in the transverse directions (parallel to the surface of the plate) arise when the particle moves above the plate? Though much theoretical prediction could be found for the quantum friction on a particle moving above a dielectric surface, the extreme case of quantum friction in the presence of a perfectly conducting plate seems largely ignored by the theoretical community. We investigated such a case as a natural extension of our work [Phys. Rev. D 104, 116006 (2021)] on quantum vacuum friction (blackbody friction), and concluded that there does exist a quantum frictional force on a neutral but polarizable particle moving above a perfectly conducting plate.

As expected, the quantum frictional force in the presence of a perfectly conducting plate reduces to the quantum vacuum friction in the limit of $aT \gg 1$. Here, a is the fixed distance between the particle and the plate, while T is the radiation temperature. Therefore, the new physics is the behavior of the frictional force at short distances or low temperatures. Very interestingly, the distance dependence, the temperature dependence and even the sign of the frictional force strongly depends on the polarization state of the particle. If the particle is only polarizable in the transverse directions, the frictional force is found to be proportional to $a^4 T^{12}$ in the limit of $aT \ll 1$, and therefore decays to zero as the particle gets very close to the surface. If the particle is only polarizable in the normal direction, we find the frictional force in the limit of $aT \ll 1$ precisely quadruples the corresponding quantum vacuum friction, which is independent of a and proportional to T^8. In both of these situations, the frictional force is negative. However, if the particle is polarizable both in the normal direction and in the direction of motion, another positive contribution to the frictional force exists, which goes as $a^2 T^{10}$. For an isotropic particle, the contributions to the frictional force from different polarization states can be added together. The resultant frictional force is found to be negative definite and therefore a true drag.

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Nb and NbN constriction Josephson junctions and nanoSQUIDs patterned by He and Ne focused ion beams

Timur Griner, Simon Pfander, Julian Linek, Jamie Potter, Oscar Kennedy, Ute Drechsler, Thomas Weimann, Reinhold Kleiner, Paul Warburton, Armin Knoll, Oliver Kieler, Dieter Koelle

MC22: Nanoscale Fabrication of Superconducting Devices and Their Applications X, August 25, 2022, 2:00 PM - 3:30 PM

Nanopatterning of superconducting thin film structures with focused He or Ne ion beams (He/Ne-FIB) offers a flexible tool for creating constriction-type Josephson junctions (cJJs) and strongly miniaturized superconducting quantum interference devices (nanoSQUIDs) based on cJJs for applications in magnetic sensing on the nanoscale. We present our attempts to use He/Ne-FIB for fabricating Nb and NbN cJJs and nanoSQUIDs which shall provide ultra-low noise and high spatial resolution for their application in scanning SQUID microscopy (SSM). The nanoSQUIDs are designed as sensors for magnetic flux and dissipation. They shall be integrated on custom-made Si cantilevers, which will provide the possibility of simultaneous conventional topographic imaging by atomic force microscopy (AFM). We will discuss the status of this project and challenges that have to be met on the way to combine SSM and AFM on the nanoscale.

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Far-From-Equilibrium Processing of Materials under Extreme Conditions

Dr. Eric O'Quinn, Mr. Alexandre Solomon, Dr. Gianguido Baldinozzi, Prof. Dr. Christina Trautmann, Prof. Dr. Maik Lang

MC38: Controlled irradiation Disorder in Model Systems: Organisation, Dynamics, and Transformations VII, August 24, 2022, 2:00 PM - 3:30 PM

High energy ball milling and exposure to energetic heavy ion beams are two material processing methods that rapidly impart enormous amounts of energy into small volumes, yielding disordered material states that are otherwise inaccessible. The innovative strategy of this project involves the application of neutron total scattering experiments, coupled with advanced modeling, to investigate the nature of structural disorder in far-from-equilibrium processed complex oxides over a range of length-scales. This approach presents a significant improvement over conventional long-range characterization techniques, using X-ray and electron probes, that are less sensitive to anion sublattices and the unique aperiodic, short-range structural features produced by extreme processing conditions. Using pyrochlore and other fluorite-derived oxides as model systems, we show that defect behavior in hemically disordered (equilibrium) and mechanically milled and ion irradiated ceramics (far-from-equilibrium) is far more complex than previously thought. We demonstrate that locally ordered structural motifs that are arranged such that the average, long-range structure does not represent the actual atomic configuration (1). The disordering process appears to be decoupled across structural length scales, proceeding locally at different rates than over longer length scales (2). This finding is important as the formation of disorder is inherent to many energy-related applications under which materials must perform in harsh conditions, such as nuclear materials as well as electrolyte and catalyst materials. In this contribution, we show that by using these oxides as model systems, we produce well-defined metastable phases with a variety of disorder and defect structures (3, 4). Systematic analysis of the structural behavior with coupled experiments and modeling identifies the underlying processes that drive the formation of intricate disorder across all material length scales. This research helps to build a robust atomic- and meso-scale understanding of highly defective and disordered phases but will also show how far-from-equilibrium processing techniques can be used to induce specific atomic arrangements and tailor physical properties (e.g., oxygen transport) to enhance functionality in technological applications (e.g., solid oxide fuel cells).

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Near quantum limited superconducting flux tunable sensors using niobium nanobridge rf SQUIDs working towards single spin and single photon detection

Laith Meti, Jamie Potter, Gemma Chapman, George Long, John Gallop, Ed Romans, Ling Hao

MC23: Superconducting Circuits for Quantum Technologies VI, August 23, 2022, 4:30 PM - 5:30 PM

Superconducting Quantum Interference Devices (SQUIDs) embedded in resonators have developed as tools for a wide range of techniques in quantum sensing and QIP applications. Single step fabrication of niobium nanobridge (SQUIDs) on silicon substrates using electron beam lithography (EBL) has produced the exceptional noise performance from ultra-sensitive flux sensors with potential applications in quantum technology; working towards single spin and single photon detection. The devices based on these nano scale constrictions exhibit flux sensitivity quantised to Φ_0~h/2e and are embedded into a niobium co-planar waveguide resonator (CPW). Combining these sensors with dispersive microwave readout circuitry enables further advantages: the achievement of near quantum-limited noise performance up to high frequencies and the mediation of exploitable parametric effects through the inherent non-linearity of the nanobridge weak-link. A controlled external field (which can be applied by a direct on-chip fast flux line) couples the flux to the weak link SQUIDs providing a hybrid flux tunable superconducting resonator circuit for quantum technologies with sensitivity working towards to 30 $n\Phi_o/Hz^{1/2}$ at 30 mK [1] or more typically sub $\mu\Phi_o/Hz^{1/2}$ at 3.6K. Furthermore, one or more single junction rf SQUIDs allow for the manifestation of parametric three-wave mixing, where a “signal” tone (f_s) can be amplified via energy transfer with a “pump” tone (f_p). The coupling in this regime is inherently stronger significantly away from the signal band; operated at pump frequencies at the second harmonic 2f_s. Here we present the design and measurement of our CPW embedded structures incorporating one or more flux-tunable niobium nanobridge rf SQUIDs fabricated using e-beam lithography and plasma etching. We compare the measured device performance with the predictions of superconducting circuit simulations.

Acknowledgement: This work was supported by the UK National Measurement System and UCL Impact Studentship.

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Mechanical overtone frequency combs

Matthijs De Jong, Dr. Adarsh Ganesan, Andrea Cupertino, Dr. Richard Norte

MC17: Nanomechanical and Electromechanical Systems VI, August 23, 2022, 4:30 PM - 6:00 PM

Mechanical frequency combs are a recent development, following the successes and widespread use of optical frequency combs. We report on a new mechanism to create frequency combs consisting of overtones (integer multiples) of a mechanical eigenmode, by putting a suspended membrane in a counter-propagating optical trap generated via its own back plane. The optical field exerts a dielectrophoretic force on the membrane that efficiently creates overtones which form a frequency comb. Based on the same optical field, we also demonstrate a strong, parametric thermal driving mechanism that requires no frequency tuning nor additional signal or control to operate. The combination of these effects result in a versatile frequency comb platform with excellent uniformity and stability that is agnostic to optical wavelength or material platform, features in-situ control and tuneability using a single, mW optical beam and standard microscope objective.

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Investigating ballistic charge transport and spin injection via 1D graphene/FM junctions

Dr Christopher Anderson[University of Manchester], Mr Noel Natera Cordero[University of Manchester], Mr. Jesus Carlos Toscano-Figueroa[University of Manchester], Mr Daniel Burrow, Ivan Vera-Marun

MC14: Beyond Charge Transport in Nanostructures and 2D Materials via Geometric Design VII, August 24, 2022, 2:00 PM - 3:30 PM

Despite its great promise for spintronics, experimental values for spin transport parameters extracted from graphene are currently significantly below theoretical predictions. Our group recently reported encouraging results from a novel spintronic device architecture constituting a fully encapsulated single layer graphene channel that employs one-dimensional (1D) ferromagnetic (FM) contacts (Fig. 1a) [1]. Encapsulation of the channel in hexagonal boron nitride preserves the quality of the graphene, resulting in high charge mobilities, while use of 1D contacts mitigates many of the problems associated with tunnel contacts, such as doping and Fermi level pinning [2, 3]. Additionally, the geometry of the contact area places transport across the junction in the ballistic regime. This not only allows for achieving sizeable contact resistance without the need for tunnel barriers, but also allows for studying previously unexplored phenomena such as quantized conductance across the 1D graphene/FM junction. Recent results from our novel device architecture have focussed on transport through these junctions, at low temperature. Bias spectroscopy measurements demonstrate conductance through the junction quantized in fractions of the conductance quantum - indicating a transmission factor $T \approx 0.5$ (Fig. 1b). Furthermore, application of an out-of-plane magnetic field leads to better defined quantization, resulting from a transition into the quantum Hall regime [4,5]. Finally, in our spin transport experiments we observe an electrically tuneable spin polarization reversal, implying a spin split density of states in the graphene region adjacent to the FM contact, which occurs due to the magnetic proximity effect. Quantized conductance in a nanoscale 1D FM contact, in the absence of a fabricated graphene nanoconstriction, is a previously unreported result, and could offer a path to ballistic spintronics.

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Figure 1 caption: (a) 3D schematic and 2D cross section (inset) of the device architecture. Figure adapted from [1]. (b) Bias spectroscopy conductance measurement of a 1D contact, for electron transport (VBG > Vneutrality) under an applied out-of-plane magnetic field B = 1 T.

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Counting charges in interacting one-dimensional conductors

Oleksiy Kashuba, Roman Riwar, Fabian Hassler, Thomas Schmidt

MC24: Quantum Electronics at Ultra-low Temperatures XII, August 26, 2022, 9:00 AM - 10:00 AM

The calculation of the moment generating function of a given observable, such as the charge or Wigner-Jordan-like exponentials is nontrivial even for the non-interacting systems. This problem is closely connected to the problem of Toeplitz eigenvalues and Szegö-Kac theorem [1]. The application of the latter leads to a violation of charge quantization, which manifests as a breaking of the moment generating function periodicity along the counting field. This periodicity can be restored using the Fisher-Hartwig conjecture, as was shown for non-interacting electrons on a line [2]. Here, we aim to go beyond and include interactions. For weak interactions, a modification of the Masubara diagrammatic approach was developed, allowing us explicit calculation of the interaction corrections to the characteristic function. All obtained terms preserve the periodic constraint of the moment generating function. This result allows us to show that, surprisingly, the Wigner crystal paradigm, usually reserved for strong interactions, can be continued to weak interactions, allowing us to study charge fluctuations for all interaction strengths.

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DMFT study of the effect of the f orbital on high-temperature superconducting lanthanide hydride

Yao Wei, Elena Chachkarova, Cedric Weber

With the current hype to search for high-temperature superconducting materials, lanthanide's high-temperature superconductivity has become a hot research topic. A series of materials such as LaH16, CeH16, CeH9 have been verified to show high temperature superconductivity in an environment of 200-300 GPa. Recent studies of these materials have shown that an increase in the f character of the Fermi level leads to an increase in the superconducting temperature of lanthanide hydrogen rich materials. Here, we compare the characteristics of three different hydrogen-rich materials, LaH10, CeH10 and PrH10, with the same ratio by DMFT method, and further elaborate on the influence of the f orbital of these substances in these extreme cases and hope that with this study we will provide ideas for the structure prediction and material properties research of hydrides in the future.

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Structural and dynamical features of a suspension of active ring polymers under confinement

Juan Pablo Miranda, Chantal Valeriani, Emanuele Locatelli

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

We have studied the properties of an active ring polymer confined between two parallel plates. The activity is inplemented as a force that acts on the tangential direction of the polymer's backbone.
We have not only analyzed the system’s dynamic properties, but also examined the structural configurations that the polymer explores, and the relevance of activity. One important aspect is the role played by confinement and active force, which makes the system behave in interesting ways.
First we have studied the beahavior of the isolated rings, and then we proceed to examine the properties of those rings in a suspension where they interact repulsively with each other.
By changing the confinement distance between the plates and the activity, we find several states, such as collapsed or expanded an we characterise its properties and its general form studying the radius of gyration, and other parameters derived also from the gyration tensor. We also found interesting collective behaviour on the solution and studied its dynamical properties.

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Control of the local magnetic states in graphene with voltage and gating

Fei Gao

MC12: Physics in 2D Nanoarchitectonics III, August 22, 2022, 4:30 PM - 6:00 PM

Magnetism of graphene can be created by atomic defects, either hydrogen adsorption or single-carbon vacancy formation, owing to the unpaired π electrons around the defects. Here we explore, based on rigorous first principles calculations, the possibility of voltage manipulation of two such types of π magnetism in graphene via a scanning tunneling microscope tip. We find a remarkably different behavior. For the hydrogen, the magnetic moment can be switched on and off with voltage-induced doping, whereas, for the carbon vacancy, the spin splitting of the π bands persists, almost independent of the extent of doping, due to the coupling between the π and the σ bonds. Furthermore, the local atomic structures near the vacancy can be reversibly manipulated by a coordination mechanism between an intermediate tip-defect distance and a moderate tip voltage, consequently leading to the reversal of spin polarization of the π bands. Voltage control of the local magnetic states may open a new avenue for potential applications in spintronics.

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Coherent quantum phase slip qubits coupled to superconducting resonators

Teresa Hoenigl-Decrinis, Ilya Antonov, Kyung Ho Kim, Jacob Dunstan, Rais Shaikhaidarov, Vladimir Antonov, Oleg Astafiev

MC23: Superconducting Circuits for Quantum Technologies V, August 23, 2022, 2:00 PM - 3:30 PM

We present spectroscopy studies of coherent quantum phase slip (CQPS) qubits coupled to a superconducting λ/2 resonator. The CQPS qubit consists of a highly inductive superconducting loop with a nanowire across which the CQPS occurs. We investigate both inductive and capacitive coupling between the qubit and the resonator. For both couplings, we can detect and couple qubits on several resonator modes. Previously the CQPS qubit was only inductively coupled to the readout resonator-the new capacitive coupling demonstrated can add flexibility in design, materials, and fabrication by avoiding galvanic contact between qubit and readout environment. Transmission measurements show a loaded quality factor in the order of 1000 and resonance modes in the order of 1 GHz. With 12 CQPS qubits capacitively coupled to the resonator, two-tone spectroscopy as a function of external magnetic field and probe frequency reveals energy spectra of the coherent quantum state in each qubit. We extract phase slip energy from 8 qubits that ranges from 1 to 3 GHz, which agrees well with the theory taking into account the widths of the superconducting nanowires. We also observe avoided crossings which allow us to estimate the intermediate coupling strengths with the resonator.

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Interactions, Disorder and Localization in 2D and 1D

Professor Michael Pepper, Dr Yilmaz Gul, Dr Stuart Holmes, Dr Sanjeev Kumar, Dr Ian Farrer, Dr Maksym Myronov, Professor David Ritchie

MC40: Strongly Disordered Insulators I, August 22, 2022, 11:30 AM - 12:30 PM

The transition between localized and “extended” states in 2D systems has been of interest for a considerable time. It is now known that in 2D all states are localized but the coherent back-scattering which is essential for the localization is cut off by phase incoherent, Landau, scattering, which creates at observable temperatures metallic conduction and extended states. The role of incoherence is maximised as the disorder decreases resulting in an increasing electron mobility, a consequence of the cutting off of the coherent back-scattering is the observation of Mott’s Minimum Metallic Conductivity, MMC, Conductance in 2D, which becomes subject to logarithmic corrections when the phase scattering length becomes greater than the elastic scattering length. In this talk we present our recent data showing how the electron-electron interaction modifies the conductance behaviour leading to a quantized 2D resistivity as pre-exponential factor in the Mott and Efros-Shklovskii variable range hopping conductances. We show how the MMC emerges as the disorder at the Fermi energy is altered.
In the regime of ballistic transport when the dimensionality is between two and one we have found non-magnetic fractional quantization of conductance in both Ge and GaAs. This phenomenon occurs when the electron-electron interaction determines the energies of the confined states and the ground state wavefunction changes its nature. The dependence of the quantization on the disorder will be discussed and the relationship to possible models of the process.

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Rotobreather dynamics in the two-dimensional XY model

Yaroslav Zolotaryuk

It is shown that rotobreathers are generic solutions of the
two-dimensional nearest neighbour XY model with constant magnetic field. The XY model describes a two-dimensional lattice of pinned interacting rotators that can rotate only in the plane. It is widely used to describe magnets and arrays of Josephson junctions. Rotobreathers are periodic and spatially localized modes that consist of several sites that rotate with some given frequency, while the rest of the lattice oscillates with the same frequency. The allowed range of the
rotobreather frequency begins from the upper edge of the linear
spectrum and continues to the arbitrarily large frequencies.
The energy-frequency dependence has a local minimum and increases both in the limits of high and low frequencies. Connection to discrete breathers in the ferromagnetic easy-plane lattice is discussed.

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Quantum and Casimir Friction: Energetics and Forces

Kim Kimball Milton

MC19: Advances in the Casimir Force and Heat Transfer Phenomena II, August 22, 2022, 2:00 PM - 3:30 PM

Quantum and Casimir Friction:
Energetics and Forces

Kimball A. Milton, Xin Guo, Gerard Kennedy, Nima Pourtolami, Yang Li, and William McNulty

For some time, we have been systematically exploring frictional forces on a particle moving uniformly through vacuum near a conducting or dielectric surface. Friction occurs classically for a charged particle or a dipole moving parallel to an imperfectly conducting surface. So-called Casimir friction occurs for a neutral, nonpolar particle when an electric dipole moment emerges through quantum fluctuations, which necessarily involve dissipation. Even in empty space, quantum vacuum friction occurs, which is a generalization of the Einstein-Hopf effect. In general, fluctuations occur in both the dipole moments and in the electromagnetic fields. These two types of fluctuations are characterized by different temperatures; if the dipole fluctuations are induced by those of the electromagnetic fields, there is a correspondence between these two temperatures, which corresponds to a nonequilibrium steady state, where the particle neither gains nor loses energy. Such a configuration appears to be stable. For high velocities, the temperature of the particle can be significantly higher than that of the background blackbody radiation. This might be a viable signature of quantum vacuum friction, since the quantum vacuum frictional forces themselves are quite small. When a metallic or dielectric surface is present, a synergic effect occurs as a competition between the vacuum friction due to radiation reaction, and that due to dissipation within the material below the surface. We are continuing to study various models for the particle and the background. Previously, these phenomena have mostly been studied in the nonrelativistic, low-temperature, and nonretarded regimes. In contrast, our work is relativistic, explores phenomena at high temperature, describes anisotropic particles, and properly incorporates retardation.

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Synthesis of mesoporous films of vanadium and vanadium-oxide nanoparticles by means of gas aggregation source

Anna Kuzminova, Tereza Kosutova, Adela Hankova, Jan Hanus, Jan Prokes, Marek Prochazka, Ondrej Kylian

MC9: Recent Developments in Gas Phase Synthesis of Nanoparticles and Applications X, August 25, 2022, 2:00 PM - 3:30 PM

Nanoparticles (NPs) and nanoparticles-based nanomaterials receive steadily growing interest in the scientific community. The popularity of this family of materials is foremost due to their unique physicochemical properties and high surface-to-volume that make them highly attractive for use in various technological fields. This is especially true in the case of metal-oxide NPs that were reported to be advantageous, for instance, for bio-detection, photo-catalysis or gas sensing. Naturally, the critical step is the controlled and reliable synthesis of nanoparticles with the required structure/functionality. One of the possibilities, which receives increasing importance is the use plasma-based of gas aggregation sources, i.e. the technique reported by many research groups to be well-suited especially for the production of various metallic NPs. Such produced nanoparticles may be subsequently annealed which allows their conversion to metal-oxide ones.

In this study, the aforementioned strategy is used for the synthesis of mesoporous vanadium oxide nanoparticle films. It is shown that under optimized conditions the gas-phase synthesis of nanoparticles by gas aggregation source allows for the production of vanadium NPs 30 nm in diameter at a deposition rate reaching 1 mg/hour. This extremely high deposition rate results in the formation of mesoporous vanadium nanoparticle films. Furthermore, by the precise control of the annealing conditions, porous vanadium nanoparticle films might be transformed either to VO_2 or V_2O_5 ones as witnessed by XRD, XPS and SEM analysis of produced coatings. While the coatings with a high fraction of VO_2 phase were found to exhibit thermally induced switching of electrical conductivity, V_2O_5 nanoparticle films were found to be suitable for the use as substrates for non-plasmonic surface-enhanced Raman spectroscopy (SERS). As indicated by the preliminary results, V_2O_5 nanostructured SERS-active platforms offer not only a high detection limit but also excellent spectral reproducibility and stability, i.e. features problematic for conventionally used metallic SERS substrates.

This work was supported by grants GAČR 22-16667S and SVV 260 579/2022.

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Ultrafast magnetic switching using polarized phonons

Carl Davies

MC45: Interfaces between Magnonics and Phononics V, August 23, 2022, 2:00 PM - 3:30 PM

All-optical switching (AOS) of magnetization – the process in which ultrashort optical pulses switch magnetization in the absence of bias magnetic fields – represents a fascinating area of condensed matter physics. Multiple avenues for AOS have emerged in recent years [1] ranging from thermal single-shot exchange-driven switching in ferrimagnets [2] and helicity-dependent switching in ferromagnets [3] to non-thermal switching mechanisms driven by the resonant excitation of electronic [4] or phononic [5] subsystems.

Here, we explore further how magnetization can be switched by the resonant excitation of infrared-active optical phonons. Using narrow-band infrared optical pulses delivered by the free-electron laser facility FELIX [6], with wavelength ranging between 10 and 50 μm (frequency between 6 and 30 THz), we drive longitudinal or transverse optical phonons at resonance in different systems.

We find that an ultrafast resonant excitation of the longitudinal optical phonon modes in magnetic iron-garnet films switches magnetization in to a peculiar quadrupolar domain pattern. This unusual fingerprint unambiguously reveals its rooting in the magneto-elastic mechanism [5]. In contrast, the resonant excitation of strongly-absorbing transverse phonons results only in thermal demagnetization. The demonstrated displacive mechanism of switching is also found to operate in other materials such as weak ferromagnets and antiferromagnets [7] that have very different crystallographic, symmetry and magnetic properties.

We have also recently discovered that optical phonons in fused-silica and sapphire substrates, when driven at resonance by circularly-polarized infrared pulses, can generate a transient magnetic field that is capable of impulsively switching magnetization [8]. In these experiments, we sweep circularly-polarized optical pulses across thin GdFeCo films mounted on fused-silica or sapphire. The resulting helicity-dependent magnetic switching scales in efficiency with the phonon spectrum characteristic of the substrate.

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Nanostructure and Evolution of Hydrated MAPbBr3(100) at Low Water Vapour Exposure

Robin Kerr, Dr. Thomas Macdonald, Jiangdong Yu, Dr. Alex Tanner, Prof. Geoff Thornton

MC48: Multi-modal Characterisation of Thin Film Optoelectronics for Energy Applications V, August 23, 2022, 2:00 PM - 3:30 PM

Hybrid organic-inorganic perovskites (HOIPs) have shown great promise as an active material in a wide range of optoelectronic applications, including light-emitting diodes, lasers, and highly efficient solar cells. However, this performance is inhibited by the surface sensitivity of HOIPs to various environmental factors, particularly, high levels of relative humidity [1]. Here, we use scanning tunnelling microscopy to reveal the surface restructuring of in-situ cleaved MAPbBr3 single crystals upon exposure to water vapour. The restructuring is shown to occur in isolated regions which grow in surface area with increasing exposure. Nanostructured features are presented which match those imaged previously on the same material exposed to ambient air [2], providing insight into the initial degradation mechanism of HOIPs. The formation of the hydrated surface was monitored via X-ray photoelectron spectroscopy, while ultraviolet photoemission spectroscopy showed an increased density of band gap states following hydration, which was attributed to surface defect formation due to lattice swelling. This work will help to inform the surface engineering and designs of future perovskite-based optoelectronic devices.

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Water under soft and hard confinement

Dr Fausto Martelli

MC7: Exploring liquid properties in confined geometry (up to mesoscopic scales) VIII, August 24, 2022, 4:30 PM - 6:00 PM

Water at the interface plays a pivotal role in both biology and technology. In this talk, we present recent advancements in understanding how water interacts and is affected by the presence of soft and hard surfaces. Adopting the perspective of topology, we show how the hydrogen bond network (HBN) of water is affected in the proximity of different surfaces. In the case of biological membranes, our investigations show that the presence of a soft surface affects the properties of water at distances almost double than previously believed, suggesting that the concept of “biological water” intended as the thin layer of water in contact with membranes and with biological relevance should be revised (1-3). In the case of hard surfaces, our investigations uncover a phase transition from a two-dimensional HBN to a three-dimensional HBN occurring in water under different degrees of confinement (4,5).

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5) Z. Wei, M. Chiricotto, J. D. Elliott, F. Martelli, P. Carbone, Under review

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Magnetism and spin-polarized bound states in semiconductor-superconductor-ferromagnetic wires

Dr. Rubén Seoane Souto, Dr. Saulius Vaitiekenas, Mr. Andrea Maiani, Dr. Yu Liu, Prof. Peter Krogstrup, Dr. Andras Gyenis, Dr. Constantin Schrade, Prof. Karsten Flensberg, Prof. Martin Leijnse, Prof. Charles M. Marcus

MC21: Bound States in Hybrid Superconductor Nanostructures I, August 22, 2022, 11:30 AM - 12:30 PM

Topological superconductors are attractive platforms for fault-tolerant quantum devices. In 1-dimension, they host well-separated Majorana quasiparticles at their ends, which can encode information in a protected way. The first proposed platforms for topological superconductivity require relatively large magnetic fields, setting constraints on the device's geometries [1]. Ferromagnetic insulating materials (FIM), such as EuS or EuO, can help overcome these limitations, eliminating the requirement of external magnetic fields. Recently, robust zero-energy states have been reported in the semiconductor-superconductor-ferromagnetic insulator platform [2], consistent with the presence of Majorana bound states.

In this presentation, I will discuss how FIMs can help inducing topological properties in the device. I will discuss recent Coulomb blockade measurements of semiconducting InAs nanowires, partially covered with Al and EuS shells and tunnel-coupled to normal leads. By comparing experimental results to a theoretical model, we associate inelastic cotunneling features in even-odd periodic Coulomb-blockade spectra with spin-polarized subgap Andreev levels. Our study suggests spin-splitting exceeding the induced superconducting gap at zero magnetic field [3]. I will also discuss the transport properties of spin-polarized Andreev bound states in Josephson junctions, analyzing the role of magnetic domains [4].

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A non-perturbative cross-Kerr coupling to achieve high fidelity quantum non-demolition superconducting qubit measurement

Vladimir Milchakov

MC23: Superconducting Circuits for Quantum Technologies I, August 22, 2022, 11:30 AM - 12:30 PM

The most common technique of qubit readout in cQED relies on the transverse coupling between a qubit and a microwave cavity, leading to the Jaynes-Cummings Hamiltonian description and dispersive readout. However, despite important progresses, implementing fast high fidelity and Quantum Non Demolition (QND) measurement remains a major challenge. Indeed, inferring the qubit state is limited by the trade-off between speed and accuracy due to Purcell effect and unwanted transitions induced by readout photons in the cavity. To overcome this, we propose and experimentally demonstrate a new measurement scheme based on a transmon molecule inserted inside a 3D-cavity_[1,2]. The full system presents a transmon qubit mode coupled to a readout mode through an original non-perturbative cross-Kerr coupling, which is definitely different from Jaynes-Cummings Hamiltonian. This novel coupling is a key point of our readout scheme which imprint new properties in our qubit such as a protection from Purcell effect and a robust QNDness.
A first generation of transmon molecule had presented promising results [2]. A novel circuit with optimized parameters such as the circuit geometry, the electric circuit parameters, the nanofabrication process leading to relaxation time of about 20us has recently developed. We will present the readout performance based on the cross-Kerr coupling of this second generation of transmon circuit with readout fidelity higher than 99%, QND estimation near 99%. We will also discuss the effect of readout photon number on the measurement and its QNDness.
This work is supported by the French Agence Nationale de la Recherche (ANR-CE24-REQUIEM).
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Nonlinear bandgap transmission in a discrete flat-band lattice

Dr Alain Bertrand Togueu Motcheyo, Prof J. E. Macias-Diaz

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter XI, August 25, 2022, 4:30 PM - 6:00 PM

We consider a cross-stitch lattice [1,2] modelled by coupled time-dependent discrete nonlinear Schrödinger (DNLS) equation. The study of the linear equations reveals the presence of the additional frequency which is not a function of the wave vector in the Brillouin zone. By considering one complex wave component proportional to another, we depict the homoclinic connection of the 2D map [3,4] helps to understand the types of the gap solutions present in the lattice. Contrary to the longitudinal dust grain oscillations in dusty plasma crystals [5], the train of bright soliton (see FIG. 1) generated by driving the lattice with a periodic source is carried by a travelling kink

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Quench dynamics in a disordered two-dimensional electron system: Long-range vs short-range Coulomb interactions

Prof. Dragana Popovic

MC40: Strongly Disordered Insulators V, August 23, 2022, 2:00 PM - 3:30 PM

Understanding the dynamics of isolated disordered systems and its dependence on the range of interactions has been attracting a lot of research attention, but many questions remain open, especially in two spatial dimensions. At the same time, experiments have been limited mostly to those on synthetic quantum matter, such as ultracold atoms. This talk will describe experiments on a strongly disordered, two-dimensional electron system (2DES) in Si metal-oxide-semiconductor field-effect transistors (MOSFETs), with a very weak thermal coupling of the 2DES to the environment. Two sets of practically identical devices have been studied, the only difference being the thickness of the oxide that separates the 2DES from the metallic gate. In thin-oxide MOSFETs, the metallic gate screens the long-range Coulomb interaction, reducing it to a short-range, dipolelike form.

We find that there is practically no difference in the dc transport, including the critical behavior near the metal-insulator transition, between the two sets of devices [1]. In contrast, there is a striking difference in their dynamics, measured after taking the 2DES far from equilibrium by a rapid change of carrier density. In the long-range case, the dynamics is glassy, and the thermalization time diverges as temperature T->0 [2]. In the short-range case, on the other hand, there is no evidence of glassy behavior, but the thermalization is anomalously slow and strongly sensitive to thermal coupling to the environment, suggesting the proximity to a many-body-localized (MBL) phase [3]. Our results demonstrate that the MBL phase in a 2D electron system can be approached by tuning the interaction range, thus paving the way to further studies of the breakdown of thermalization and MBL in real materials. These findings provide qualitatively new insights into the problems of dynamics and thermalization in strongly disordered, interacting systems.

*This work was supported by NSF Grants Nos. DMR-1307075, DMR-1707785, DMR-2104193 and the National High Magnetic Field Laboratory (NHMFL) through the NSF Cooperative Agreements Nos. DMR-1157490, DMR-1644779, and the State of Florida.

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Measurement driven quantum clock implemented with a superconducting qubit

Xin He, Prasanna Pakkiam, Adil Gangat, Alejandro Gomez Frieiro, Gerard J. Milburn, Arkady Fedorov

MC23: Superconducting Circuits for Quantum Technologies IV, August 23, 2022, 11:30 AM - 12:30 PM

In classical physics, clocks are open dissipative systems driven from thermal equilibrium and necessarily subject to thermal noise. Here we consider the case of quantum clocks near zero temperature driven in part by entropy reduction through measurement and necessarily subject to quantum noise. The experimental setup is a superconducting transmon qubit dispersively coupled to an open co-planar resonator. The cavity and qubit are driven by coherent fields and the cavity output is monitored with a quantum noise-limited amplifier. When the continuous measurement is weak, it induces sustained coherent oscillations (with fluctuating period) in the conditional moments. Strong continuous measurement leads to an incoherent cycle of quantum jumps. Both regimes constitute a clock, whose signal can be extracted from the observed measurement current and analysed to determine the relation between clock period noise and dissipated power. The experiment demonstrates for measurement driven quantum clocks a fundamental principle of all clocks: good clocks require high rates of energy dissipation.

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Random-matrix approach to ergodicity breaking and slow dynamics in quantum systems

Dr. Ivan Khaymovich, Prof. Vladimir Kravtsov

MC42: Broken Ergodicity and Localisation in Quantum Many-Body Systems IX, August 25, 2022, 11:30 AM - 12:30 PM

Ergodicity breaking based on the coherent quantum nature of interacting systems inevitably appear and play a crucial role in technological applications, such as computing, classical or quantum, and machine learning.

Great efforts have been applied to ergodicity breaking over the last decades, motivated by the fact that ergodic systems keep no information about their initial state.

Currently, the attention is focused on many-body localization (MBL) where all degrees of freedom are localized via disorder in the on-site potential of the system and break ergodicity, being a prototype of a quantum memory.

However, the complexity of quantum many-body systems prevents one from the analytical description of it.

Thus, it is of particular concern and high demand to model essential attributes of these phenomena on a universal level.

Random matrix theory (RMT) provides such a universal and powerful approach to describe the thermalizing many-body quantum systems and sets the basis for a quantum eigenstate thermalization hypothesis, (ETH).

However unlike the thermalizing case, there is no framework of the same generality to ETH to describe them.

In this talk, I will focus on an alternative RMT framework for description of ergodicity breaking phenomena, basing on the random-matrix theory and statistical mapping of the Hilbert-space structure of many-body systems to RMT.

The similarity between non-ergodic delocalized phase, found in a so-called Rosenzweig-Porter model, with the wave-function structure of the MBL phase in the Hilbert space allows one to develop the mapping between these systems.

The same is also true for the graphs prototypes of MBL.

This statistical mapping opens a simple and universal way to describe the ergodicity-breaking physics of the many-body models in the Hilbert space and on the disordered hierarchical graphs, similar in spirit of how RMT describes the ergodic behavior.

As a generic example of this approach, we consider the static and the dynamical phases in a Rosenzweig-Porter random matrix ensemble with a distribution of off-diagonal matrix elements of the form of the large-deviation ansatz, relevant for the MBL description.

We show that our model contains four possible phases. These are not only the localized and the fully ergodic (RMT-like) phases which existence is known long ago. Our model supports also the genuine multifractal phase which is currently vigorously discussed in connection with MBL and which local spectrum is multifractal, and a “bad metal” one related to slow dynamics.

We present a general theory of dynamical properties (survival probability) in such a random-matrix model and show that the averaged survival probability may decay with time as a simple exponent, as a stretch-exponent and as a power-law or slower. Correspondingly, we identify the exponential, the stretch-exponential and the frozen-dynamics phases.

We consider the mapping of the Anderson localization model on Random Regular Graph, the known proxy of MBL, onto the RP model and find exact values of the stretch-exponent kappa in the thermodynamic limit.

Our theory allows to describe analytically the finite-size multifractality and to compute the critical length with the exponent 1 associated with it.

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Typicality of nonequilibrium (quasi-)steady currents

Dario Poletti

MC20: Recent Advances in Quantum Thermodynamics with a Focus on Many-body Interactions V, August 23, 2022, 2:00 PM - 3:30 PM

The understanding of the emergence of equilibrium statistical mechanics has progressed significantly thanks to developments from typicality, canonical and dynamical, and from the eigenstate thermalization hypothesis. Here we focus on a nonequilibrium scenario in which two nonintegrable systems prepared in different states are locally and non-extensively coupled to each other. Using both perturbative analysis and numerical exact simulations of up to 28 spin systems, we demonstrate the typical emergence of nonequilibrium (quasi-)steady current for weak coupling between the subsystems. We also identify that these currents originate from a prethermalization mechanism, which is the weak and local breaking of the conservation of the energy for each subsystem.

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Charge transport in pinned, gapless charge density waves

Blaise Goutéraux

MC31 : The Physics of Cuprates XI, August 25, 2022, 4:30 PM - 6:00 PM

Gapped, pinned charge density waves are charge insulators. Charge density wave states in strongly-correlated materials are often gapless. Using effective field theory methods, I will show how this gives rise to a nonzero electric dc conductivity. Remarkably, the leading contribution is independent from the strength of disorder in the system. I will comment on the potential relevance of this mechanism to strange metallic transport in cuprate high Tc superconductors.

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Stokes experiment in an active cellular material: understanding the emergence of a Maxwell rheology

Marc Karnat, Jean-François Rupprecht, Sham Tlili, Shao-Zhen Lin

MC3: Tissue Dynamics: From in Vivo Experiments to in Silico Modelling XII, August 26, 2022, 9:00 AM - 10:00 AM

Dragging a finger into a fluid is arguably the most intuitive means to estimate its viscosity. Letting the fluid flow past your finger is an equivalent method. Controlled experiments and theory were historically introduced by Stokes for simple fluids [1] and later applied to more complex materials such as foams [2]. Inspired by the Stokes experiment, a recent work considered the flow of a Madin-Darby Canine Kidney epithelial tissue past a circular spot without fibronectin coating [3].
Here, I will discuss our implementation of the Stokes experiment within an active viscous vertex model framework. Accounting for co-rotational and drift terms, we find a linear correlation between the cell deformation and the cell rearrangement rate tensors. Such a linear relation is indicative of a Maxwell viscoelastic liquid rheology, as observed in MDCK experiments [3]. Our vertex-model simulations allow us to relate the measured viscoelastic time to both tissue-scale and cell-cell mechanical properties, as well as to interpret epithelial tissue experiments in alternative confining geometries.

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Lifshitz transition-induced tuning of charge density waves in 2H-TaSe2

Yiwei Li, William Luckin, Juan Jiang, Surani Gunasekera, Dharmalingam Prabhakaran, Felix Flicker, Yulin Chen, Marcin Mucha-Kruczynski

MC50: Fermi Surface Topological Transitions - Effects of Interactions VIII, August 24, 2022, 4:30 PM - 6:00 PM

2H-$TaSe_2$ is a metallic transition metal dichalcogenide which consists of weakly coupled sandwich-like layers in which an atomic plane of transition metals is embedded between two planes of seleniums. All the atoms are arranged in hexagonal lattices, with the chalcogen layers in each sandwich directly above/underneath each other. The consecutive sandwich-layers are rotated by 180 degrees and stacked so that the transition metals are placed on top of each other. Below 90 K, 2H-$TaSe_2$ exhibits a (3×3) charge density wave. As suggested by this high critical temperature, the electronic band reconstruction in this phase is quite strong, with the associated gap 50-100 meV. For this reason, 2H-$TaSe_2$ serves as a model to understand the mechanisms behind charge density wave formation in other materials (including other transition metal dichalcogenides).

Here, we study the interplay between the charge density order and a Lifshitz transition by surface doping 2H-$TaSe_2$ with potassium. Using angle-resolved photoemission spectroscopy, we map out directly the electronic dispersion in the (3×3) charge density wave state and how it changes as the previously unoccupied electronic states in the topmost layers are filled so that the chemical potential crosses a saddle point in the dispersion. Based on calculations of generalized susceptibility within a minimal two-band model and symmetry arguments, we conclude that the change in the Fermi surface topology drives a change in the charge density order from a (3×3) to a (2×2) superlattice.

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Exploration of emerging chirality of chemically non-chiral systems in mixtures with LC nanoparticles

Georg Mehl, Wanhe Jiang, Haifa Ojaym, Huanan Yu, Stephan Conopo-Holyoake, Feng Liu, Yangyang Zhao, Xiangbing Zeng, Giuliano Siligardi

MC8: Complex Phases in Soft Matter V, August 23, 2022, 2:00 PM - 3:30 PM

There has been considerable attention of exploring the organization of metallic nanoparticles (NPs) by liquid crystals (LC), either in defects of optical textures or fully dispersed in an LC matrix. Nematic like systems have been in the focus, as the nematic tends to tolerate additives well. This research has been extended to the use of chiral groups bound to NPs to induce helical structures with high efficiency into nematic hosts. [1-3] The interplay of NPs functionalized with nematogenic groups with the recently observed new nematic phases such as the Ntb phase and the Nf phase has not yet been explored very much.
Here we show the results of our investigations of combining nematogenic LC functionalized NPs functionalized with nematogens as well as chiral groups in the Ntb and the Nf phase. [4] We will provide details of the superstructures of the NP systems, based on TEM, OPM, DSC and XRD analysis and the results of our studies of combing the NPs systems with suitable Ntb dimers and Nf forming materials such DIO using OPM, UV/vis data and CD spectroscopy in thin films in the LC phases. [5] These results shown and data from the CD 2D mapping of thin films; showing both P and M domains will presented. Overall the investigated systems will be compared with related materials and structure properties relationships will be discussed.

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Multiplexed readout of superconducting qubits with a 3D waveguide

Michele Piscitelli, James Wills, Giulio Campanaro, Shuxiang Cao, Simone Fasciati, Peter Leek

The use of superconducting qubits as sensitive detectors of microwave photons has recently emerged, in particular for application in searches for dark matter candidates [1,2]. The superconducting qubits typically need to be embedded inside high quality microwave cavities to protect them from the electromagnetic environment, limiting detection to a narrow cavity frequency band. Here we explore an approach that utilizes the frequency cutoff of a waveguide to enable a wide range of possible detection frequencies (above cutoff), while maintaining qubit isolation from the environment (below cutoff). We present preliminary work on a proof-of-principle device in which an array of lumped circuit resonators and superconducting qubits are embedded in a 3D microwave waveguide. The lumped resonators with frequencies above the waveguide cutoff (~8 GHz) couple to the waveguide port, which can be employed for multiplexed readout of the device.

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Nonequilibrium non-Markovian steady states in open quantum many-body systems: Persistent oscillations in Heisenberg quantum spin chains

Ms Regina Finsterhoelzl, Mr Manuel Katzer, Mr Alexander Carmele, Andreas Knorr

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter XI, August 25, 2022, 4:30 PM - 6:00 PM

We investigate the effect of a non-Markovian, structured reservoir on an open Heisenberg spin chain by applying coherent time-delayed feedback control to it. The structured reservoir couples frequency-dependent to the spin chain and therefore induces a memory, thus the spin chain interacts partially with its own past. We demonstrate that with this new paradigm of non-Markovian temporal driving scheme, it is possible to generate persistent oscillations within the many-body system and thus induce highly non-trivial states which dynamically store excitation within the chain. These oscillations occur at special points in the stability landscape and persist for different chain lengths and different initial excitations within the chain. We propose a non-invasive partial characterization of the chain by exploiting the fact that the different trapping conditions which arise each relate to specific steady states within the chain.

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Clusters in the real world

Richard Palmer

MC9: Recent Developments in Gas Phase Synthesis of Nanoparticles and Applications XI, August 25, 2022, 4:30 PM - 6:00 PM

Compared with the notional case of an isolated cluster at T=0, as addressed in some foundation theoretical treatments, two factors will shape the behaviour of clusters in the real, that is to say, experimental, world: (i) the radiative environment (including temperature and charged beams) and (ii) the material environment (including pressure, reactive gas and support). We will discuss five examples of the influence of these (coupled) factors; the work is mostly unpublished.

(1) Aberration-corrected electron microscopy at elevated temperature probes the melting and isomeric energy differences of arrays of size-selected gold clusters bound to point defects on a carbon surface (while subject to irradiation by 200keV electrons) [1,2].

(2) Video imaging of a single cluster at room temperature (plus beam heating) under conditions as (1) shows fluctuations between isomers, enabling both equilibrium properties and dynamical behaviour (branching ratios) to be explored.

(3) The case of 1 nm silver clusters (on carbon) stored in vacuum versus exposed to ambient shows dramatic differences in the isomer proportions (fcc dominant versus Ih dominant), probably due to the effect of sulphur contaminants on the structural energetics.

(4) For clusters assembled on the carbon surface from sputtered gold atoms, the transition from 2D to 3D morphology versus size appears to be delayed substantially compared with the free cluster.

(5) Implantation of lead clusters from the scaled-up MACS cluster beam into porous carbon supports provides a means to create an electrode architecture, illustrated by the electrochemical generation of oxidising species for water treatment.

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Quantum Synchronization of Josephson Photonics Devices with Shot Noise

Florian Höhe, Brecht Donvil, Lukas Danner, Ciprian Padurariu, Björn Kubala, Joachim Ankerhold

MC23: Superconducting Circuits for Quantum Technologies VI, August 23, 2022, 4:30 PM - 5:30 PM

Phase stability is an important characteristic of radiation sources. For quantum sources exploitation and characterization of many quantum properties, such as entanglement and squeezing, may be hampered by phase instability. Josephson photonics devices, where microwave radiation is created by inelastic Cooper pair tunneling across a dc-biased Josephson junction connected in-series with a microwave resonator, are particularly vulnerable lacking the reference phase provided by an ac-drive. To counter this issue, sophisticated measurement schemes have been used in [1] to prove entanglement, while in [2] a weak ac-signal was put in to lock phase and frequency of the emission.

The intrinsic shot noise of the Josephson-photonics device inevitably diffuses the oscillators phase and requires an extension of the classical theory [3] describing locking and synchronization to the quantum regime. This description relies on linking the current shot-noise at a residual in-series resistor to the Full Counting Statistics of emitted radiation. Modeling a Josephson-photonics device in that manner, we numerically recover dynamics typical of a self-sustained oscillator with a phase which undergoes diffusion and can synchronize to an external locking signal, see figure.
We perform multi-time scale perturbation theory to derive from this full numerical description an effective Fokker-Plank equation for the phase. This allows us to analyze quantum locking and synchronization in an Adler-type equation. Injection locking and synchronization lead to a strong narrowing of the photon emission statistics, while the shot noise induces phase slips.

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Fabrication and measurement of niobium nanoSQUIDs using focused ion beam lithography for single spin detection

George Long, David Cox, Elias Polychroniou, Jamie Potter, John Gallop, Ling Hao

Quantum technologies and metrology are driving the need for single particle detection across different areas of physics. The detection of a single spin is desired for quantum information processing as well as quantum metrology. NanoSQUIDs are a new manifestation of a well-established but exciting technology which addresses some of these requirements.

By reduction of the SQUID loop dimensions to the nanoscale (nanoSQUID) allows for greatly increased sensitivity to the tiny localised magnetic field associated with a magnetic nanoparticle. In this work we report on niobium nanoSQUIDs utilising nanobridge junctions with SQUID loop dimensions of order ~50 nm. These devices are fabricated using (gallium) focused ion beam lithography, where the nanobridge weak link constrictions as well as the nanoscale SQUID loop is defined in a single step process.

We present measurement results characterising the performance of our nanoSQUID devices, including their current-voltage relation, magnetic field dependence and demonstrate their noise performance using a SQUID series array amplifier to give estimates of the spin sensitivity.

Acknowledgment: This work was supported by the UK National Measurement System and Imperial College London PhD studentship.

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Electrical glassy effects in disordered insulators: current experimental situation

Julien Delahaye, Thierry Grenet

MC40: Strongly Disordered Insulators VIII, August 24, 2022, 4:30 PM - 6:00 PM

Earliest evidence of electrical glassy effects in disordered insulators were reported more than 30 years ago. In 1991, Zvi Ovadyahu and co-workers described for the first time in insulating indium-oxide films around 4K what they called an “anomalous” field effect. It became clear later that this “anomalous” field effect was indeed an out of equilibrium property, which reflects the practical impossibility for the films to equilibrate at low temperature. Since then, similar electrical glassy features have been observed in disordered insulating systems as diverse as amorphous, microcrystalline and granular thin films. Simultaneously, the explanations based on the existence of an electron glass, i.e. a glassy state of the electrons induced by the coexistence of disorder and ill-screened interactions, have strengthened over time.

During this presentation, we will give a review of the current experimental situation. We will begin by recalling what are the hallmarks of these electrical glassy features. Then, we will discuss some striking properties which have so far not received a satisfactory explanation, such as the temperature dependence of the dynamics and the memory effects observed upon cooling. Last, we will present recent results which show how the glassy features evolve when the temperature is raised up to 300K and when the films are brought close to the insulating-metal or insulating-superconducting transition.

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Organic molecular doping of single and bilayer graphene: Band engineering and THz Physics

David Carey, A Samuels, M Dashti

MC52: Heterostructures, Combining Organic Molecules and 2D Materials VI, August 23, 2022, 4:30 PM - 6:00 PM

Graphene's electrical and mechanical properties are attractive for lightweight, flexible, and conformal electronic devices and its tunable electrical, optoelectronic, and plasmonic characteristics allow for operation at microwave, terahertz, infrared, or optical frequencies. In particular, next generation device-to-device communication systems will employ THz frequency bands capable of transferring large amounts of data, however, current THz technology is limited by the upper limits of device cut-off frequencies. In this study we explore the GHz and THz properties of graphene via molecule doping to engineer the intra- and interband contributions to the dynamical conductivity. For example, n-type doping of graphene is achieved using cobaltocene and tetrathiafulvalene (TTF) with a calculated charge transfer of 0.41 and 0.24 electrons donated per adsorbed molecule, respectively. We show organic and organometallic molecules can efficiently dope graphene to carrier densities in excess of 10^13 cm−2 with conductivities at gigahertz frequencies in excess of 60 mS. Calculation of the high-frequency conductivity shows dispersion-less behaviour of the real component of the conductivity over a wide range of gigahertz frequencies. Potential high-frequency applications in graphene antennas and communications that can exploit these properties are discussed.

The ability to induce an energy band gap in AB stacked bilayer graphene is important, here we report the emergence of permanent electronic and optical band gaps in bilayer graphene upon adsorption of organic π electron containing molecules due to an asymmetric charge distribution between the top and bottom layers. The resultant band gap scales linearly with induced carrier density though a slight asymmetry is found between n-type dopants, where the band gap varies as 47 meV/10^13 cm-2, and p-type dopants where it varies as 40 meV/10^13 cm-2. Decamethylcobaltocene (DMC, n-type) and 3,6-difluoro-2,5,7,7,8,8-hexacyanoquinodimethane (F2-HCNQ, p-type) are found to be the best molecules at inducing the largest electronic band gaps up to 0.15 eV. Comparison is made between the band gaps calculated from adsorbate-induced electric fields and from average displacement fields found in dual gate bilayer graphene devices. Non-Pauli blocked optical adsorption transitions in the 2.8-4 μm region can result. A key advantage of using molecular adsorption with π electron containing molecules is that the high binding energy can induce a permanent band gap and open up possible uses of bilayer graphene in mid-infrared photonic or electronic device applications. The broader impacts of these studies show how molecular doping can advantageously modify 2D van der Waals materials for a wide range of applications.

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Using an active patterned shell model to understand the mechanics of sea urchin gastrulation

Nicolas Cuny, Barthélémy Delorme, Grégoire Malandain, Jenifer Croce, Matteo Rauzi, Guillaume Salbreux

MC3: Tissue Dynamics: From in Vivo Experiments to in Silico Modelling IX, August 25, 2022, 11:30 AM - 12:30 PM

The sea urchin is one ideal model system to study embryo gastrulation and tubulogenesis in living systems. At early stage of embryonic development the sea urchin blastula undergoes an inward folding of its epithelium at the vegetal pole (cf attached image showing cross-section of sea urchin P. lividus embryo at different stages of the gastrulation). This inpocketing deepens with time until reaching the opposite pole of the embryo (the animal pole), resulting in a tubular epithelium that will constitute the primordial gut of the future sea urchin larva. It has been shown that a ring of cells apically constricted in an isotropic way around a group of quiescent cells at the vegetal pole play an important role in the initiation of the invagination [1]. Recently, we also observed that a ring of cells surrounding the apically constricted ones exhibits orientational order of cell junctions with circumferential junction cables that seem to play a role in the invagination deepening. Micropipetting experiments also revealed that tension on the basal side of the epithelium is much lower than on the apical side, giving rise to bending moments on the epithelium.

In this work, we use a recently developed active shell model [2] to modelize the sea urchin epithelium during the gastrulation process. In this model, the epithelium is reduced to one infinitely thin surface behaving as an active viscoelastic fluid. Cells activity generate tensions but also active torques accounting for tension difference between apical and basal sides. Those active tensions and torques can be either isotropic or anisotropic, in which case they orientate through a nematic tensor field deriving from a Frank-Landau-de Gennes energy. Numerical simulations of this active patterned shell model in an axisymmetric formulation starting from a sphere with one ring of active isotropic tensions and torques accounting for the apically constricted cell region surrounded by another ring of active anisotropic tensions and torques representing the circumferential junction cable zone allow us to reproduce the gastrulation process observed in sea urchin. This model help us sheding light on the role of each active region in the inward folding process. In particular, we highlight the importance of active torques generated by the difference of tensions between basal and apical side for allowing inward folding of the epithelium. Moreover, our model allows us to study the influence of various parameters like, for example, the respective size of the active regions or the magnitude of tensions and torques in each region on the shape and the dynamics of the invagination.

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Optimization of the hysteresis effect in Nb superconductor open nanotubes

Igor Bogush, Prof. Vladimir M. Fomin

MC13: Topological and Geometrical Effects in Complex Nanostructures II, August 22, 2022, 2:00 PM - 4:00 PM

Superconductor nanoarchitectures, including self-rolled films, are highly promising for advancements in nano- and meso-scale magnetic sensors, superconductor qubits, spintronics devices, and single-photon detectors. It is a challenging technical problem, to create an arbitrary profile of a magnetic field applied to a flat film. To get around this problem, one gives a complex shape to films by bending a flat film into a curved surface. We consider the Nb superconductor open nanotube under a strong subcritical transport current and external homogeneous magnetic field. The operating state of the nanotube can include two types of topological defects: vortices and phase slips. The regime with a phase slip generates a higher resistivity of the tube than that with a vortex pattern [1]. We have found the dependence of the final superconducting state on the way how the transport current and/or magnetic field is switched on [2]. This implies a memory effect in open superconductor nanotubes. As a result, the hysteresis effect in current–voltage characteristics is found numerically using the time-dependent Ginzburg-Landau equation [2]. The hysteresis effect occurs due to the existence of an energy barrier between vortex-pattern and phase-slip regimes in some window of the external parameters (transport current and magnetic field). We have studied the dynamics of the order parameter in the course of state transitions in such hysteresis loops. Besides, we have investigated the characteristics of the hysteresis loops (width, height, and area) as a function of the external magnetic field. For higher magnetic fields, the loop is wider along the transport current axis, but shorter along the voltage axis. The area of the loop possesses a maximum for a certain value of the magnetic field (Figure). Similar hysteresis effects in current–voltage characteristics are found theoretically and/or experimentally in superconductor nanowires, micro-bridges, mesoscopic superconductor square with attached contacts, and NbN superconductor nanowires. The explanation of the hysteresis effect is attributed to the change of the effective temperature of quasiparticles due to the Joule heating, a finite relaxation time of the order-parameter magnitude, or the coupling of the order-parameter dynamics with the heat equation. In the case of the open nanotube, the hysteresis effect appears at a constant temperature owing to the energy barrier. The present work has been partly supported by the DFG project #FO 956/6-1 and by the COST Action CA16218 (NANOCOHYBRI) of the European Cooperation in Science and Technology.

Figure: Hysteresis loop area as a function of the external magnetic field for different values of the nanotube radius. Upper inset: voltage as a function of the transport current density for different values of the magnetic field for increasing (left) and decreasing (right) current. Lower inset: vortex and phase-slip patterns of the order parameter, providing lower and upper branches of the hysteresis loop correspondingly.

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Topology effects on the acoustic phonon spectra in nanostructures

Igor Bogush

MC13: Topological and Geometrical Effects in Complex Nanostructures II, August 22, 2022, 2:00 PM - 4:00 PM

The effects of nontrivial geometry and topology of nanostructures are highly promising to make use of the diversified properties of quantum and classical fields in modern nanophysics. The nontrivial geometry introduces effects at the local level, modifying dynamics due to, e.g., the presence of curvature or a nontrivial vector projection onto the tangent or normal direction with respect to the surface. On the other hand, the nontrivial topology takes into account the shape of the nanostructure as a whole, leading to new quantization rules of the continuous fields. However, it is not always evident, whether the effect is attributed to the geometrical or topological one. We focus on the phonon dynamics in three-dimensional nanostructures with one-dimensional translational symmetry and different topologies of the two-dimensional cross-section. Also, we reduce the result to two-dimensional thin films. Such topologies include a rectangle with boundaries, a ring with a boundary, a Möbius ring with a boundary, a Klein bottle, and a sphere, where boundaries can be either free or fixed. Though some of the topologies are not physical, they shed light on the topological effects or represent an ideal approximation. We demonstrate and compare the energy dispersion and average velocity of the acoustic phonons for different topologies at low temperatures, where quantization effects are pronounced. We use the continuous elastodynamic model which gives a good approximation at small wave vectors and low temperatures. This provides us an important tool for the optimization of thermal properties of nanostructures, which is important for an efficient way to remove and dissipate the heat or the thermoelectric effect. The author is grateful to Prof. V.M. Fomin for helpful suggestions and discussions.

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Adhesion percolation controls the deformation of biomimetic emulsion packings

Lorraine Montel, Iaroslava Golovkova, Silvia Grigolon, Élie Wandersman, Alexis M. Prevost, Thibault Bertrand, Léa-Lætitia Pontani

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Adhesion plays a central role in the mechanical properties of tissues, ensuring its cohesion and transmitting forces. We use a biomimetic emulsion, in which the droplets are functionnalized with adhesive binders, as a model for tissues. Oil droplets are functionnalized with either biotinylated lipids and streptavidins, or complementary DNA sequences. In this system, we can tune the binding energy and the fraction of adhesive contacts in static packed monolayers of droplets. We show that, as the packing fraction increases, adhesion prevents local hexagonal order by preventing droplet rearrangements. Conversely, below jamming, adhesive emulsions retain more connectivity than repulsive ones.
As we increase the fraction of adhesive contacts, we measure a consistent increase in droplet deformation, with a sharp increase at all densities above a threshold of 40 % of adhesive contacts. Moreover, we observe that the deformation is increased similarly for all the droplets in the packing, irrespective of their local amount of adhesive contacts. We show that the threshold corresponds to the percolation of our adhesive network of contacts, mechanically connecting all droplets of the packing and distributing the deformation. For biological tissues, it implies that tuning the adhesion of a part of the cell population could have global consequences on its mechanical properties.

Legend of the image : Confocal images of adhesive droplets monolayers. Droplets are functionnalized with complementary DNA sequences in red and blue. Yellow lines connect adhesive complementary droplets. Below percolation, adhesive droplets are connected in small independent clusters (A). Above percolation, all the droplets are connected in a giant cluster (B).

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Towards the Heisenberg limit in microwave photon detection by a qubit array

Dr Patrick Navez, Dr Alexander Balanov, Prof Sergey Savel'ev, Dr Alexandre Zagoskin

MC28: Condensed-matter Quantum Technology on the Hunt for Dark Matter II, August 22, 2022, 2:00 PM - 3:30 PM

Using an analytically solvable model, we show that a qubit array-based detector allows to achieve the fundamental Heisenberg limit in detecting single photons. In case of superconducting qubits, this opens new opportunities for quantum sensing and communications in the important microwave range.

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Supercurrent noise in short ballistic graphene Josephson junctions

Francesco. M. D. Pellegrino, Giuseppe Falci, Prof. Elisabetta Paladino

MC23: Superconducting Circuits for Quantum Technologies III, August 22, 2022, 4:30 PM - 6:00 PM

Short ballistic graphene Josephson junctions sustain superconducting current with a non-sinusoidal current-phase relation up to a critical current threshold. The current-phase relation, arising from proximitized superconductivity, is gate-voltage tunable and exhibits peculiar skewness observed in high quality graphene super-conductors heterostructures with clean interfaces. These properties make graphene Josephson junctions promising sensitive quantum probes of microscopic fluctuations underlying transport in two-dimensions. Understanding material-inherent microscopic noise sources possibly limiting the phase-coherent behavior of GJJ-based quantum circuits represents an essential, still unexplored, prerequisite. An especially relevant issue is understanding the impact on ballistic GJJs of fluctuations responsible for current noise with 1/f power spectrum [1], which is observed in a variety of graphene devices [2]
In this presentation we first demonstrate that fluctuations with 1/f power spectrum of the critical current of a short ballistic GJJ directly probe carrier density fluctuations of the graphene channel induced by the presence of charge traps in the nearby substrate, modeled by a spatially uniform distribution of independent generation–recombination centers [3]. Tunability with the Fermi level, close to and far from the charge neutrality point, and temperature dependence of the noise amplitude are clear fingerprints of the underlying material-inherent processes. Secondly, we study the effect of a dilute homogeneous spatial distribution of non-magnetic impurities on the equilibrium supercurrent within the Dirac-Bogoliubov-de Gennes approach and modeling impurities by the Anderson model. We find a modification of the current-phase relation with a reduction of the skewness induced by disorder, and a nonmonotonic temperature dependence of the critical current. The potentialities of the supercurrent power spectrum for accurate spectroscopy of the hybridized Andreev bound states-impurities spectrum are highlighted. In the low temperature limit, the supercurrent zero frequency thermal noise directly probes the spectral function at the Fermi energy [4]. Our results suggest a roadmap for the analysis of decoherence sources in the implementation of coherent devices by hybrid nanostructures.

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Gas-Phase Synthesis of Nanoparticles: a Unique Technique for Nanomagnetism

Prof. Jose A. De Toro, Peter Normile, Raúl López Martín, Benito Santos Burgos, Josep Nogués, Chris Binns

MC9: Recent Developments in Gas Phase Synthesis of Nanoparticles and Applications X, August 25, 2022, 2:00 PM - 3:30 PM

I will present a small collection of results on the magnetism of granular thin films prepared by co-depositing gas-phase nanoparticles (from a sputtering cluster source) with a sputtered matrix, highlighting the particle-matrix interactions and giving some examples on how to exploit them to enhance the magnetic properties. These include: (i) the creation of an artificial antiferromagnet by proximity effects between CoO and NiO, with both high anisotropy and Néel temperature, thus able to stabilize through exchange coupling the magnetic moment of small Co particles beyond room temperature [1], and (ii) the optimization of exchange bias by lattice matching between the particle oxide shell (CoO) and a copper oxide matrix [2]. The advantages of gas-phase synthesis for the nanomagnetism community will be underlined, including those enabling ongoing efforts to increase the saturation magnetization further beyond the Slater-Pauling limit [3]. Finally, now from a purely synthetic perspective, a simple method to prepare highly coherent nanostripes (≃ 200 nm) of nanoparticles (≃ 5 nm), magnetic or not, will be presented [4].

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3. The behaviour of nanostructured magnetic materials produced by depositing gas-phase nanoparticles. C. Binns et al, J. Phys D: Appl. Phys. 38, R357 (2005).

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Theory of transport between superconducting states bound to magnetic impurities

Ciprian Padurariu, Haonan Huang, Björn Kubala, Christian R. Ast, Joachim Ankerhold

MC21: Bound States in Hybrid Superconductor Nanostructures III, August 22, 2022, 4:30 PM - 6:00 PM

The realization of the Majorana chain [1], a 1D-chain of Yu-Shiba-Rusinov (YSR) states, superconducting states bound to magnetic impurities, suggests that Majorana states emerging at the edges can be probed by the superconducting tunnelling microscope (STM).

Recently, we have developed an ideal tool to probe and manipulate the edge states of a Majorana chain. It consists of a superconducting STM tip with its own in-gap YSR state created by a magnetic impurity on the tip. With this device we have studied the sharp resonant transport between the YSR state on the tip and another YSR on the sample, and have developed its theory [2].

This presentation will summarize and expand on the theory of YSR-YSR tunnelling by discussing phenomena present when one YSR state occurs close to zero energy, near its quantum phase transition. If the zero-energy state is, in addition, at the edge of a Majorana impurity chain, theory predicts that the topological edge state will transfer from the chain to the tip. This may provide a first step towards realizing braiding of edge states using the STM.

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Coupling between Surface Acoustic Waves and Spin Waves in Uniform or Patterned Magnetic Films

Jarosław W. Kłos, Grzegorz Centała

MC45: Interfaces Between Magnonics and Phononics IV, August 23, 2022, 11:30 AM - 12:30 PM

The simplest structure in which the magnetoelastic coupling between spin waves (SWs) and surface acoustic waves (SAWs) can be observed is the magnetostrictive layer deposited on the non-magnetic substrate. The surface localization of SAW ensures the co-existence of both kinds of waves in the magnetostrictive layer. The strength of the magnetoelastic interaction depends on the direction of the static magnetic field. Moreover, this interaction is different for different types of SAWs, specifically, Rayleigh-SAWs (R-SAW) and Love-SAWs (L-SAW). Thus, the coupling is strongly anisotropic and cannot be observed for arbitrary selected SAWs and SWs, even if their frequencies and wave vectors match. This effect is well-known and broadly discussed in the literature [1]. Our study shows an additional factor limiting the interaction between SAWs and SWs. The SAW/SW coupling proves to require an appropriate profile of the elastic wave near the surface of the magnetostrictive structure, at distances much smaller than the wavelength. For R-SAWs the tangential component of displacement can have nodes within the magnetic layer, resulting in a reduction of the net strength of magnetoelastic interaction even if the related strain is locally significant, whereas for L-SAW the displacement does not have any nodes (changes monotonously in the normal direction). We have shown [2] that this additional factor plays a role for some types of surface acoustic waves (R-SAWs), while other types (L-SAWs) are insensitive to it.

We extended our work and considered the impact of the patterning on magnetoelastic interactions. We calculated the magnetoelastic dispersion relation for an array stripes (of the width 200 nm or 100 nm) differing in saturation but identical in terms of elastic properties. Such structure can be potentially fabricated from the CoFeb/Au by ion implantation in the selected strip areas. We found that (i) the higher SAW dispersion branches, folded into 1st BZ, are exhibited only due to the magnetoelastic interactions, (ii) the partial confinement of SWs within the stripes and non-uniform changes of SWs' phase affect their coupling with freely propagateing SAWs.

We studied CoFeB/Au multilayer as a magnetostrictive medium deposited on Si substrate. In CoFeB layers (2.1 nm) the magnetization is oriented in-plane and the presence of Au layers (0.9 nm) reduces the SWs' frequencies due to out-of-plane anisotropy.

We measured the dispersion relations of thermally excited SAWs and magnetostatic SWs in non-patterned multilayer using a six-pass tandem Brillouin spectrometer. The finite element method (COMSOL Multiphysics) was used to solve numerically the coupled equations of motion for magnetization and mechanic displacement both for uniform and patterned multilayer.

The authors would like to acknowledge the support from the National Science Center – Poland (grants No. 2020/39/O/ST5/02110, and 2016/21/B/ST3/00452)

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Negative Spin Cross-Correlation in a Cooper Pair Splitter

Christian Schönenberger, Arunav Bordoloi, Andreas Baumgartner, Valentina Zannier, Lucia Sorba

MC21: Bound States in Hybrid Superconductor Nanostructures II, August 22, 2022, 2:00 PM - 3:30 PM

The control and measurement of the spin degree of freedom of solid-state electrons has a wide range of prospective applications, be it in spintronics logic devices or in fundamental research, for example to demonstrate spin correlations in quantum mechanical systems. To this end, we have introduced ferromagnetic split-gates (FSGs) to individually polarize the electron spins in semiconductor quantum dots (QDs) [1]. We first demonstrate the working principle of such electronic spin filters in a double QD spin valve [2], consisting of two individually polarized, weakly coupled QDs in series, showing spin polarization up to 80%. We then implement such spin filters in a Cooper pair splitting (CPS) device [3] with two FSG/QD elements coupled in parallel to a superconducting reservoir to demonstrate a negative correlation between the spin currents emitted from the 'splitting' of spin-singlet Cooper pairs. We measure a strong negative spin correlation of -1/3, which deviates from the ideal value of -1 mainly due to the finite spin polarization of the QD states [4]. Such QD spin filters are suitable for various applications, for example in spin projection experiments investigating spin structures in Rashba nanowires [5], or, in equal spin Andreev reflection [6] at Majorana-type bound states.

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AC Josephson effect in higher-order topological insulator WTe2

Christian Schönenberger, Artem Kononov, Martin Endres, Fabian Oppliger, Roy Haller, Hashita S. Arachchige, Jiaqiang Yan, David Mandrus, Kenji Watanabe, Takashi Taniguchi

MC12: Physics in 2D Nanoarchitectonics IV, August 23, 2022, 11:30 AM - 12:30 PM

WTe2 is a layered transitional metal dichalcogenide, known for its topological properties. In the form of a monolayer it is a 2D topological insulator and as a bulk material it is a type-II Weyl semimetal. Recently, another topological phase in WTe2 has been predicted. The new phase is a higher-order topological insulator with helical hinge states. The evidence of such 1D states along certain crystallographic directions in thin WTe2 has been obtained in a number of experiments employing Josephson junctions.
Here, we study the AC Josephson effect in the few-layer thick WTe2. Our measurements indicate a strong contribution of the multi Cooper pair tunnelling events to the supercurrent. This observation suggests non-sinusoidal current-phase relation of the studied Josephson junctions due to the presence of superconducting modes with high transparency. We connect these modes with the hinge states in WTe2.

We acknowledge support by the Georg H. Endress foundation, the European Research Council project Top-Supra (787414), the Swiss National Science Foundation (SNSF) project 200020B_192027 and project NCCR-QSIT and the Swiss Nanoscience Institute (SNI).

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Measurements on a Localized Anderson Chain

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Prof. Yuval Gefen, Paul Popperl, Dr. Sthitadhi Roy, Pd Igor Gornyi

MC40: Strongly Disordered Insulators V, August 23, 2022, 2:00 PM - 3:30 PM

We study the dynamics of a monitored single particle in a one-dimensional, Anderson-localized system. The time evolution comprises a hybrid of Hamiltonian dynamics interspaced with by local projective measurements. We address measurement readout-averaged quantities, which form a manifestation of the competition between disorder induced localization and measurement induced jumps. Specifically we find that measurements at random positions delocalize the average particle position, resulting in motion akin to classical random walk. Along each individual quantum trajectory the particle remains localized, albeit with a modified localization length. In contrast to measurement induced delocalization, controlled measurementsmay be used to introduce transport in the system and localize the particle at a pre-selected site. In other words, the measurements provide a controlled environment for the particle.

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Shape-Persistent Mesogens and Intrinsic Void – A New Design Tool for Complex Functional Liquid Crystal Materials

Prof. Dr. Matthias Lehmann, Dr Moritz Dechant, Mr Martin Lambov, Mrs Lisa Gerbig, Mrs Katja Noll, Mr Maximilian Baumann

MC8: Complex Phases in Soft Matter I, August 22, 2022, 11:30 AM - 12:30 PM

Unlike metallorganic (MOFs) or covalent organic (COFs) frameworks, liquid crystal materials do not possess porous structures. Nevertheless, liquid crystals are full of defects, in which guest molecules accumulate and either to stabilise or even change the LC structure. Recently, shape-persistent mesogens have been reviewed, which provide intrinsic free space by design.[1] They offer another possibility of structural control by incorporation of guests within the intrinsic free space of their mesogenic scaffold either be physical mixing, supramolecular interaction (H-bond) or by covalent link via spacers. Using this design tool we were able to generate complex LC structures via hydrogen bonding. For example, co-assemblies of two different chromophores side-by-side in one column and donor-acceptor structures of phthalocyanines and fullerenes were realised by triple nanosegregation. Most recently the guests even induced the formation of bicontinous cubic phases.
This contribution will highlight that the new design tool allows a whole new family of soft functional matter to be envisioned with a high level of control on structure and alignment.

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Growth kinetics of cellular aggregation mediated through different kind of interaction mechanisms

Dr. Rumi De, Ms. Debangana Mukhopadhyay

One of the most fundamental aspects of developmental biology is the ability of cells to aggregate and form tissue patterns. Cellular aggregation is a complex process orchestrated by various kinds of interactions depending on its environments. Different interactions give rise to different pathways of cellular rearrangement and the development of specialized tissues. To distinguish the underlying mechanisms, based on a theoretical framework, we investigate the spontaneous emergence of tissue patterns from an ensemble of single cells on a substrate following three leading pathways of cell-cell interactions, namely, direct cell adhesion contacts, matrix mediated mechanical interaction, and chemical signalling. Our analysis shows that the growth kinetics of the aggregation process is distinctly different for each pathway and bears the signature of the specific cell-cell interactions. Interestingly, we find that the average domain size and the mass of the clusters exhibit a power law growth in time under certain interaction mechanisms hitherto unexplored. Further, as observed in experiments, the cluster size distribution can be characterized by stretched exponential functions showing distinct cellular organization processes.

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Consistent evidences of Planckian dissipation in the resistivity, specific heat, and optical conductivity of cuprates

Bastien Michon, Christophe Berthod, Antoine Georges, Dirk van der Marel

MC31: The Physics of Cuprates X, August 25, 2022, 2:00 PM - 3:30 PM

The T-linear resistivity of cuprates in the strange-metal phase has long been associated with non-Fermi liquid behavior, possibly resulting from quantum criticality and Planckian dissipation. The recently observed enhancement of the electronic specific heat at the quantum critical point and its logarithmic divergence at low temperature confirm this picture [1,2]. The optical conductivity is also expected to show signatures of quantum criticality, in the form of power laws and frequency/temperature scaling relations. Such signatures have indeed been observed, but they indicate ``sub-Planckian'' behavior with power-law exponent smaller than unity [3]. We present new optical data for La$_{2-x}$Sr$_x$CuO$_4$ that confirm sub-Planckian power laws in the infrared conductivity. However, these same data show remarkably Planckian frequency/temperature scaling of the scattering rate and effective mass, as well as a logarithmic temperature dependence of the mass. We propose a universal theory for the optical response of Planckian systems, that reconciles these apparently conflicting observations. The theory predicts the observed behaviors and provides a numerically consistent picture of the resistivity, specific heat, and optical conductivity in this material.

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Intramolecular force mapping at room temperature

Timothy Brown, Dr Phil Blowey, Jack Henry, Dr Adam Sweetman

MC18: Developments at the Frontiers of High-resolution Scanning Probe Microscopy I, August 22, 2022, 11:30 AM - 12:30 PM

Non-contact atomic force microscopy (NC-AFM) has yielded enormous progress in our ability to characterise materials at the atomic scale, including the acquisition of dense 3D molecular force fields with intramolecular resolution [1, 2]. To date, intramolecular imaging has almost exclusively been performed at cryogenic temperatures, as the standard CO functionalisation of the metallic tip is only stable at low temperature. In this paper we present the first demonstration of high-resolution three-dimensional force mapping of a single organic molecule at room temperature. The challenges of operating in a room temperature experimental environment are overcome using semiconducting materials to inhibit molecular diffusion and create more robust tip apexes, whilst challenges due to thermal drift are overcome with atom tracking based feedforward correction [3, 4]. Three-dimensional force maps comparable in resolution to those acquired at low temperature are demonstrated, permitting a quantitative interpretation of the adsorption induced changes in the geometry of the molecule.

Figure: (A) Constant height mode image of single NTCDI molecule on Si(111)-(7x7) surface. Image is an average of 19 scans, made possible by continual corrections to the drift compensation. (B), (C) molecular cross sections of the force, measured via grid spectroscopy along the short and long axes respectively. The positions of the cross sections are represented by the dotted lines in (A).

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Casimir Physics: Quantum Metrology and the Casimir Energy

Prof David Bishop, Prof David Campbell

MC19: Advances in the Casimir Force and Heat Transfer Phenomena III, August 22, 2022, 4:30 PM - 6:00 PM

The Casimir Effect is a profound physical phenomenon, theoretically deep and with great technological potential. It arises from the influence of quantum fluctuations on physically measureable, typically nanoscale, objects. It is a direct and clear manifestation of the quantum nature of the universe, whose experimental observations are at odds with a purely classical interpretation. In its simplest form, it predicts an attractive interaction between two identical uncharged, perfectly conducting plates held a short distance apart, usually well less than a micron. Classically, if the plates are electrically uncharged and not magnetic, the only attractive force between them is gravity which produces forces in the 10-8 pN range for typical Micro-Electro-Mechanical System (MEMS) plates, a vanishingly small number. What was predicted theoretically by Casimir in 1948 and has been seen experimentally many times since, is a force in the range of 1-1000 pN when the plates are ~100 nm apart. This is a force solely due to the effects of quantum fluctuations of the vacuum. It is fundamentally a nanoscale phenomenon and understanding and exploiting it holds great technological promise. In our presentation, we will discuss two important application areas, the Casimir energy and Casimir metrology and their potential impact on both science and technology. We believe both hold great promise to provide revolutionary new capabilities and scientific insights.

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Proposal for a nanomechanical qubit

Dr Fabio Pistolesi

MC17: Nanomechanical and Electromechanical Systems VII, August 24, 2022, 2:00 PM - 3:30 PM

Mechanical oscillators have been demonstrated with very high quality factors over a wide range of frequencies. They also couple to a wide variety of fields and forces, making them ideal as sensors. The realization of a mechanically based quantum bit could therefore provide an important new platform for quantum computation and sensing. Here, we show that by coupling one of the flexural modes of a suspended carbon nanotube to the charge states of a double quantum dot defined in the nanotube, it is possible to induce sufficient anharmonicity in the mechanical oscillator so that the coupled system can be used as a mechanical quantum bit. However, these results can only be achieved when the device enters the ultrastrong coupling regime. We discuss the conditions for the anharmonicity to appear, and we show that the Hamiltonian can be mapped onto an anharmonic oscillator, allowing us to work out the energy level structure and find how decoherence from the quantum dot and the mechanical oscillator is inherited by the qubit. Remarkably, the dephasing due to the quantum dot is expected to be reduced by several orders of magnitude in the coupled system. We outline qubit control, readout protocols, the realization of a CNOT gate by coupling two qubits to a microwave cavity, and finally how the qubit can be used as a static-force quantum sensor.

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Nonequilibrium spintronic transport through Kondo impurities

Mr Anand Manaparambil, Dr. habil. Andreas Weichselbaum, Dr. habil. Jan von Delft, Dr. habil. Ireneusz Weymann

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter XIII, August 26, 2022, 10:00 AM - 11:00 AM

Spin and electronic transport through Kondo impurities under equilibrium conditions can be well described using the numerical renormalization group. This method is not directly applicable, though, for describing non-equilibrium transport through such Kondo impurities while treating the correlations exactly. We implement a recently-developed hybrid technique combining the Numerical Renormalization Group (NRG) and time-dependent Density Matrix Renormalization Group (tDMRG) methods in a thermofield quench framework.

In particular, we theoretically investigate the electronic transport through a quantum dot coupled to ferromagnetic leads under finite potential bias conditions. The behavior of the zero-bias conductance peak - exhibited by Kondo impurity systems - has been thoroughly studied against the influence of spin polarization on the leads and other external parameters. We observe a characteristic reduction in the Kondo energy scale when the impurity orbital level is at the particle-hole symmetry point, and a suppression of the zero-bias conductance due to the emergence of an exchange field when the impurity is tuned out of the particle-hole symmetry point. We further analyze the behavior of the split-Kondo peak - formed when exchange field is greater than the Kondo energy scale - against external parameters, such as magnetic field and temperature. Our work provides quantitatively accurate results for nonequilibrium behavior of quantum dot spin valves that may serve as a benchmark for future theoretical and experimental research.

This work was supported by the Polish National Science Centre from funds awarded through the decision No.2017/27/B/ST3/00621.

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New Examples of Ferronematic Materials Showing Evidence for the Antiferroelectric Smectic-Z Phase

Mr. Pierre Nacke, Atsutaka Manabe, Melanie Klasen-Memmer, Xi Chen, Vikina Martinez, Eva Korblova, Guillaume Freychet, Mikhail Zhernenkov, Matthew A. Glaser, Joseph E. Maclennan, David M. Walba, Matthias Bremer, Frank Giesselmann

MC8: Complex Phases in Soft Matter II, August 22, 2022, 2:00 PM - 3:30 PM

The recent discovery of the ferroelectric nematic phase (NF) [1, 2] opens completely new perspectives in the science and applications of liquid crystals. In this contribution we report a detailed investigation into new NF-type materials, namely AUUQU-2-N and its higher homologues (Fig. 1a). In AUUQU-2-N for instance the two nematic phases – dielectric N at higher temperatures and ferroelectric NF at lower temperatures – are separated from each other by another phase, which clearly shows antiferroelectric response to external electric fields in polarization reversal measurements (Fig. 1b) as well as in dielectric spectroscopy. Interestingly, however, these intermediate phases also show characteristic zig-zag defects (Fig. 1c) that indicate the presence of a layered (or at least modulated [3]) structure, as in common smectics. All in all, these observations suggest that the intermediate phases in the AUUQU−n−N series are new examples of the recently proposed antiferroelectric smectic Z-phase (SmZA) phase [4].

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A new form of ergodicity breaking from quantum many-body scars

Maksym Serbyn, Zlatko Papic, Dmitry Abanin

MC42: Broken Ergodicity and Localisation in Quantum Many-body Systems VI, August 23, 2022, 4:15 PM - 5:30 PM

In my talk I will review a new mechanism of the weak ergodicity breaking relevant for the experimentally realized Rydberg-atom quantum simulator [1]. This mechanism arises from the presence of special eigenstates in the many-body spectrum that are reminiscent of quantum scars in chaotic non-interacting systems [2]. In the single-particle case, quantum scars correspond to wave functions concentrated in the vicinity of unstable periodic classical trajectories. I will demonstrate that many-body scars appear in the Fibonacci chain, a model with a constrained local Hilbert space which can be realized by a Rydberg chain. The quantum scarred eigenstates are embedded throughout the otherwise thermalizing many-body spectrum but lead to direct experimental signatures, as I show for periodic recurrences that reproduce those observed in the experiment [1]. Using algebraic approach, I will construct the weak deformation of the Rydberg chain Hamiltonian that makes revivals virtually perfect [3]. In a different direction, using variational approach I will predict new initial states that lead to long-lived oscillations. I will conclude with discussing a new opportunities for the creation of novel states with long-lived coherence in systems that are now experimentally realizable [4] and a brief overview of the recent experiments [5] that uncovered surprising interplay between scars and and time crystalline physics [6].
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Weak anisotropy of band gap modulation using uniaxial strain in MoS2

Alex Armstrong

Strain in nanomaterials is often a useful parameter to examine, especially for light emitting materials due to its potential to modify band gap and photoluminescence efficiency. Although strain
is known to reduce the band gap in monolayer transition metal dichalcogenides such as MoS2, the effect of strain direction has not yet been fully investigated. The variation of band gap with strain in few-layer systems is also yet to be systematically studied. Here, density functional theory is used to investigate the effects of uniaxial strain on monolayer MoS2 as well as the effect of biaxial strain in monolayer and few-layer systems. For monolayer MoS2 the linear band gap variation is found to only weakly depend on the direction of applied strain. The direct band gap gradient with respect to strain varies by only 4.6 meV/% (from -52.7±0.6 meV/% to -57.3±0.1 meV/%) for strain applied along the armchair and zigzag directions respectively. These gradients are also shown to decrease when biaxial strain is applied to an increasing number of layers. These findings should be directly applicable to the other hexagonal-shaped Van der Waals-bonded transition metal dichalcogenides.

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Understanding Wet Impregnation Synthesis for Sustainable Hydrogenation Catalysts via In-situ TEM Observation

Rongsheng Cai, Lifeng Xiao, Meenakshisundaram Sankar, James Paterson, Sarah Haigh

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Wet impregnation method is the most common way to synthesize commercial heterogeneous catalysts, especially on oxide supports. However, many questions remain about the mechanism of the catalyst formation process and how this depends on interactions between metal to metal and metal to support. Recently it was found that the addition of excess Cl- ions to the metal precursors dramatically influence the particle size, distribution and composition of PdAu nanoparticles supported on titania1, a good catalyst system for aerobic oxidation of alcohols and hydrogenation/hydrogenolysis of bioderived feedstock, although the mechanism remains unknown. Therefore, understanding this behaviour could open the door to new multi-metallic nanoparticle materials, with control of size, shape and composition, providing the industrial catalysts needed to address the current energy emergency. Scanning transmission electron microscopy (STEM) imaging was employed to investigate the size and elemental distribution of wet impregnated PdAu catalysts synthesized with different salt concentrations and reduced for different times (0-12 hrs). We found that for the samples synthesized with HCl as the promoter, the particle size decreases with the reduction time whereas for the samples synthesized without promoters, the particle size does not change significantly. Combined the in-situ STEM experiments with theoretical calculations on metal to metal and metal to support interactions, the role that the excess Cl- ions play in the nanoparticle growth was investigated. This suggests the addition of excess HCl to the precursors can slow down the diffusion of the metal ions on the support during the reduction, due to a strong interaction with HCl modified TiO2. Therefore, newly formed smaller particles shift the particle size distribution.

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Mobility, quantum efficiency and defect density from multi-modal spectroscopy of surface-guided strained CsPbBr3 microstructures

Stephen Church, Hoyeon Choi, Nawal Al-Amairi, Ruqaiya Al-Abri, Ella Sanders, Eitan Oksenberg, Ernesto Joselevich, Patrick Parkinson

MC48: Multi-modal Characterisation of Thin Film Optoelectronics for Energy Applications V, August 23, 2022, 2:00 PM - 3:30 PM

Surface guided in-plane CsPbBr3 microwires (MWs) are promising structures for nano-photonic applications, showing good waveguiding [4] and luminescence properties [3] as well as demonstrating lasing at elevated carrier densities [5]. These MWs exhibit strong strain fields originating from the heterointerface [6]: it is crucial to understand how this impacts the optoelectronic behaviour of the MWs in order to facilitate the design of optimised devices. However, it is challenging to investigate these effects experimentally due to inter and intra-MW variation in the structural and material properties that modifies functional performance [1].

In this study, we tackle this problem by adopting a data-led experimental approach that uses a bespoke optical microscope to automatically identify, locate and characterise >10,000 individual points using a suite of experimental techniques. This multi-modal approach uses machine vision imaging, to find the structure dimensions, room temperature photoluminescence spectroscopy, to assess the MW bandgap and disorder, and time correlated single photon counting to find the carrier lifetimes. To isolate the impact of the heterointerfaces, these measurements were performed on the same set of MWs whilst exciting carriers at the air/MW interface and the substrate/MW interface. This methodology generates a multidimensional dataset consisting of 15,576 individual measurements that, when analysed, provide a holistic picture of this emerging material.

To draw conclusions from this dataset, the carrier dynamics were assessed using a carrier recombination model, combined with a machine learning model that had been trained on Monte-Carlo carrier diffusion simulations. This model demonstrates that non-radiative recombination at the surface is the dominant recombination pathway and that the MW width is the key parameter in determining the recombination behaviour. Additionally, we observe a blueshift in the bandgap, both with increasing distance from the heterointerface and with reducing MW width: a consequence of tensile strain and lattice deformation effects [6]. This model, when applied to the large volume of experimental data, provides a comprehensive view of information about the growth, and can simultaneously determine values for the diffusion length, carrier mobility, trap densities and internal quantum efficiency (IQE). These values are compatible with those from small-scale studies in the literature, and the IQE was verified independently using temperature dependent PL. Importantly, the model requires minimal a-priori knowledge and can therefore be applied to other material ensembles in a statistically rigorous way, including those which have not been previously studied.

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NEAR-FIELD RADIATIVE HEAT TRANSFER ENHANCEMENT VIA EXTERNAL MAGNETIC FIELDS

Dr. Shunashi Guadalupe Castillo Lopez, Alonso Marquez Hernandez, Dr. Raul Esquivel-Sirvent

MC19: Advances in the Casimir Force and Heat Transfer Phenomena VI, August 23, 2022, 4:30 PM - 6:00 PM

NEAR-FIELD RADIATIVE HEAT TRANSFER ENHANCEMENT VIA EXTERNAL MAGNETIC FIELDS

We show that the radiative heat transfer between a flat SiC surface and an InSb nanosphere can be increased when we apply an external magnetic field. This happens as we couple the plasmonic resonance of the nanosphere with the polaritonic resonance of the surface, achieving an enhancement of two orders of magnitude compared with the same setting in the absence of an external magnetic field.[1]

Magnetoplasmons have been widely studied in nanoparticles; for instance, nanospheres display an analogous behavior to atoms in an external magnetic field in the presence of external magnetic fields. We can observe a splitting of the resonance into two new modes, where the resonance frequency of these modes shifts as we modify the external magnetic field (Plasmonic Zeeman Effect). [2]

This effect allows us to tune the new plasmonic modes of the nanosphere. By choosing an adequate magnetic field, we can couple one of these with the phonon-polariton frequency of the SiC surface, thus obtaining the enhancement.

This enhancement can be achieved with other combinations of materials, where we can achieve a similar enhancement for different magnetic fields. This depends on the material properties such as the sphere and surface resonant frequency and the effective electron mass of the sphere.

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Geometric tuning of stress in pre-displaced silicon nitride beam resonators

Menno Poot

MC17: Nanomechanical and Electromechanical Systems V, August 23, 2022, 2:00 PM - 3:30 PM

Silicon nitride is a material with high intrinsic stress, enabling mechanical resonators with very high quality factors. This makes SiN the ideal material for optomechanical experiments. Typically, the film stress can only be changed via the deposition process, making the study of stress-dependent properties such as the damping rate very challenging. In this talk, we show that we can control the stress geometrically. Our double-S-shaped beams are designed with a pre-displacement and thus initially longer than the distance between the two clamping points. When releasing them, they straighten and partially relax their stress; how much depends on the design.

First, using scanning electron microscopy, the static shapes before and after release are compared quantitatively, confirming the straightening of the beam. The observed relaxation matches very well with finite-element simulations of the resonators, allowing a quantitative extraction of the final longitudinal stress in our beams. Longer and more pre-displaced beams give a larger geometric tuning of the stress, something that can be understood from the interplay between the curve length, bending rigidity and the potential to buckle.

Next, we use on-chip Mach-Zehnder interferometers to optically sense the driven motion of the resonators and extract the the eigenfrequencies and quality factors for devices with different parameters. This way, the stress dependence of eigenfrequencies and quality factors are obtained.
First of all, a strong dependence of the resonance frequency on the initial displacement and length is observed; this tuning again closely matches our finite-element simulations. We find that for a large range of parameters, the pre-displaced resonators act as strings under - a now geometrically tunable - tension. Interestingly, at low stresses, the ratio between the in- and out-of-plane modes becomes tunable. Also, we find that the quality factor changes with tension and that the damping rate is a better metric. The stress dependence of the dissipation is captured by a semi-analytical model. It builds on previous insights that the curvature of the modal displacement determines the amount of dissipation and uses the mode profile calculated using the Euler-Bernoulli equation with tension included. The intrinsic quality factor is the only free parameter in the model, which describes our data well in the high and intermediate tension limits. Initial measurements seem indicate that the internal damping is different for the in- and out-of-plane modes, which may provide another important clue for the understanding of dissipation in silicon nitride.

Finally, we study the influence of different pre-displacement shapes on the mechanical properties. Overall, our devices not only provide valuable insight in the role of stress in the damping of SiN resonators, but also adds geometrically-tunable stress as a new degree of freedom for a variety of optomechanics experiments, such as synchronization, state transfer, and cooling.

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Hall effect in overdoped cuprates and its link to Fermi surface reconstruction

Antony Carrington

MC31: The Physics of Cuprates IX, August 25, 2022, 11:30 AM - 12:30 PM

In a conventional single-band metal the Hall number n_H measures directly the carrier density. Strong k-space anisotropy in the mean-free path can complicate the interpretation of n_H, but the simple relation to the carrier density is recovered in the high field limit. In YBa_2Cu_3O_6+x (Y123), an apparent transition from n_H=p, to n_H=1+p was observed which was linked to the emergence of the pseudogap regime [1]. Our high field measurement of n_H in the overdoped cuprates Tl_2Ba_2CuO_6+x (Tl-2201) and Bi_2Sr_2CuO_6+x (Bi-2201), show a similar cross-over from p to 1+p but over a much broader range of doping where there is no evidence of a pseudogap [2]. In this regime, we have discovered evidence for a charge density wave (CDW) in Tl-22012, with a remarkably long coherence length (up to 200Å) for p<0.265, which provides a possible explanation for the evolution of the transport properties [3]. In this talk I will review these experiments and show calculations which show the CDW could lead to the observed p->1+p transition in n_H.
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[2] C. Putzke et al, Nature Physics 17, 826 (2021).
[3] C.C. Tam et al, Nature Comms 13, 570 (2022).

220

Confinement-induced columnar crystals: A route to new architecture in the scientific world

Asso. Prof. Ho-kei Chan

MC8: Complex Phases in Soft Matter IV, August 23, 2022, 11:30 AM - 12:30 PM

Identical spheres in cylindrical confinement exhibit a complex variety of densest-packed columnar structures. Such densest-packed structures can serve as theoretical models for the structures of a variety of quasi-one-dimensional physical systems, such as nanotube-confined fullerenes, nanochannel-confined copolymers, colloidal crystal wires, capillary-tube-confined thermoresponsive microspheres, capillary-tube-confined microbubbles, and fluid-driven self-assemblies of polymer beads. On the other hand, there have been comparatively few studies of this kind for shape-anisotropic particles. Thanks to their rotational degrees of freedom, shape-anisotropic particles in cylindrical confinement exhibit densest-packed structures with non-trivial orientational order, and therefore they demonstrate a greater variety of densest-packed crystal structures than their spherical counterparts.

In this talk, I will present a historical overview of research on the densest-packed structures of identical hard spheres in cylindrical confinement [Phys. Rev. Lett. 106, 115704 (2011)], and then present our recent extensions of such research to shape-anisotropic particles [Phys. Rev. Lett. 124, 248002 (2020); Phys. Rev. Research 3, 013053 (2021)]. For packings of spheres, I will introduce a variety of columnar crystals as discovered computationally in the past two decades, and explain how a wide range of such structures can be obtained through a method of sequential deposition [Phys. Rev. E 84, 050302(R) (2011)]. I will also discuss how some ordered but non-densest crystal structures can be discovered through this specific method of sequential deposition. For packings of shape-anisotropic particles, I will present a variety of densest-packed columnar crystals as discovered recently for identical spheroids in cylindrical confinement and for identical ellipses within a parallel strip. For the case of spheroids, I will explain how the corresponding densest-packed structures arise from a competition between confinement-induced chiral ordering and shape-anisotropy-induced orientational ordering. For the case of ellipses, I will explain why the corresponding densest-packed structures are all affine transformations of particular densest-packed structures of circular disks. It is believed that the confinement-induced crystal structures presented in this talk could constitute a basis for the development of novel low-dimensional materials with tailored translational or orientational order.

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Is the tendency for all living systems to do work universal?

Dr Elsen Tjhung

MC3: Tissue Dynamics: From In Vivo Experiments to In Silico Modelling X, August 25, 2022, 2:00 PM - 3:30 PM

Not long ago, it was found that swimming bacteria are able perform a useful macroscopic work. If we look at the trajectories of swimming bacteria, they look completely random with no coherent motion. And yet, as soon as we put an asymmetric rotor inside a bath full of bacteria, the bacteria can somehow rotate the rotor in one direction. In this talk, we will try to establish if this tendency to extract work from all living system is universal by looking at another biological system, which is living tissue. Biological living tissues are continuously regenerated through cellular division and apoptosis (or cell death). I will discuss how we can extract useful work from these division and apoptosis process alone.

Reference:
Mitchell, E. and Tjhung, E., Macroscopic current generated by local division and apoptosis in a minimal model of tissue dynamics, Soft Matter, https://doi.org/10.1039/D1SM00928A (2022)

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High pressure study of CsPbBr3: dynamical and mechanical stability

Prof. Alfonso Muñoz, Dr. Raouia Ben Sadok, Dr. Placida Rodriguez-Hernandez, Dr. Dalila Hammoutène

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

By means of ab initio simulation using Density Functional Theory, we study a new ferroelectric phase transition from the Pnma structure to the P212121 polar structure is predicted under a hydrostatic pressure above 3.6 GPa for CsPbBr3 compound. This phase transition results from the softening of the silent mode Au at the center of the Brillouin zone. The off-center displacement of Pb is dominated relative to that of Cs and Br atoms in this soft mode. Besides, the structural, elastic, and dynamic properties of both structures are reported in the present work. The Pnma structure shows mechanical stability under pressure and a large resistance to unidirectional compression along y-axis comparing to the shear deformation. The application of pressure decreases the ductility and enhances the stiffness of the compound

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Multi-modal Characterisation of Thickness Dependent Small Molecule Thin Films for Effective Orientation Control

Dongkuk Kim, Dr. Daphné Lubert-Perquel, Dr. Jessica Wade, Dr. Rachel Kilbride, Demetris Soukeras, Dr. Sebastian Schneider, Prof. Michael Toney, Prof. Sandrine Heutz

MC48: Multi-modal Characterisation of Thin Film Optoelectronics for Energy Applications VI, August 23, 2022, 4:15 PM - 5:45 PM

Pentacene is an archetypal p-type organic semiconductor well-researched for its high charge carrier mobility and singlet fission properties. Molecular orientation control of small organic molecules has been extensively researched as a means to optimise optoelectronic devices. Pentacene thermodynamically favours a standing herringbone arrangement on non-interacting substrates such as standard metal electrodes and functional organic materials. This preferred orientation severe limits the applicability of pentacene in a broad range of optoelectronic devices, such as photovoltaics, where a flat-lying orientation is desired. Although extensive research has focused on effectively controlling pentacene molecular orientation, limited success has been achieved in producing flat-lying molecules over a long-range order.

In our work, we have effectively controlled the pentacene molecular orientation through the use of copper (I) iodide deposited at elevated temperatures via structural templating. Structural templating is a commonly implemented approach to govern morphology and structure. Through the use of a combination of grazing incidence X-ray diffraction (GIXRD) and Raman spectroscopy, pentacene was found to undergo a structural transition from a standing orientation to a flat-lying orientation with lattice parameters within 1.7 – 3.5% of the indexed herringbone structures. The orientation transition suggests competing intermolecular interactions between the negatively charge copper (I) iodide surface and quadrupolar coupling of the pentacene molecules. The GIXRD findings are supported by Raman spectroscopy in which the long axis C-C mode, indicative of a flat-lying orientation, appears for the templated films.

Further investigation on the functional properties of the templated pentacene was carried out via kelvin probe force microscopy (KPFM) and UV-Vis spectroscopy. The flat-lying arrangement was found to double the absorption as a result of the increased absorption cross-section. A 0.25 eV increase in the work function was also observed in the templated pentacene due to a vacuum level alignment mechanism. Through the combined use of KPFM and UV-Vis spectroscopy, we find this new molecular orientation to provide application opportunities for fission and photovoltaic devices as the copper (I) iodide templating layer also encourages charge transport due to favourable energy alignments.

As a result, we can confirm the use of copper (I) iodide as a templating layer is an effective means to control the molecular packing of small organic molecules for a wide range of optoelectronic devices. The combined use of various characterisation techniques in this work underline the power of multi-modal characterisation to fully understand the changes in orientation of small organic molecules and its effect on functional properties.

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Aharonov-Bohm oscillations on a kagomé network of Lifshitz transition trajectories as a precursor of Brown-Zak fermions in graphene superlattices.

Dr Sergey Slizovskiy, Dr Folkert de Vries, Dr Aitor Garcia-Ruiz, Mr Petar Tomic, Dr Giulia Zheng, Prof. Klaus Ensslin, Prof. Vladimir Fal'ko, Dr Peter Rickhaus

MC50: Fermi Surface Topological Transitions - Effects of Interactions VIII, August 24, 2022, 4:30 PM - 6:00 PM

Brown-Zak magnetic minibands for electrons are common for metals with a rational value of magnetic field flux, φ =φ0 p/q, piercing the unit cell of a crystal. Here, we study how this ultra-quantum phenomenon, usually, attributed to strong magnetic fields emerges at low magnetic fields and moderate temperatures from the interplay between peculiar dynamics and interference of electrons at the fundamental Lifshitz transition (LT), realised using moiré superlattice miniband in twistronic graphene. We show that precursors of Brown-Zak minibands appear in the form of Aharonov-Bohm oscillations of conductivity produced by electrons propagating along entwining paths with a kagomé network topology, Fig.1. We report the observation of coinciding features in the vicinity of LT for both twisted double bilayer graphene and in highly aligned graphene - hexagonal boron nitride heterostructures. In particular, the maximal amplitude of conductance oscillations is located in the vicinity of LT, displacing from the LT by the amount growing linearly in the magnetic field, Fig.2. These findings are naturally explained by the topology of interfering paths, which implies a different number of left and right turns at the saddle-point regions of dispersion.

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First-order quantum breakdown of a bosonic disordered superconductor

Thibault Charpentier, Sébastien Léger, Kazi Rafsanjani Amin, Mikhail Feigel'man, Lev Ioffe, Denis Basko, Olivier Buisson, Thierry Grenet, Nicolas Roch, Benjamin Sacépé

MC40: Strongly Disordered Insulators VI, August 23, 2022, 4:30 PM - 6:00 PM

Strongly disordered superconductors undergo a transition to insulation upon increasing disorder, driven by the localization of preformed Cooper pairs. A key question implicit in this transition is the fate of the superfluid density as the critical disorder approaches. By measuring the kinetic inductance of superconducting resonators of amorphous indium oxide, we show that the transition to superconductivity is bosonic with a critical temperature ruled by superconducting phase fluctuations. Upon reaching the critical disorder terminating superconductivity, the superfluid stiffness remains surprisingly finite at the transition to insulation. This indicates an unexpected first-order nature of the disorder-driven quantum phase transition to insulator, opening a new paradigm for superfluid disordered systems of quantum particles.

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Cryogenic electronics for the QSHS microwave axion search

Deepanjan Das, Patrick Steger, Saba Khan, Scott Henderson, Dr. Edward Laird

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Detecting galactic axions could solve one of the greatest challenges in physics, the identification dark matter. This requires cutting-edge quantum electronics and highly advanced measurement techniques. In a strong magnetic field axions decay into photons resulting an extremely weak electromagnetic signal. To measure such tiny signal, a low noise amplifier and a robust low temperature platform are highly desirable to meet the standard quantum limit.

This poster will describe the cryogenic wiring and noise temperature measurement of a parametric amplifier. We have set up two dry dilution fridges with base temperature below 10 mK. We mounted cryogenic circulators, directional couplers, HEMT amplifiers, microwave filters, a noise source and cryo-attenuators in order to be able to control and measure a sensitive quantum device at GHz frequency. To optimise the sensitivity and therefore maximise the readout fidelity, we have also installed a parametric amplifier from VTT Technical Research Centre of Finland Ltd [1]. One of these fridges is equipped with a vector magnet. We are planning to utilize this low temperature platform to develop electronics for the QSHS axion search experiment currently under construction.

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A local relativistic approach to light scattering through mirrors and optical cavities

Dr Almut Beige

MC25 : Emerging Trends in Many-Body Cavity Quantum Electrodynamics X, August 25, 2022, 2:00 PM - 3:30 PM

The Casimir effect [1, 2], which predicts the emergence of an attractive force between two parallel, highly reflecting plates in vacuum, plays a vital role in various fields of physics, from quantum field theory and cosmology to nanophotonics and condensed matter physics. Nevertheless, Casimir forces still lack an intuitive explanation and current derivations rely on regularisation procedures to remove infinities. Moreover, their standard derivation simply assumes that mirrors restrict the field inside the cavity to standing waves with a discrete set of frequencies. However, standing wave mode models cannot take into account from which direction light enters an optical cavity and therefore cannot reproduce the typical behaviour of Fabry-Perot cavities [3]. Discrete mode models also imply that no light is permitted inside a cavity with mirror distances well below typical optical wavelengths, which contradicts recent nanocavity experiments [4]. An alternative approach is needed.

Starting from special relativity and treating space and time coordinates equivalently, we overcome no-go theorems of quantum electrodynamics and obtain a local relativistic quantum description of the electromagnetic field in free space [5, 6, 7]. When extended to cavities, our approach can be used to calculate Casimir forces directly in position space without the introduction of cut-off frequencies. Our local relativistic description provides additional insight into light scattering by optical mirrors and optical cavities.

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Structural, Electronic and Mechanical Properties of Re
Doped FeMnP 0.67 A 0.33 (A=Ga and Ge): A DFT Study

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Mr Gabriel Chirchir

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Abstract

The structural, electronic and mechanical properties of Re doped FeMnP 0.67 A 0.33 (A= Ga and Ge) were examined by use of density functional theory (DFT) within the generalized gradient approximations as demonstrated
in Quantum ESPRESSO code. The optimized structural parameters as well as derived lattice parameters are in
consistent with other computational and achievable experimental results. The computed independent elastic
constants confirm the mechanical stability of the investigated materials. The computed Poisson's and Pugh's ratios
as well as Cauchy pressure, verify that FeMn 0.67 Re 0.33 P 0.67 Ga 0.33 is the most ductile among the studied compounds.
The calculated values of bulk modulus, shear modulus and Young's modulus confirm high values of bond strength, hardness and stiffness of the investigated materials respectively. Therefore, the four compounds considered may be
appropriate for industrial applications. The results report that FeMn 0.67 Re 0.33 P 0.67 Ga 0.33 compound is more ductile and
mechanically stable compared to other investigated compounds. This is the first qualitative computational prediction
of the elastic properties of FeMnP 0.67 Ge 0.33 , FeMnP 0.67 Ga 0.33 , FeMn 0.67 Re 0.33 P 0.67 Ge 0.33 and FeMn 0.67 Re 0.33 P 0.67 Ga 0.33 compounds and this awaits experimental ratification. The calculated electronic density of states confirms that the Re_2p states are located in the conduction band (CB) in the unite cell while Re_3d dominate the CB in the supercell. Results from the doped compounds could not be compared with experimental or computational findings because to the best of our knowledge, this has not been done.

Keywords : DFT, doping, ductility, electronic density of states, mechanical stability, elastic constants

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Magnon – phonon coupling in magnetostrictive nanostructures

Andrew Rushforth, Alexey Scherbakov, Andrey Akimov, Manfred Bayer

MC45: Interfaces between Magnonics and Phononics V, August 23, 2022, 2:00 PM - 3:30 PM

Coupling excitations in different systems allows scientists and engineers to harness and exploit the beneficial properties of each system and can lead to new ways to investigate fundamental physics. Magnon and phonon modes can be engineered to exist in the low GHz frequency range in nanostructures. Magnons can be tuned by magnetic field and methods exist and are being developed to couple magnons to microwave and optical photons. Phonons can have longer lifetimes than magnons and can be propagated over larger distances, and methods already exist to manipulate and utilise surface acoustic waves in communications technologies. It would be desirable to develop methods to couple magnons and phonons in the same structure. Recent works have reported methods to drive magnons with phonons (and vice versa) and to achieve the strong coupling limit in which the magnon and phonon modes hybridise [1]. Key challenges include the development of materials possessing strong magnetostriction, capable of supporting magnon and phonon modes with long lifetimes, and engineering structures in which the coupling between the magnon and phonon modes is optimised. This presentation will discuss the development of a suitable material system – epitaxial thin layers of galfenol (Fe81Ga19), which possesses favourable properties including strong magnetostriction, large moment and magnetocrystalline anisotropy, and magnon modes with long lifetimes [2]. Our recent experimental progress in developing device concepts for achieving magnetisation precession driven by coherent phonons [3], and hybridisation of magnon and phonon modes [4] will be described.

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Exploring the third dimension in magnonics

Gianluca Gubbiotti

MC44: New Perspectives in Magnonics, from 2D to 3D Systems I, August 22, 2022, 11:30 AM - 12:30 PM

Magnonics, the research field that uses spin waves, the collective excitations of ordered magnetic materials, or magnons (their quanta) as a tool for signal processing, communication, and computation have rapidly grown during the last decade due to the low-energy-consumption property.[1,2]

Magnonics systems investigated up to now are mainly planar systems that can be patterned out of an extended layer that is deposited on a flat substrate.

The interest in 3D magnonic nanostructures follows the latest trend in CMOS electronics based on the expansion from two-dimensional planar to three-dimensional vertically integrated structures. In order to remain at the same technological level, a similar expansion should be realized in magnonics.[3]
3D magnonic systems might offer several advantages over 2D systems, such as permitting more functionality in a smaller space, allowing for a large number of vertical connections between planar layers, or increasing the density of elements for the fabrication of scalable and configurable magnonics.
In this talk, I will review the different strategies to build the next generation of magnonic systems. The first of them is an extension of planar patterned nanostructures, where arrays of patterned magnetic dots or antidots have a layered structure. In this case, the vertical stacking of ferromagnetic materials, placed in direct contact or separated by a non-magnetic spacer, adds new functionality and an additional degree of freedom for controlling the spin-wave band structure.
An alternative approach to physical patterning is based on the use of hybrid heterostructures in the form of bilayer systems. These include metal-insulator, metal-heavy metal, metal-antiferromagnet, and metal-ferroelectric, where new properties of spin waves such as confining and filtering, guiding and steering, non-reciprocity and reconfigurability, direct and indirect gap in the magnonic band structure, emerge from the interaction between the continuous (flat) magnetic film, where spin waves propagate, and the vertical magnetic/nonmagnetic layers which induce periodic modulation of either the static or the dynamic internal magnetic field of the magnetic film itself.[4-9]
Moreover, 3D MCs in the form of meander-shaped ferromagnetic films fabricated on top of pre-patterned substrates have been proposed as prototypes for the transmission of SW signals in 3D magnonic networks.[10-11]

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Engineering interactions in cavity qed materials

Juan Román-Roche

MC25: Emerging Trends in Many-Body Cavity Quantum Electrodynamics IX, August 25, 2022, 11:30 AM - 12:30 PM

The field of cavity qed materials seeks to modify the properties of bulk materials by coupling them to an electromagnetic cavity at equilibrium. When the material is composed of magnetic dipoles, the resulting system is described by a generalized Dicke model. Under certain conditions, the cavity modes can be traced out, leaving a spin Hamiltonian with cavity-mediated (effective) spin-spin interactions. Here, we study the relationship between the effective spin model and the underlying Dicke model. We reverse the mapping and tackle the fundamental question of which effective interactions can be engineered via coupling to a cavity. The range of the effective interactions and the number of modes required in the cavity field are inversely related.

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The Pressure Driven Superconductor-Insulator-Transition in 2D Films

Roy Cohen, Professor Aviad Frydman

MC40: Strongly Disordered Insulators VI, August 23, 2022, 4:30 PM - 6:00 PM

The Superconductor Insulator Transition (SIT) in 2D films has been in the front of condensed-matter research for the past few decades. The SIT is a quantum phase transition which occurs at zero temperature and is thus driven by quantum fluctuations and controlled by a non-thermal tuning parameter. So far, several tuning parameters have been used to drive the transition, such as thickness, external magnetic field, level of disorder etc. We explore a new tuning parameter - hydrostatic pressure. For this we fabricate thin films of amorphous Indium Oxide directly on a diamond and apply pressure on the samples by using a diamond anvil cell, a device that can apply pressure up to 100 GPa.
We find that for pressures up to 1.5 GPa, superconductivity is improved, and the critical temperature increases with increasing Pressure. Applying higher pressure suppresses superconductivity and drives the films into the insulating state. These results imply two competing effects of the pressure on the superconductivity of thin films. Furthermore, we observed signs that the pressure induced insulator may be with different nature than the disordered induced insulator.
In my talk I will discuss the implications of the pressure induced SIT and the nature of the insulating phase in these films.

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Universal dynamical onset in water at distinct material interfaces

Lirong Zheng

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Interfacial water remains liquid and mobile much below 0 C, imparting flexibility to the encapsulated materials to ensure their diverse functions at subzero temperatures. However, a united picture that can describe the dynamical differences of interfacial water on different materials and its role in imparting system-specific flexibility to distinct materials is lacking. By combining neutron spectroscopy and isotope labeling, we explored the dynamics of water and the underlying substrates independently below 0 C across a broad range of materials. Surprisingly, while the function-related anharmonic dynamical onset in the materials exhibits diverse activation temperatures, the surface water presents a universal onset at a common temperature. Further analysis of the neutron experiment and simulation results revealed that the universal onset of water results from an intrinsic surface-independent relaxation: switching of hydrogen bonds between neighboring water molecules with a common energy barrier of 35 kJ mol1

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A surface-polarity-driven valence-ordered non-periodic surface reconstruction

Prof Chi-Ming Yim, Ms Olivia Armitage, Ms Dibyashree Chakraborti, Mr Craig Wells, Dr Seunghyun Khim, Prof Andrew Mackenzie, Prof Peter Wahl

MC18: Developments at the Frontiers of High-resolution Scanning Probe Microscopy III, August 22, 2022, 4:30 PM - 6:00 PM

Chemical and electronic properties of surfaces and interfaces are important for many technologically relevant processes, be it in information processing where properties of interfacial electronic states are crucial for device performance, or for catalytic properties of surface which depend on types and densities of active nucleation sites for the chemical reactions. Quasi-periodic and non-periodic crystalline surfaces afford new opportunities due to their inherent inhomogeneity, resulting in localization and properties vastly different from the surface of crystals described by the conventional Bravais lattices. Here, we demonstrate a new route to stabilization of a non-periodic surface reconstruction at the surface of a high-quality single crystal with a tetragonal unit cell. The surface reconstruction exhibits no long-range periodicity, but comprises few-atom hexagonal domains filling up the whole space. We demonstrate that this reconstruction is stabilized by a valence disproportionation driven by the surface polarity. Measurement of the local density of states by tunneling spectroscopy demonstrates the exciting opportunities arising from localization in the surface layer. Our results therefore indicate that non-periodic orders can emerge directly from a periodic solid, creating a new class of emergent order.

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Hexatic phase and rheological properties in model epithelial tissues

Massimo Pica Ciamarra, Anshuman Pasupalak, Ran Ni, Matteo Paoluzzi, Yan-Wei Li

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

We investigate (i) the jamming transition of the Voronoi model of epithelial cell tissues and its dynamical properties as induced by (ii) stochastic forces mimicking tension fluctuations and (ii) self-propelling forces mimicking the lamellipodium induced motility. In all cases, an intermediate hexatic phase occurs between the solid and the liquid ones, suggesting this phase might have an unexpected biological relevance.
We further demonstrate that the Voronoi model of epithelial cell tissues and other Voronoi based tesselation models undergo a shear-induced rigidity transition.

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Long-wavelength fluctuations and dimensionality crossover in confined liquids

Massimo Pica Ciamarra, Jing Yang, Yan-Wei Li

MC7: Exploring Liquid Properties in Confined Geometry (up to mesoscopic scales) X, August 25, 2022, 2:00 PM - 3:30 PM

We develop a Debye model for the density of vibrational states of confined systems to investigate the crossover from a two- to a three-dimensional dynamics of liquids in a slit geometry and validate it via extensive numerical simulations.
In confined systems, Mermin-Wagner fluctuations enhance the amplitude of vibrational motion—or the Debye-Waller factor—by a quantity scaling as the inverse gap width and proportional to the logarithm of the aspect ratio, as a clear sign of a two-dimensional behaviour. As the temperature or lateral system size increases, the crossover to a size-independent relaxation dynamics occurs when structural relaxation takes place before the vibrational modes with the longest wavelength develop.

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Interplay between jamming and MIPS in persistent self-propelling particles

Massimo Pica Ciamarra, Jing Yang, Ran Ni

MC6: Emergent Phenomena in Driven Soft, Active and Biological Matter III, August 22, 2022, 4:30 PM - 6:00 PM

In living and engineered systems of active particles, self-propulsion induces an unjamming transition from a solid to a fluid phase and phase separation between a gas and a liquid-like phase.
We demonstrate an interplay between these two nonequilibrium transitions in systems of persistent active particles.
The coexistence and jamming lines in the activity-density plane meet at the jamming transition point in the limit of hard particles or zero activity. This interplay induces an anomalous dynamics in the liquid phase and hysteresis at the active jamming transition.

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Role of coherence and degeneracies in quantum synchronization

Parvinder Parvinder, Noufal Jaseem, Michal Hajdušek, Sai Vinjanampathy

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Synchronization in quantum systems has been largely driven by specific examples of frequency entrainment as well as mutual synchronization. Here we study quantum synchronization as a Liouville space perturbation theory. We begin by clarifying the role of centers, symmetries, and oscillating coherences in the context of quantum synchronization. We then analyze the eigenspectrum of the Liouville superoperator generating the dynamics of
the quantum system and determine the conditions under which synchronization arises. We apply our framework to derive a powerful relationship between energy conservation, degeneracies, and synchronization in quantum systems. Finally, we demonstrate our approach by analyzing two mutually coupled thermal machines and prove that nondegenerate thermal networks cannot be simultaneously energy conserving and synchronous.

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Seeding Crystallization in Time

Parvinder Parvinder, Michal Hajdušek, Sai Vinjanampathy, Rosario Fazio

MC20: Recent Advances in Quantum Thermodynamics with a Focus on Many-body Interactions VI, August 23, 2022, 4:00 PM - 6:00 PM

We introduce the concept of seeding of crystallization in time by studying the dynamics of an ensemble of coupled continuous time crystals. We demonstrate that a single subsystem in a broken-symmetry phase acting as a nucleation center may induce time-translation symmetry breaking across the entire ensemble. Seeding is observed for both coherent and dissipative coupling, as well as for a broad range of parameter regimes. In the spirit of mutual synchronization, we investigate the parameter regime where all subsystems are in the broken-symmetry phase. We observe that more broadly detuned time crystals require weaker coupling strength to be synchronized. This is in contrast to basic knowledge from classical as well as quantum synchronization theory. We show that this surprising observation is a direct consequence of the seeding effect.

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Comparison of d-wave and p-wave pairing models in Sr2RuO4

Professor James Annett, Dr Reena Gupta, Professor Sam Shallcross, Dr Jorge Quintanilla, Dr Martin Gradhand

MC50: Fermi Surface Topological Transitions - Effects of Interactions V, August 23, 2022, 2:00 PM - 3:30 PM

For many years the prevailing view of Sr_2RuO_4 was of a well understood Fermi liquid state with a phase transition to an unconventional p-wave triplet superconductor of chiral p_x +ip_y order parameter at T_c = 1.5 K. However recent experiments have challenged this picture. In particular the suppression of the Knight shift below Tc appears to exclude the chiral p-wave scenario. Employing a realistic tight-binding model well describing the Fermi surface in the normal state of Sr_2RuO_4 we map out magnetic field versus temperature phase diagrams for d_x^2−y^2 and d_xz + id_yz pairing types. Both produce (i) a similar Knight shift suppression of ~ 80% and (ii) a bicritical point at T = 0.88 K separating low field second order phase transitions from high field Pauli limiting first order transitions. We find, however, strikingly different phase behaviour between the two scenarios in the high field Pauli limiting region. For the case of d_x^2−y^2 pairing symmetry an additional lower critical line of first order transitions is found, which is absent in the d_xz + id_yz case. We investigate the strength of spin-orbit coupling and its effect on normal state Fermi surface topology on these results. Finally we compare these results to our earlier calculations for helical p-wave triplet pairing [2] and to other recent experimental constraints on the pairing state.

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Molecular dynamics simulations of radiation damage in disordered waste forms

Kostya Trachenko

MC38: Controlled Irradiation Disorder in Model Systems, Organisation, Dynamics, and Transformations XII, August 26, 2022, 9:00 AM - 10:00 AM

Modelling high-energy radiation damage in waste forms has been limited to crystalline waste forms. These waste forms become amorphous under irradiation fairly quickly, therefore it is important to understand radiation damage effects in disordered materials. This modelling in amorphous zirconolite and zircon reveals a number of interesting effects.
Amorphous systems are found to be “softer”than crystalline zirconolite with a much larger number of atoms becoming displaced and changing coordination during a 70 keV cascade. The local coordination and connectivity analysis shows that the amorphous structure continues to evolve as a result of repeated radiation damage, changes which cannot be identified from globally averaged prop- erties such as pair distribution functions. We also find large density inhomogeneities at the local level which we suggest may play an important role for future developments in nuclear waste storage. Finally, we find a correlation between the changes in enthalpy and local coordination, suggesting that measure- ments of enthalpy change can be linked quantitatively to structural radiation damage. Our results raise an interesting possibility of whether an evolution of the amorphous structure due to radiation damage can converge to a new equilibrium amorphous regime, posing the fundamental question of what that structure may be.

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Finite field transport response of a dilute magnetic topological insulator based hybrid Josephson junction

Pankaj Mandal, Mr. Nicolai Taufertshöfer, Mr. Lukas Lunczer, Dr. Martin P. Stehno, Prof. Charles Gould, Prof. Laurens W. Molenkamp

MC21: Bound States in Hybrid Superconductor Nanostructures IX, August 25, 2022, 11:30 AM - 12:30 PM

We report on a hybrid Josephson junction made from the superconductor MoRe and the dilute magnetic topological insulator – Mn doped HgTe [1]. Dilute magnetic semiconductor (DMS) materials are typically II-VI semiconductors, containing a few percent of magnetic atoms. The material system has been the subject of intense study for over half a century, and is known to exhibit a large Zeeman effect due to exchange interaction between the magnetic ions and the semiconductor band structure, as well as for having paramagnetic behaviour with no remanent magnetization [2]. Mn doped HgTe quantum wells are two dimensional topological insulators where, at lowest temperatures, the spin Hall conductance is quantized due to Kondo screening of the magnetic impurities [3], and they have been demonstrated to show chiral quantum Hall edge modes at fields as low as 50 mT [4]. Combining (Hg,Mn)Te with superconductors thus opens the prospect of inducing superconductivity in chiral edge modes, and is a promising platform for exploring exotic new transport physics.

We examine a Josephson junction of such a system. In the zero and very low field limit the device shows, for the first time, induced supercurrent through a DMS, which in this case is also a topological insulator. At higher fields, a rich and “anti”-hysteretic magnetoresistance is revealed. Careful analysis shows that the explanation of this behaviour can be found in magnetic flux focusing stemming from the Meissner effect in the superconductor, without invoking any role of proximity-induced superconductivity. The phenomenon is important, as it will ubiquitously coexist with any exotic new physics that may be present in this class of hybrid devices.

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Electronic spectra of complex materials from real-space simulations

Johannes Lischner

MC41: Real Space Simulations of Topological Matter and Disordered Materials I, August 22, 2022, 11:30 AM - 12:30 PM

In this talk, I will describe different tight-binding based approaches to compute electronic spectra of complex materials. First, I will describe a tight-binding based Hartree theory calculation of twisted bilayer graphene. Near the magic angle of 1.1 degrees, this system contains more than 10,000 atoms in its unit cell making standard electronic structure approaches based on density-functional theory challenging to apply. Our calculations predicted a dramatic deformation of the electronic band structure upon electron or hole doping which was later verified by scanning tunnelling spectroscopy measurements. Next, I will describe calculations of charged defects on transition-metal dichalcogenide monolayers. In these calculations, the effect of electron-electron interactions is incorporated into the screened defect potential which decays very slowly as function of distance necessitating the use of very large supercells. Finally, I will discuss the generation of energetic or “hot” electrons and holes resulting from the decay of localized surface plasmons in large noble metal nanoparticles containing more than one million atoms. This is achieved by coupling a tight-binding description of the nanoparticle electronic states with a solution of the Maxwell equations in matter. Our findings reveal a complex interplay of intra- and interband transitions as function of nanoparticle size, composition and environment.

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Large scale tight-binding calculations on deformed TMD monolayers

Bert Jorissen

MC41: Real Space Simulations of Topological Matter and Disordered Materials III, August 22, 2022, 4:30 PM - 6:00 PM

Experiments on large scale monolayers of Transition Metal Dichalcogenides (TMDs) systems have found interesting electronic phenomena, like localized excitons in strained or twisted multilayer structures.

To obtain accurate predictions for these deformed structures, a large-scale real-space calculation is needed. These systems are typically too large to handle accurately with ab-initio methods. In order to tackle large systems, with an adequate level of accuracy, we will instead use tight-binding (TB) implementations of available models in the literature. This is done within the open-source software Pybinding, developed and maintained at UAntwerp.

In this presentation, I will first show how the tight-binding models for TMDs can incorporate strain. These models are compared with DFT results in the presence of uniaxial strain to assess their performance. Furthermore, I will show results for 1D periodically buckled structures that give rise to flat mini-bands and localized states in the valence and conduction bands. These are compared with DFT results for small scale superlattices. Using these results, I will turn to larger-scale TMD structures beyond those that are obtainable by ab-initio methods, like bound states in 2D periodically buckled structures and realistic nanobubbles.

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High-pressure synthesis of β- and α-In2Se3-like structures in Ga2S3

Samuel Gallego Parra, Rosario Vilaplana, Óscar Gomis, Plácida Rodríguez Hernández, Alfonso Muñoz, Jesús González, Juan Ángel Sans, Catalin Popescu, Francisco Javier Manjón

MC46: Structure, Dynamics and States in Matter under High Pressure VI, August 23, 2022, 4:30 PM - 6:00 PM

Nowadays, alternative synthesis of ferroelectric materials and the capacity of tailoring their properties such as strong dipole moment, piezoelectricity and pyroelectricity are being demanded. Ferroelectric materials under high temperature (HT) or varying composition transform into paraelectric materials, where spontaneous polarization vanishes. This is rooted in the non-centrosymmetric-to-centrosymmetric phase transition (PT) promoted by such changes. In this way, these PTs are used to switch the properties of these materials.

We are witnessing the A2X3 (A=Al, Ga, In; X=S, Se, Te) compounds being studied to find novel ferroelectric and paraelectric 2D materials and, in addition, to switch between them easily. Among all these compounds, only In2Se3 exhibits these structures experimentally: α-In2Se3 (space group (s.g.) R3m, hexagonal, No. 160, Z=3, non-centrosymmetric), stable at room temperature (RT), and β-In2Se3 (s.g. R-3m, hexagonal, No. 160, Z=3, centrosymmetric), observed at HT [1-3]. For the rest of this family, a few theoretical works have highlighted possibilities for obtaining such structures and switching them via increasing/decreasing temperature. More precisely, α-In2Se3-like structure is dynamically stable for the all family at RT [4], unlike the β-In2Se3-like structure [5]. However, this structure becomes stable above the theoretical Tc calculated, following a tendency of Al2X3 > Ga2X3 > In2X3 [4].

When it comes under extreme conditions, such as high pressure, related to both structures, α-In2Se3 undergoes a PT to β-In2Se3 at above 10-12 GPa, after transforming into β'-In2Se3 at 1 GPa [6]. Until now, no previous works have focused on this α- β PT under HP in the A2X3, apart from In2Se3. Among this family of compounds, just α'-Ga2S3 happens to turn into β-In2Se3-like structure (β'-Ga2S3) at about 16 GPa [7]. Evidence of such PT has been stressed in subsequent works [8, 9]. What is more unexpected, after this α'-β' PT on Ga2S3, two other polymorphs have been synthesized upon decreasing pressure, at 9.0 and 3.0 GPa, respectively [8]. However, further information about the nature of both polymorphs was not given.

In this work, we have confirmed this β'-Ga2S3 under HP via XRD and Raman measurements, joint theoretical simulations. Upon decreasing pressure, α-In2Se3-like structure matches quite well with the 1st polymorph observed at 9.0 GPa (ϕ-Ga2S3). Raman signatures and pressure dependence of structural parameters have allowed us to discern such β'- ϕ PT. The 2nd polymorph below 1.0 GPa has been identified with a disordered zincblende (γ-Ga2S3). To complement our results, we discuss the relation between the PTs of both Ga2X3 and AGa2X4 compounds.

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Andreev reflection and electron-hole coherence in proximitized core-shell semiconductor nanowires

Kristján Ó. Klausen, Dr. Anna Sitek, Dr. Andrei Manolescu, Dr. Sigurdur I. Erlingsson

MC21: Bound States in Hybrid Superconductor Nanostructures III, August 22, 2022, 4:30 PM - 6:00 PM

We consider core-shell semiconductor nanowires (i.e. a radial heterostructure), based on III-V materials, with an n-doped shell and an intrinsic core, such that they can be seen as tubular conductors. The cross section of such a nanowire is typically hexagonal, but sometimes triangular. In such a geometry the low-energy electrons within the shell are usually localized at the corners of the polygon. We assume a nanowire of this type in contact with a metallic superconductor. The electron-hole coherence within such a partially proximitized nanowire is investigated numerically, by solving the Bogoliubov-DeGennes Hamiltonian, and compared with the Andreev reflection interpretation of proximitized superconductivity. Partial proximitization is considered to quantify the effects of a diminished coherence length. Three cases are explored: radial, angular and longitudinal asymmetry of proximitization of the shell. For the radial case, it is found that the boundary conditions impose wave function maxima in the center of the shell in spite of the off-center radial proximitization. The induced superconductivity gap is calculated as a function of the ratio of area and radius of the semiconducting and superconducting parts, and the result is found to be independent of the shell thickness for a fixed diameter of the nanowire. In the angular case, a hexagonal wire with a single proximitized side is found to display the essence of Andreev reflection in the total probability density by lengthwise summation of the lowest energy state. In the longitudinal case, a clear correspondence with Andreev reflection is seen per site of the shell for a halfway proximitized wire. Effects of shell geometry on the Bogoliubov-DeGennes wave functions, and the oscillations of the superconducting gap due to an external magnetic field are also discussed.

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Non perturbative numerical simulation of the non-linear optical response of type-II 2D Weyl materials

Dr Leone Di Mauro Villari, Mr Yaraslau Tamashevich, Prof Marco Ornigotti

MC41: Real Space Simulations of Topological Matter and Disordered Materials II, August 22, 2022, 2:00 PM - 3:30 PM

We present a theoretical model to study the non-linear optical response of materials with a low-energy spectrum characterised by strongly tilted, type-II, Weyl cones in two dimensions (2D). Our findings reveal that the tilted nature of the Weyl cones is responsible for the appearance of even harmonics in the non-linear signal, as well as its strong polarisation dependence. We discuss how it is possible to control such non-linear response and envision how 2D Weyl materials can be used to realise novel photonic devices for sensing applications.

Materials with a nodal band crossing point in two and three dimensions can be classified based on the nature of their low-energy dispersion, namely if they admit Dirac or Weyl (DW) cones. Dirac materials contain both time reversal and spatial inversion symmetry. When one of these symmetries is broken, the Dirac points are split into two constituent Weyl points, and the medium becomes a Weyl material (WM). DW cones (fermions) can be further classified into Type I and Type II cones. While the former present DW cones that are straight, and preserve Lorentz invariance, the latter are tilted and with broken Lorentz invariance. Type II cones typically occur when Type I DW nodes are tilted enough, along some specific direction, that a Lifschitz transition occurs and the system acquires a finite density of states at the DW node. While the electronic properties of such media are fairly well studied, understanding the non-linear optical processes, and harnessing their potential applications for photonics, constitutes a less explored territory. This work envisions the characterisation of the non-linear optical properties of materials with a low energy spectrum described by strongly tilted (Type-II) Weyl cones in two dimensions. We present a non perturbative numerical simulation based on the formalism of the Dirac Bloch equations (DBEs) which has been introduced relatively recently to study the non-linear optical response of type-I Dirac materials. In this work after deriving and solving the dynamical equations we characterise the non-linear response by studying the current spectrum in different light polarisation configurations and tilting parameters. We show that there is a polarisation dependent even harmonic amplification and that the tuning of the tilting leads to a non-linear modulation of the intensity of the harmonic signal.

In summary, we have shown how the tilted nature of Type-II Weyl cones results in a natural polarisation-dependent anisotropy of the non-linear signal, and in a significant polarisation-dependent amplification. We have discussed how it is possible to control the non-linear response of such materials, by engineering its properties, in terms of velocity tensor and tilting vector. The results presented here suggest that 2D-WMs possess a significant potential for photonic devices.

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Noise-resilient time crystals in quantum computers

Dr Max Mcginley, Sthitadhi Roy, Siddharth Parameswaran

MC36: Integrating Quantum Computers in Condensed Matter Physics Simulations IV, August 23, 2022, 11:30 AM - 12:45 PM

Quantum systems driven out of equilibrium can exhibit phenomena that have no equilibrium analogues. One example of much recent interest is the discrete time crystal (DTC) [1,2,3], which exhibits a type of spatiotemporal order that breaks time-translation symmetry. Programmable quantum devices offer a promising platform to experimentally realise such phases, and progress is already being made in this direction [4,5]. However, these platforms inevitably suffer from noise, which destabilises the DTC order beyond some fixed timescale. In this talk, I will describe how to realise a DTC that is intrinsically robust against all noisy perturbations that are present in real devices. This scheme uses projective measurements combined with conditional feedback to counteract noise, thus stabilizing the required spatiotemporal order against dissipative processes. This results in infinitely long-lived DTC order in the thermodynamic limit. I will discuss how our model of dynamics can be implemented on present-day quantum devices, and more generally highlight the potential utility of measurement-feedback loops for synthesizing novel dynamical phases of matter in quantum computers.

This talk is based on arXiv:2111.02499

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Dynamic electron correlations with charge order wavelength along all directions in the copper oxide plane

Prof. Eduardo Da Silva Neto, Prof. Fabio Boschini, Prof. Alex Frano, M Minola, R Sutarto, E Schierle, M Bluschke, S Das, Y Yang, M Michiardi, Y-C Shao, X Feng, S Ono, R.D. Zhong, J Schneeloch, G Gu, E Weschke, F He, Y-D Chuang, B Keimer, A Damascelli

MC31: The Physics of Cuprates XII, August 26, 2022, 9:00 AM - 10:00 AM

In strongly correlated systems the strength of Coulomb interactions between electrons, relative to their kinetic energy, plays a central role in determining their emergent quantum mechanical phases. We performed resonant x-ray scattering on BSCCO 2212, a prototypical cuprate superconductor, to probe electronic correlations within the CuO2 plane. We discover a dynamic quasi-circular pattern in the x-y scattering plane with a radius that matches the wave vector magnitude of the well-known static charge density wave [1]. Our experiments reveal a picture of charge density wave competing with superconductivity where short-range domains along x and y can dynamically rotate into any other in-plane direction. This quasi-circular spectrum, a hallmark of Brazovskii-type fluctuations, has immediate consequences to our understanding of rotational and translational symmetry breaking in the cuprates. We discuss how the combination of short- and long-range Coulomb interactions results in an effective non-monotonic potential that may determine the quasi-circular pattern. Finally, we discuss the relation of these quasi-isotropic charge density wave fluctuations to the strange metal behavior in the cuprates, as recently proposed [2].

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Pico-electrodynamics in Silicon

Dr. Sathwik Bharadwaj, Dr. Todd Van Mechelen, Prof. Zubin Jacob

MC19: Advances in the Casimir Force and Heat Transfer Phenomena III, August 22, 2022, 4:30 PM - 6:00 PM

The concept of photonic frequency (ω) - momentum (q) dispersion has been extensively studied in artificial dielectric structures such as photonic crystals and metamaterials. However, the ω-q dispersion of electrodynamic excitations hosted in natural materials at the atomistic level is far less explored. Here, we develop a Maxwell Hamiltonian theory of matter combined with the quantum theory of atomistic polarization to obtain the electrodynamic dispersion of natural materials interacting with the photon field. We apply this theory to silicon and discover the existence of anomalous atomistic waves. These waves occur in the spectral region where propagating waves are conventionally forbidden in a macroscopic theory. Our findings demonstrate that natural media can host a variety of yet to be discovered waves with sub-nano-meter effective wavelengths in the pico-electrodynamics regime.

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Electrical and thermal transport in twisted TMDC/CrI$_3$-superconducting TMDC junctions

Leyla Majidi, Reza Asgari

MC21: Bound States in Hybrid Superconductor Nanostructures IX, August 25, 2022, 11:30 AM - 12:30 PM

Wide tunability of the proximity exchange effect between transition metal dichalcogenides (TMDCs) and Chromium iodide (CrI$_3$) heterostructures provides fascinating opportunity for using TMDCs in two-dimensional magnetoelectrics. In this paper, the effect of the twist angle between the monolayer CrI$_3$ and the TMDC layer as well as the gate electric field on the electrical and thermal transport through a TMDC/CrI$_3$-superconducting TMDC junction are investigated by making use of Dirac-Bogoliubov-de Gennes equation. We show substantial quantities can be controlled by spin-splitting of band structures owing to the spin-orbit interaction, and exchange splitting of the bands originates from the proximity effect. The property of Andreev reflection process strongly depends on the spin-valley polarized states owing to the spin-orbit coupling. Remarkably, perfect spin-valley polarized Andreev reflection is possible over a large bias voltage range by using a gate voltage to tune the local Fermi energy and varying the type of charge doping. It is detected that the proposed structure with p-type doping has greater spin-valley polarized Andreev conductance and the high thermal conductance. We further demonstrate that twisting can lead to the suppression or significant enhancement of the Andreev conductance depending on the TMDC material and the chemical potential of the TMDC/CrI$_3$ layer as well as the amplification of the thermal conductance for the chemical potentials less than that of the superconducting region.

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Mixed active-passive suspensions: from particle entrainment to demixing

Marco Polin, Steve Williams, Raphaël Jeanneret, Idan Tuval

MC6: Emergent Phenomena in Driven Soft, Active and Biological Matter III, August 22, 2022, 4:30 PM - 6:00 PM

Understanding the properties of active matter is a challenge which is currently driving a rapid growth in soft- and bio-physics. Some of the most important examples of active matter are at the microscale, and include active colloids and suspensions of microorganisms, both as a simple active fluid (single species) and as mixed suspensions of active and passive elements. In this last class of systems, recent experimental and theoretical work has started to provide a window into new phenomena including activity-induced depletion interactions, phase separation, and the possibility to extract net work from active suspensions. Here I will present our work on a paradigmatic example of mixed active-passive system, where the activity is provided by swimming microalgae. Macro- and micro-scopic experiments reveal that microorganism-colloid interactions are dominated by rare close encounters leading to large displacements through direct entrainment. Simulations and theoretical modelling show that the ensuing particle dynamics can be understood in terms of a simple jump-diffusion process, combining standard diffusion with Poisson-distributed jumps. Entrainment length can be understood within the framework of Taylor dispersion as a competition between advection by the no-slip surface of the cell body and microparticle diffusion. Building on these results, we then ask how external control of the dynamics of the active component (e.g. induced microswimmer anisotropy/inhomogeneity) can be used to alter the transport of passive cargo. As a first step in this direction, we study the behaviour of mixed active-passive systems in confinement. The resulting spatial inhomogeneity in swimmers' distribution and orientation has a dramatic effect on the spatial distribution of passive particles, with the colloids accumulating either towards the boundaries or towards the bulk of the sample depending on the size of the container. We show that this can be used to induce the system to de-mix.

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Ultrafast X-ray Coherent Imaging of the Light-Induced Phase Transition in VO2

Dr Allan Johnson

MC47: X-ray Free Electron Lasers for Condensed Matter & Materials Physics (XFELs for CMMP) II, August 22, 2022, 2:00 PM - 4:00 PM

Optically driven materials can show complex nanoscale phase dynamics including domain nucleation and the emergence of non-equilibrium phases. Studying transient phases requires ultrafast probes which to date have been spatially integrating, despite photo-generated domain growth or topological defects leading to nanoscale inhomogeneity. Here we demonstrate femtosecond time-resolved hyperspectral X-ray nanoscale imaging of the prototypical photoinduced phase transition in vanadium dioxide. Using resonant coherent X-ray imaging at the PAL X-ray free electron laser (Figure 1), we map the insulator-to-metal transition with 50 nm spatial and 140 fs temporal resolution. We find that the transition proceeds by a prompt, sub-140 fs switching followed by further few-picosecond dynamics across all domains. The transitions occurs via a step-like transition to the metallic phase which launches strain waves into the sample. Fast relaxation of out-of-plane strain leads to a long-lived transient orthorhombic phase, with a heterogeneous response only emerging after in-plane relaxation several hundred picoseconds later. Hyperspectral x-ray imaging spectroscopy of the transient phase formed at 20 ps corroborates this interpretation.

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Exploring the electronic and transport properties of Li-decorated nanoporous graphene

Xabier D. de Cerio, Rodrigo E. Menchón, Cesar Moreno, Aitor Mugarza, Aran Garcia-Lekue

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

The on-surface synthesis of atomically precise nanoporous graphene (NPG), achieved by the lateral fusion of graphene nanoribbons (GNRs), was a milestone in the field of nanostructured 2D materials [1]. Besides being a semiconductor, NPG exhibits a strongly anisotropic electronic character and, thus, the current flow is highly directional [2]. Recent works have demonstrated the possibility of tuning such properties by changing the morphology and chemical composition of the carbon network [3,4]. Alternatively, one might envision to modify the electronic structure of NPG by alkali atom decoration. In fact, this approach has proven effective in other carbon-based systems like graphene [5] and GNRs [6].

In this work, we study the influence of Li atom decoration on the electronic and transport properties of NPG. Using Scanning Tunneling Microscopy (STM) and Density Functional Theory (DFT), we analyse different adsorption sites and concentrations. Interestingly, modifications in the electronic structure are governed by the specific arrangement of Li atoms. Adsorption on the backbone of the GNRs n-dopes only the electronic bands confined within such region. In contrast, Li deposition on the inter-ribbon linkers induces remarkable energy downshifts of the electronic bands dispersing perpendicular to the nanoribbons. These effects are ultimately determined by the specific charge redistribution and electrostatic interplay between Li and NPG, and are expected to significantly alter the electron propagation along the system. Our results may be transferable to similar nanoarchitectonics with tunable anisotropic characteristics.

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Multiscale modelling of organic photovoltaic devices: Reconciling models of interfacial state kinetics and device performance in organic solar cells.

Mohammed Azzouzi, Nathaniel Gallop, Flurin Eisner, Artem Bakulin, Jenny Nelson

Achieving the simultaneous increases in the open circuit voltage , short circuit current and fill factor necessary to further increase the power conversion efficiency of organic photovoltaics (OPV) requires a unified understanding of how molecular and device parameters affect all three characteristics. In this work, we introduce a framework that for the first time combines different models that have been used separately to describe the different steps of the charge generation and collection processes in OPV devices: a semi-classical rate model for charge recombination processes in OPV devices, zero-dimensional kinetic models for photogeneration process and exciton dissociation and one-dimensional semiconductor device models. Using this unified multi-scale model in conjunction with experimental techniques (time-resolved absorption spectroscopy, steady-state and transient optoelectronic measurements) that probe the various steps involved in charge generation we can shed light on how the energy offsets in a series of polymer: non-fullerene devices affect the charge carrier generation, collection, and recombination properties of the devices. We find that changing the energy levels of the donor significantly affects not only the transition rates between local-exciton (LE and charge-transfer (CT) states, but also significantly changes the transition rates between CT and charge-separated (CS) states, challenging the commonly accepted picture of charge generation and recombination. These results show that in order to obtain an accurate picture of charge generation in OPV devices, a variety of different experimental techniques under different conditions in conjunction with a comprehensive model of processes occurring at different time-scales are required.

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DC and optical signatures of the reconstructed Fermi surface for electrons with parabolic band

Dr Zoran Rukelj, Dr Danko Radić

We study the main intra-band and inter-band transport properties at zero temperature of free electron-like system undergoing a topological reconstruction of the Fermi surface for the two-dimensional and three-dimensional case. The calculated intra-band properties include the single-particle density of states, the total and the effective concentrations of electrons and the thermopower. As for the inter-band case, the real part of the conductivity has been calculated within the vanishing inter-band relaxation approximation as a function of the incident photon energy. Within this approach, it is shown that the optical conductivity has a nonvanishing component parallel to the reconstruction wave vector and the shape which depends on the value of the Fermi energy. Each dimensionality has its particular features in the transport quantities presented in the paper, which are discussed and compared with those in the free electron scenario. Finally, we identify the signature of the topological reconstruction of the Fermi surface in the intra-band and inter-band transport functions.

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Magnetoconductivity of a metal with a closed Fermi surface reconstructed by a biaxial charge density wave

Dr Danko Radić, Barbara Keran, Dr Anatoly Kadigrobov

We investigate quantum dynamics and kinetics of a 2D conductor with a closed Fermi surface reconstructed by a biaxial density wave, in which electrons move along a two-dimensional periodic net of semiclassical trajectories coupled by the magnetic breakdown tunneling under a strong magnetic field [1, 2]. We derive a quasiparticle dispersion law and magnetoconductivity tensor. The quasiparticle spectrum is found to be the alternating series of two-dimensional magnetic energy bands with gaps between them. The longitudinal magnetoconductivity shows giant oscillations with change of magnetic field, while the Hall coefficient changes sign and is absent in a wide range of the magnetic fields in between.[3] Preliminary estimations show that the suggested magnetoconductivity
mechanism may be the origin of such behavior of the Hall coefficient versus magnetic field, as observed in experiments in materials with analogous topology of the Fermi surface, such as the high-Tc superconducting cuprates.

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Electronic and thermoelectric transport through hybrid double quantum dot nanostructure with Majorana bound states

Piotr Majek, Krzysztof P Wójcik, Weymann Ireneusz

MC21: Bound States in Hybrid Superconductor Nanostructures VI, August 23, 2022, 4:30 PM - 6:00 PM

Majorana fermions are expected building blocks for topological quantum computers. The last decade has been devoted to the hunt for topological phases. These are essential for the emergence of Majorana quasiparticles in the system. Some of the earliest proposals to look for the signatures of Majoranas were related to the quantum transport through well-known devices – quantum dots [1,2]. Quantum dot was also proposed as an element to design scalable quantum computers made with topological superconducting nanowires [3]. With the development of nanofabrication, the feasibility of such hybrid systems has significantly increased [4]. We investigate a related system consisting of a double quantum dot coupled with a topological superconducting nanowire in terms of electronic and thermoelectric transport properties. Using the numerical renormalization group method, we look for the features induced by Majorana zero-modes in the Kondo-correlated regime. These features include the fractional restoration of the low-temperature conductance showing the competition between Majorana and Kondo physics [5]. Within conductance, we indicated the persistence of the modified Wiedemann-Franz law. We have also shown that coupling to the topological superconductor induces finite spin polarization of the current. Moreover, in such a system, the Majorana-Kondo interplay brings about an additional sign change in thermopower. Furthermore, non-equal contributions from different spin channels induce finite spin-thermopower [6]. These results may indicate some unique features which can support the efforts toward finding the signatures of Majorana zero modes in semiconductor-superconductor nanostructures.

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Writing In Water

Nadir Möller, Lukas Hecht, Benno Liebchen, Thomas Palberg

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Writing is an ancient cultural technique, typically performed by leaving some trace in or on a solid surface. While most writing occurs in dry environments, we present a novel lithographic technique that etches lines in an aqueous medium. In general, objects moving in a gravitationally settled suspension of small tracers leave a trace by different mechanisms ranging from short hydrodynamic trails to chemical concentration fields decorated by tracers settled on the substrate surface. A reliable and suitable source of chemicals are ion exchange (IEX) resin beads moving across a charged substrate. These mobile proton or hydroxyl ion sources provide a diffuse pH trace to which the tracers are phoretically drawn to or repelled from. Continuing phoretic flows towards the trail counteract its diffusive dispersion, leading to a focusing of the written line. Deliberate tilting of the inclined surface aid in the inscription of symbols.
To understand the formation process, the chemical map is recorded via pH microphography as well as high-speed particle image velocimetry. Additionally, density distributions of the trail are measured, revealing Gaussian distributions along the trail cross-section. The creation of these is derived with a continuums model of the particle dynamics under an effective flow potential.

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Thermoelectricity in superconducting quantum devices

Dr. Gianmichele Blasi, Dr. Giampiero Marchegiani, Dr. Alessandro Braggio

Thermoelectrical effects in superconductors are expexted to be weak due to the intrinsic particle-hole (PH) symmetry characterizing these systems. In this talk, we show some relevant examples where the opposite is true. Indeed, superconductors may be very strongly thermoactive materials due to the strong energy dependence of the bands in the gap opening at the Fermi surface but it requires some tricks to clearly unveil their thermoelectrical potential.
We will discuss how thermoelectricity can be developed and manipulated in Cooper pair splitters[1] and topological Josephson junctions[2]. In the first case, the entanglement of the Cooper pair splitting will be detected by nonlocal thermoelectricity and it was even recently measured[3].
In the second case, we will show that nonlocal thermoelectrical effects can be very strong of the order of tens of μV/K at sub-Kelvin temperatures and can be manipulated by magnetic flux[2] and phase biases[4,5]. This effect can be used to clearly identify the helical nature of the topologically protected edge states with a purely three-terminal geometry.
In the second part, we will discuss how strong thermoelectricity can even be generated by spontaneous breaking of the PH symmetry with an asymmetric SIS' junction where the Josephson coupling is sufficiently suppressed[6]. Intriguingly, the thermoelectricity is strong and nonlinear Seebeck coefficients can reach values up to 300 μV/K for aluminum-based tunnel junctions at sub-Kelvin temperatures. Further, the thermoelectricity is uniquely bipolar, i.e., opposite signs of the thermo-voltage for the same thermal gradient occur, as the spontaneous breaking mechanism would imply. We will discuss the generality of the effects for different operating conditions[7], different setup configurations, phase-coherent control[8] and noise effects[9]. Finally, we will report possible experimental evidence and investigate potential applications[10].

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Self-assembly of gold nanoparticles into an adjustable plasmonic 3D lattice using twin and Janus-type forked ligands

Yang-yang Zhao, Yu Cao, Giuliano Siligardi, Georg H. Mehl, Feng Liu, Goran Ungar

MC8 : Complex Phases in Soft Matter VII, August 24, 2022, 2:00 PM - 3:30 PM

Surface plasmonic resonance (SPR) of gold nanoparticles (NPs), offer opportunities for their use in superlenses, drug delivery, memory devices and even generation of negative refractive index metamaterials. We report the formation of a 3D body-centred self-assembled superlattice of AuNPs whose interparticle gap, and hence its plasmonic properties, are adjustable exclusively in the xy-plane[1]. Thus, even though the particles are spherical, their anisotropic packing generates tailorable plasmonic dichroism. The AuNPs are coated with forked ligands containing two mesogens: either two cholesterols (“twin”), one cholesterol and one azobenzene (“Janus”), or a mixture of the two. Beside the body-centered arrangement of AuNPs, the structure also contains unusual two-dimensionally modulated smectic-like layers of mesogens in an egg-box geometry. Moreover, the presence of azobenzene mesogens allows the superlattice to be melted through UV-induced photo-isomerization; the process is reversible displaying low fatigue on repeated cycling.
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Polarization topology of ferroelectric nematics in confined space

Satoshi Aya, Jidan Yang, Wentao Tang, Mingjun Huang

MC8: Complex Phases in Soft Matter II, August 22, 2022, 2:00 PM - 3:30 PM

Magnetic and electric states are closely related. However, many fundamental magnetic states cannot find their electric counterparts especially in liquid matter systems. Typically, many complex electromagnetic states require low symmetries of matters. Thereby, their appearance is limited mostly in solid-state materials, hindering the material processibility and tunability for a wide range of applications.

The emerging new class of materials, dubbed ferroelectric nematic (NF) liquid crystalline state, exhibits the head-to-tail asymmetry. In this presentation, we report on various polarization topological structures enabled by the NF state. Especially, we discuss how polar interactions and the traditional nematic elasticity dedicates the topology.

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Hypothetical complex multi-domain network geometries with chirality: optical properties and geometric free energy estimates

Prof Gerd Schroeder-turk

MC8 : Complex Phases in Soft Matter VII, August 24, 2022, 2:00 PM - 3:30 PM

Bicontinuous geometries, with two intergrown network-like domains, have become a 'household staple' in many soft matter systems, including lipid or copolymer self-assembly and biological membranes. Polycontinuous geometries [1] where three or more network-like domains are integrown, remain less common but not elusive, found e.g. in mesoporous silicates [2], gemini-surfactants [3], and thermotropic liquid crystals [4]. In this talk, we will review some of our work on related poly-continuous geometries in terms of geometric and SCFT free energy considerations [9-11]. Interest in this structures is motivated here in parts through their chiral properties which theory and simulation predict to lead to potentially interesting chiro-optical properties [5,6], some of which have been observed in experiments on larger-scale nanofabricated specimens [7,8]. The talk will mostly review research over the last 15 years, with commentary on potential future avenues for exploration.

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Controlling the ground state of quantum spins over 2D stacks of polar insulators

Dr. David Serrate, Dr. José Martínez-Castro, Dr. Amelia Domínguez-Celorrio, Dr Manuel Vilas-Varela, Dr. Diego Peña, Dr. Véronique Langlais

MC12 : Physics in 2D Nanoarchitectonics II, August 22, 2022, 2:00 PM - 3:30 PM

When a 2D insulator is placed over a metallic surface, a broad range of physical properties are altered and the surface becomes a tool to control the state of additional adsorbates deposited on top. Some well-known consequences are the modification of the surface workfunction, the adsorbate-supporting metal electronic states hybridization suppression, and the integer charge transfer across the insulator. In the case of ionic insulators, another remarkable effect is the surge of a finite rumpling between anions and cations, which causes an out-of-plane electric polarization. Here, the necessary inversion symmetry breaking concomitant to aligned dipolar moments is introduced by the abrupt lattice discontinuity at the surface. The electric field existing at the tip-sample gap of a scanning tunnelling microscope can be used to controllably modify the local ionic displacements below magnetic adsorbates consisting of a few atoms, including also bistable configurations of the electric polarization [see Martínez-Castro et al., Nature Nanotech 13, 19-23 (2018)]. This paves the way to investigate the coupling between spin and charge degrees of freedom, and permits to envisage the application of 2D nano-architechtonics to the design of atomic scale quantum and spintronic devices. In this contribution we will discuss this approach for two different systems. First, we will show that the bistable electric polarization of NaCl monolayer on Cu2N/Cu(001) can reversibly change the spin excitation threshold between the magnetic ground state of individual Co atom and its first excited state. Second, we will discuss the role of a monolayer of MgO on Ag(001) in the spin polarization of edge states in chiral graphene nanoribbons (cGNRs) [see Yazyev et al., Phys. Rev. B 84, 115406 (2011)]. cGNRs were synthesized on the Ag(001) surface following the same reaction proved successful on Au(111) [see Li et al., Nature Comm. 12, 5538 (2021)], and subsequently repositioned on the MgO patches by atomic manipulation. The electronic decoupling provided by the MgO monolayer favours the formation of electronic states with strong spatial localization. This gives rise to magnetic instabilities of the cGNR's 1D edge state ascribed to the reinforcement of e-e correlations. In addition, the electric polarization of the surrounding MgO permits to adjust the energy, relative to the Fermi level, of the new magnetic states.

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Majorana bound states in encapsulated bilayer graphene

Fernando Peñaranda, Ramón Aguado, Elsa Prada, Pablo San-Jose

MC21: Bound states in hybrid superconductor nanostructures VIII, August 24, 2022, 4:15 PM - 6:00 PM

The search for robust topological superconductivity and Majorana bound states continues, exploring both one-dimensional (1D) systems such as semiconducting nanowires and two-dimensional (2D) platforms. In this work [1] we study a 2D approach based on graphene bilayers encapsulated in transition metal dichalcogenides that, unlike previous proposals involving the Quantum Hall regime in graphene [2,3], requires weaker magnetic fields and does not rely on interactions. The encapsulation induces strong spin-orbit coupling on the graphene bilayer, which in turn has been shown to open a sizeable gap and stabilize fragile pairs of helical edge states [4]. We show that, when subject to an in-plane Zeeman field, armchair edge states can be transformed into a p-wave one-dimensional topological superconductor by laterally contacting them with a conventional superconductor. We demonstrate the emergence of Majorana bound states (MBSs) at the sample corners of crystallographically perfect flakes, belonging either to the D or the BDI symmetry classes depending on parameters. We compute the phase diagram, the resilience of MBSs against imperfections, and their manifestation as a 4π-periodic effect in Josephson junction geometries, all suggesting the existence of a topological phase within experimental reach.

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Imaging the field-induced changes in the electronic structure of metamagnetic Sr4Ru3O10

Carolina De Almeida Marques, Izidor Benedičič, Masahiro Naritsuka, Luke C Rhodes, Weronika Osmolska, Christopher Trainer, Yoshiko Nanao, Aaron B Naden, Rosalba Fittipaldi, Veronica Granata, Mariateresa Lettieri, Antonio Vecchione, Peter Wahl

MC50: Fermi Surface Topological Transitions - Effects of Interactions V, August 23, 2022, 2:00 PM - 3:30 PM

The ground state of metamagnetic materials can be precisely controlled by the application of magnetic field, making them exciting candidates for spintronic applications. However, in order to obtain a microscopic understanding and fully control these properties, it is important that we understand the interplay of magnetism, spin- orbit coupling and structural details and their impact on a materials electronic structure.

Here we report a study of the ferromagnetic trilayer ruthenate $Sr_4Ru_3O_{10}$, which exhibits a metamagnetic transition around in-plane magnetic fields of 5T. Using low temperature scanning tunnelling microscopy and spectroscopy, we reveal the distinct changes to the electronic structure as a function of magnetic field. We find a strongly anisotropic response of the electronic structure with in-plane magnetic field, suggesting that the relatively small orthorhombic distortion has an unusually large effect on the metamagnetic electronic structure. For magnetic field applied out-of-plane, we find magnetic-field induced changes to the electronic structure, with significant variation of the effective g-factors describing the field-induced changes in the electronic structure. We discuss these field-induced changes in terms of spin-orbit coupling and the influence of electronic correlation effects.

Comparison of quasi-particle interference imaging with ab-initio simulations of the local density of states reveals how the interplay of ferromagnetism and spin orbit coupling enables us to constrain models of the microscopic electronic structure and demonstrates how a pronounced directional dependence of the electronic structure can result due to spin-orbit coupling, demonstrating a pathway to a realization of field-control of the electronic structure.

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Spectral Simulation of Spin Liquids

Francisco Brito, Aires Ferreira

MC41: Real Space Simulations of Topological Matter and Disordered Materials II, August 22, 2022, 2:00 PM - 3:30 PM

The proliferation of quantum fluctuations and long-range entanglement presents an outstanding challenge for the numerical simulation of interacting spin systems with exotic ground states. In this talk, I will present a Chebyshev iterative method [1] that gives access to the thermodynamic properties and critical behavior of frustrated quantum spin models with good accuracy. The computational complexity scales linearly with the Hilbert space dimension and the number of Chebyshev iterations used to approximate the eigenstates. I will show results obtained with this approach for the spin correlations of the Kitaev-Heisenberg model, a paradigmatic model of honeycomb iridates that exhibits a rich phase diagram including a quantum spin liquid phase. The results are benchmarked against exact diagonalization and a popular iterative method based on thermal pure quantum (TPQ) states. All methods accurately predict transitions between paramagnetic, stripy antiferromagnetic and spin-liquid phases for honeycomb layers with antiferromagnetic Heisenberg interactions. Our findings suggest that a hybrid Chebyshev-TPQ approach could open the door to previously unattainable studies of quantum spin models in two dimensions, namely α-RuCl3 in proximity to graphene [2]. This system is promising for quantum computing since it may support bond-directional Kitaev spin interactions.

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Figure 1: Nearest neighbor spin correlation for the ground state of a 24-site Kitaev-Heisenberg model on the honeycomb lattice with periodic boundary conditions, displaying two phase transitions.

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Advected percolation provides a minimal mechanism for amoeboid cell motility

Dr Silvia Grigolon

Spontaneous locomotion is a common feature of most metazoan cells, generally attributed to the fundamental properties of the actomyosin network. This force-producing machinery has been studied down to the most minute molecular details, especially in lamellipodium-driven migration. Nevertheless, how actomyosin networks work inside contraction-driven amoeboid cells still lacks unifying principles. Here, using stable motile blebs as a model amoeboid motile system, we image the dynamics of the actin cortex at the single filament level and reveal the co-existence of three phases of the actin network with distinct rheological properties. Physical modelling shows that these three phases organize spontaneously due to a rigidity percolation transition combined with an active advection of the percolated network. This spontaneous spatial organization of the mechanical properties of the actin network, which we propose to call advected percolation, constitutes a minimal and generic locomotion mechanism. It explains, down to the single actin filament level and up to the scale of the entire cell, how amoeboid cells can propel efficiently through complex 3D environments, a feature shared by immune and cancer cells.

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Self-focusing nanomechanical sensors for atmospheric pressure mass spectrometry of single viruses and nanoparticles

Mehmet Selim Hanay, R. Tufan Erdogan, Mohammed Alkhaled, Batuhan E. Kaynak, Dr. Hashim Alhmoud, Dr. Hadi S. Pisheh, Mehmet Kelleci, Dr. Ilbey Karakurt, Dr. Cenk Yanik, Z. Betul Sen, Burak Sari, Prof. Aykut Ozkul

MC17: Nanomechanical and Electromechanical Systems V, August 23, 2022, 2:00 PM - 3:30 PM

Nano-Electromechanical Systems (NEMS) have emerged as a promising technology for the mass sensing and spectrometry of nanoparticles and viruses at the single-particle level. However, a typical NEMS device has a small cross-section area, therefore it can capture only a tiny fraction of the incoming analyte particles. As a result, the limit-of-detection and throughput of NEMS mass sensors have not yet reached the levels required to analyze realistic biologic samples. Here, we overcome this problem by integrating a NEMS sensor with an on-chip polymeric ionic lens which automatically focuses the analyte ions onto NEMS. The polymeric lens charges up by accumulating the incoming analyte ions delivered through electrospray ionization (ESI) on itself. As charge is accumulated and maintained on the polymeric lens, a significant portion of incoming analytes are focused onto an open window on the polymer layer which is aligned with an active NEMS sensor.

Owing to the increased ionic flux at the NEMS location, not only the capture efficiency is increased drastically, but also the system could be operated entirely under atmospheric conditions by eliminating the need of focusing by ion optics and the vacuum conditions needed for ion optics. We show that different nanoparticles and viruses can be characterized rapidly, and under ambient conditions. We applied this technique to obtain the mass spectrum of SARS-CoV-2 in atmospheric conditions, with an analysis duration of less than twenty minutes [1]. Moreover, we have characterized another mammalian virus, BoHV-1, as a positive control experiment. The capture efficiencies obtained here are orders-of-magnitude higher than the earlier state-of-the-art NEMS systems.

The results demonstrate that a chip-based technique, rather than bulky and expensive hardware, can be developed to solve the capture efficiency problem of nanoscale sensors. With the increase in analytical throughput, the simplicity of the overall setup and the operation capability under ambient conditions, the technique presented here brings NEMS mass spectrometry one step closer to operation in the field and with realistic biological samples.

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Off-diagonal Casimir-Polder potentials in near-degenerate atomic systems

Diego Fernández de la Pradilla Viso, Esteban Moreno Soriano, Johannes Feist

MC19: Advances in the Casimir Force and Heat Transfer Phenomena V, August 23, 2022, 2:00 PM - 3:30 PM

The interaction of an atom with the electromagnetic environment supported by a macroscopic body affects its structure and induces both spontaneous emission and Casimir-Polder energy shifts of the atomic levels. The possibility to control the properties of the atom by tuning the parameters of the macroscopic body has drawn attention recently [1]. Usually, the effects of the environment are treated separately for each atomic level. However, for groups of near-degenerate states, the induced shifts can become comparable to the energy differences between levels. In that case, the standard approach fails and it becomes necessary to treat the environment-induced interaction between the levels, leading to off-diagonal terms in the field-induced decay and energy shifts.

We here present a way to treat such systems and show that the dynamics of an atom close to a macroscopic structure can noticeably deviate from those predicted by the standard diagonal formulation of the theory. Our approach is based on the framework of macroscopic quantum electrodynamics [2], together with a recent Lindblad master equation formalism that can treat near-degenerate levels while avoiding some of the problems of the standard Bloch-Redfield equation, leading to a trace-preserving master equation even without performing a secular approximation [3]. While this method includes the well-known Casimir-Polder potentials in the diagonal energy shifts, it importantly also describes off-diagonal contributions, especially relevant in near-degenerate atomic subspaces. Due to these off-diagonal contributions, the effective atomic eigenstates are linear combinations of the free-space eigenstates. The mixing of the atomic eigenstates has interesting physical consequences on, for instance, the atomic decay rates, and yet, as far as we know, these off-diagonal terms have not been discussed in the literature.

We have simulated the fine structure of a hydrogen atom coupled to an AlN nanoparticle that supports infrared phonon-polaritonic resonances. For this system, we find notable deviations of the atomic dynamics from the predictions offered by the conventional approaches to the Casimir-Polder interaction. In this regard, we have explored the influence of the Casimir-Polder interactions on the atomic decay rates derived from the master equation, as a function of the distance between the hydrogen atom and the nanoparticle. The nanoparticle offers new decay channels that become enhanced as the atom approaches it, leading to the naive expectation that the atomic decay rates will increase in a monotonic fashion, closely related to the well-known emission quenching due to nanoparticles. Our results show that this is not the case when the off-diagonal terms are taken into account. Although we recover the monotonic increase in the decay rates both far and close to the nanoparticle, for a certain range of intermediate distances, some decay rates actually decrease thanks to the state mixing induced by the off-diagonal Casimir-Polder potential. Such an effect is not present in traditional Casimir-Polder treatments lacking the off-diagonal terms.

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Slip and stress of confined systems at arbitrarily low strain rate:

The transient-time correlation function technique.

Luca Maffioli

Nonequilibrium molecular dynamics (NEMD) is an essential technique for the investigation of systems at atomistic level, and it is widely used to monitor the response of the system to an external force. On the other hand, a good signal-to-noise ratio can typically be achieved only for external fields much larger than those commonly encounterd in technological applications or experimentally accessible. We apply the transient-time correlation function (TTCF) method for the computation of the local pressure and slip velocity in a fluid undergoing a boundary driven shear flow. We show that, while the signal-to-noise ratio of the direct average (DAV) rapidly decays for low shear rates, the TTCF formalism allows one to detect the response of the system with the same level of accuracy for any magnitude of the external field employed. Hence, the TTCF formalism can be used to investigate the rheology of fluids at arbitrarly low shear rates.

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Probing the physics of 2D materials by nanomechanical resonance

Prof. Dr. Peter Steeneken

MC17: Nanomechanical and Electromechanical Systems V, August 23, 2022, 2:00 PM - 3:30 PM

The dynamics of suspended 2D materials has received increasing attention during the last decade, yielding new techniques to study and interpret the physics that governs the motion of these atomically thin layers. This has led to new insights into the role of thermodynamic and nonlinear effects as well as the mechanisms that govern dissipation and stiffness in these resonators. Here, I will present recent progress in using nanomechanical resonance as sensitive probe of condensed matter physics in ultrathin layers [1]. This progress includes detection of thermodynamics and phonon transport in 2D [2], the detection of phase transitions in magnetically and electronically ordered materials [3], and the use of linear and nonlinear dynamics to investigate dissipation mechanisms. Finally, resonant heterostructures of 2D materials and complex oxides will be discussed as platforms for studying physics and realizing applications near the atomic thickness limit [4,5].

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Reconfigurable active colloids with multi-state dynamics

Prof. Lucio Isa

MC6: Emergent Phenomena in Driven Soft, Active and Biological Matter III, August 22, 2022, 4:30 PM - 6:00 PM

Synthetic microswimmers are propelled micro-scale objects that are often thought as model systems for biological microscopic swimmers. However, most synthetic microswimmers lack any autonomous self-regulation and typically rely on external feedback schemes to control their motion and, hence, function. Simple regulation of autonomous behavior in artificial systems is however commonly achieved in larger scale machinery and robotic systems, even in the absence of on-board logic. The paradigmatic example is the one of state machines, i.e. devices that perform specific functions depending on a discretized state in which they are and which are able to transition between different states in response to external cues (a classic example is a turnstile, which opens when a token is inserted and closes after a person has passed and the token has fallen out of position).

Here, we show the that the controlled assembly of colloidal clusters made from soft PNIPAM-co-AAC thermoresponsive microgels and hard polystyrene colloids, can be utilized to fabricate reconfigurable microswimmers with multiple internal states that define different dynamical behavior [1,2]. We employ sequential capillarity-assisted particle assembly (sCAPA) to obtain precisely designed clusters comprising multiple microgels that reversibly swell and deswell at well-defined temperatures, to induce changes in shape and dielectric properties, which in turn are coupled to motility as induced by electrohydrodynamic flows in AC fields. The design of hybrid, responsive microswimmers opens the way to include a broader palette of responses towards the realization of autonomous microswimmers adapting and reconfiguring their motility to the environment.

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Learning the Crystallisation Behaviour of Bidisperse Branched Model Polymers using Coarse-Grained Molecular Dynamics Simulations.

Dr William Fall, Professor Joerg Baschnagel, Dr Olivier Lhost, Dr Hendrik Meyer

MC8: Complex Phases in Soft Matter X, August 25, 2022, 2:00 PM - 3:30 PM

Model polymer systems have long played an important role in understanding how polymers crystallise. Ungar, Zeng and co-workers for example studied mixtures of linear and branched n-alkane mixtures to 'learn' polymer crystallisation[1]. This approach is still being used today i.e. to understand the influence of substrates on polymer melting using ultra-long n-alkanes[2]. Often fundamental aspects of these studies may then be applied to real polymers. Clean systems like these are important since they provide an ideal playground to tackle fundamental questions about polymer melting and crystallisation, unobscured by the effects of polydispersity.

Molecular dynamics (MD) simulations can provide molecular level insights into these systems inaccessible to experiments but studying large lamellar structures is a challenge. This is due to the large simulations required but also the entanglement time of very long chains. Meyer and Muller-Plathe set the stage for such studies demonstrating how reproducing the local crystalline structure is essentially unimportant when large-scale crystalline and amorphous regions dominate material properties[3]. They revealed how a purely repulsive potential, combined with a high pressure and coarse-grained angular potential, is enough to trigger crystallisation.

Motivated by industrial needs and this fundamental approach, the role of short chain branches (SCBs) (C4H9) on the melt and crystalline properties of monodisperse polyethylene systems (C400H802) is first investigated, using coarse-grained MD simulations of a united-monomer model that represents a chemical monomer as one particle. A new method is introduced, whereby SCBs are grown out of the linear backbone, to minimise computational expense and 'short-cut' the entanglement time. This concept is proven by introducing differing numbers of regularly spaced SCBs along the chains and studying their influence. By growing SCBs into the melt, we demonstrate how they only marginally perturb the original topology, justifying a short equilibration time after growth. This procedure combined with the above approach provides access to larger systems.

Continuous cooling and heating cycles are performed to study crystallisation and melting at progressively slower rates. The crystalline morphology depends strongly on both cooling rate and number of branches. This method is then used to study more complex architectures and mimic industrial polyethylene morphologies. Bidisperse mixtures of ultra-long C4000H8002 and C400H802 are studied, with different short and long chain branch distributions to understand their influence on the crystalline structure. Via self-seeding, well aligned lamella are grown and morphological features, including tie chains and branch conformations, are analysed to understand their role during nucleation. We begin to address how these features influence crystalline structure and material properties.

We thank TotalEnergies for funding and GENCI/IDRIS (Orsay) and CAIUS/HPC centre at University of Strasbourg for generous grants of CPU time.

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Frank-Kasper Spherical Phases in Block Copolymers

Weihua Li

MC8: Complex Phases in Soft Matter IV, August 23, 2022, 11:30 AM - 12:30 PM

Frank-Kasper phases were originally discovered in metallic alloys more than sixty years ago. In this century, complex Frank-Kasper spherical phases were observed in various soft condensed matter systems of amphiphilic macromolecules, such as supramolecular liquid crystals and block copolymers. Inspired by these experimental works, my group have been studying the emergence and stability of Frank-Kasper phases in block copolymers using self-consistent field theory, especially focusing on revealing their stabilization mechanisms as well as designing new block copolymer systems for the formation of Frank-Kasper phases. We propose that Frank-Kasper spherical phases are stabilized in the spherical phase region of AB-type block copolymers significantly expanded by conformational asymmetry or architectural asymmetry. We further propose that the spherical region can be extremely expanded by rationally designing the asymmetric architecture of AB-type block copolymers, forming “inverted” Frank-Kasper spherical phases with the volume fraction of spheres being larger than 0.5 and even reaching 0.7. In addition, we predict that the Frank-Kasper phases, especially the Laves C14 and C15 phases, can be stabilized by adding the second polymers (homopolymer or copolymer) to enlarge the size differences. Encouragingly, some of our theoretical results have been confirmed by experiment.

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Global/Local Chirality Characterization with Resonant X-ray Scattering

Dr Yu Cao, Dr. Chenhui Zhu, Prof. Natasa Vaupotic, Prof. Carsten Tschierske, Prof. Feng Liu

MC8 : Complex Phases in Soft Matter VII, August 24, 2022, 2:00 PM - 3:30 PM

Chirality in various dimensions attracts significant attentions. Scientifically, it poses some fundamental questions of mechanistic understanding on homo-chirality in life science. In the perspective of application, chirality is critical to devices like circular polarized light emitters and chirality transfer template. To understand the origin and realize the potential of chirality, there is a high demand for going beyond the scale of electron density and down to molecule/bond/orbital. Deciphering the orientation order in such scale would be benefit to understand the observed micro- and macroscopic chiral phenomena in soft and biomaterials. Resonant X-ray scattering, working in the vicinity of absorption edges with linear polarized incident beam, is a good candidate for chiral structure characterization.

Herein, we introduce the characterization of two complex chiral systems in 1D and 3D with resonant X-ray scattering to exhibit how this technique serves as a molecular level probe of orientation order and helps elucidation the global/local chirality generation and manipulation in complex structures.

The first system is helical nanofilament (HNF) phase, a complex 1D chiral structure composed by bent-core molecules, doped by different achiral dopants, rod-like 5CB and soft octane. Characterized by resonant X-ray scattering, the phase behavior of HNFs, especially its helical pitch, is well-studied. By match the position and intensity distribution of the simulated resonant signal with experimental results, the HNF phase can be regarded as strings of twisted bent-core molecules with global chirality. Moreover, by simply switching the incident beam energy from carbon K-edge to oxygen K-edge, the superstructure of dopant 5CB can be characterized as a pseudo helical twist directed by the groove of HNFs.

For the second one, a complex bicontinuous double gyroid (DG) phase, which is an achiral meso-structure formed by two networks with opposite handedness, is chosen to learn its local helicity. DG phases formed by rod- or disc-like molecules are examined by resonant X-ray scattering at carbon K-edge. Though small-angle X-ray scattering patterns from DG phase formed by different molecules are identical, significant differences can be observed in resonant scattering patterns. Taking the symmetry of Ia3d space group into consideration, resonant signal simulations for two different molecules suggest that rod-like molecules twist in opposite directions along two networks with opposite handedness while disc-like molecules randomly packed regardless of handedness.

With these two 1D and 3D complex structures, we would like to show not only how molecules are packed to generate global/local chirality but also the strong capability of resonant X-ray scattering in chirality studies as a complementary of conventional X-ray scattering.

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High-pressure evolution of distortions in perovskites: A comparative RFeO3 vs RMnO3 study

Rui Vilarinho, Mael Guennou, Pierre Bouvier, Mads Weber, Inma Peral, Pedro Tavares, Gaston Garbarino, Mohamed Mezouar, Jens Kreisel, Abílio Almeida, Joaquim Agostinho Moreira

MC46: Structure, Dynamics and States in Matter under High Pressure VI, August 23, 2022, 4:30 PM - 6:00 PM

The physical properties of perovskite materials, with general formula ABO3, are known to be strongly dependent on their structural distortions, which can be changed through temperature, applied electric/magnetic fields, and epitaxial strain. The understanding of the delicate energy balance involving the different structural instabilities is therefore a key point for the design of multifunctional perovskite-based materials, and can give important inputs for ab initio calculations and phenomenological models [1]. Hydrostatic pressure allows modifying the interatomic distances and, thus, tuning the interactions to a much larger extent than any other external parameters.

Rare-earth orthoferrites (RFeO3), and orthomanganites (RMnO3) (with R lanthanide atom) exhibit interesting bulk and strain-engineered magnetic and multiferroic phases, motivating a better understanding of the compressibilities of these structures. All of RFeO3 and the RMnO3, with R = La to Dy, crystallize in the Pnma space group, characterized by two tilts of the oxygen octahedra: in-phase about the [010]pc axis, and out-of-phase about the [101]pc axis. For the same rare-earth, the RFeO3 and RMnO3 exhibit exactly the same the tolerance factor, as Mn3+ and Fe3+ have the same ionic radius, however, the MnO6 octahedra exhibits Jahn-Teller distortion superimposed to the intrinsic distortion arising from the out-of-phase [101]pc octahedra tilt.

In order to disclose the effect of the structural distortions on the physical properties of RFeO3 and RMnO3, their high-pressure behavior has been studied to some extend by x-ray diffraction, Mössbauer spectroscopy, and resistivity measurements. A general scenario can be summarized, wherein both types of compounds undergo compression before a structural phase transition occurs at PC in the 35 to 50 GPa range, depending on the rare-earth ion [2-3]. At PC, there is a volume collapse around 5%, accompanied by an insulator-to-metal transition, which has been explained by a high-spin to low-spin state change of the Fe3+ and Mn3+ cations. This work focuses on the similarities and differences found in the high-pressure behavior of RFeO3 and RMnO3, explaining how the structural distortions can be either enhances or suppressed, giving special evidence to the role played by the Jahn-Teller distortion, namely on the degree of anisotropy, volume compression, and symmetry of the high-pressure crystallographic phase.

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Influence of sintering methods on piezoelectric K0.5Na0.5NbO3 ceramics

Mariana Gomes, Rui Vilarinho, Rui Pinho, Ricardo Serrazina, Abílio Almeida, Ana Senos, M. Elisabete Costa, Paula Vilarinho, J. Agostinho Moreira

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

There is a growing interest in lead-free materials as substitutes of lead zirconate-titanate (PZT) based materials, due to their poisonous nature. Some promising piezoelectric and friendly environment compounds are attracting attention, namely KxNa(1-x)NbO3 [1]. For the case of x=0.5, K0.5Na0.5NbO3 (KNN), the high-temperature cubic symmetry changes to a non-symmetric ferroelectric tetragonal structure at T3=700 K, becoming orthorhombic at T2=465 K, and finally stabilizing in a rhombohedral symmetry below T1=135 K [2,3]. The sintering conditions play an important role in the enhancement of the electromechanical properties of this material [4,5].

In this work, we revisit the phase transition sequence and the effect of the sintering process on the structure, lattice dynamics, and dielectric/polar properties of KNN ceramics prepared by conventional sintering, spark plasma sintering, spark plasma texturing, and FLASH sintering. From a comparative analysis of the overall experimental obtained results, we have observed that the phase transition sequence includes an unreported structural and polar phase at low temperatures, independently on the processing method. Moreover, apparent changes of the stability temperature interval of the different phases have been ascertained. A comparison between the conventional and FLASH processes allows us to detect an internal stress state arising from the FLASH by using X-ray diffraction and Raman spectroscopy. In addition, the internal stress state, and its dependence on the local temperature during FLASH sintering is established by Finite Element Modelling. The results here reported clearly point out towards the possibility to change physical properties following different sintering routes to improve device performance.

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Magnetic, thermal, and topographic imaging with a nanometer-scale SQUID-on-lever scanning probe

Daniel Jetter

MC22: Nanoscale Fabrication of Superconducting Devices and their Applications X1, August 25, 2022, 4:30 PM - 6:00 PM

Scanning superconducting quantum interference device (SQUID) microscopy is a magnetic imaging technique combining high field sensitivity with nanometer-scale spatial resolution. We demonstrate a scanning probe that combines the magnetic and thermal imaging provided by an on-tip SQUID with the tip-sample distance control and topographic contrast of a non-contact atomic force microscope (AFM). We pattern the nanometer-scale SQUID, including its weak-link Josephson junctions, via focused ion beam milling at the apex of a cantilever coated with Nb, yielding a sensor with an effective diameter of 365 nm, field sensitivity of 9.5 nT/√Hz and thermal sensitivity of 620 nK/√Hz, operating in magnetic fields up to 1.0 T. The resulting SQUID-on-lever is a robust AFM-like scanning probe that expands the reach of sensitive nanometer-scale magnetic and thermal imaging beyond what is currently possible.

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Emergent Hyper-Magic Manifold in Twisted Kitaev Bilayers

Dr Alessandro Principi, Mr Samuel Haskell

MC16: Spin Control in Twisted Van Der Waals Heterostructures VI, August 23, 2022, 4:30 PM - 6:00 PM

Kitaev quantum spin liquids have been the focus of intense research effort thanks to the discovery of various materials (e.g., RuCl3) that approximate their intriguing physics. Here we present a mean-field approximation for a moire superlattice emerging in twisted Kitaev bilayers in terms of solutions of commensurate bilayers. We show that the band structure of deconfined spinons, defined on the mini-Brillouin zone of the superlattice, is greatly modified. The system exhibits a hyper-magic manifold: a series of nearly perfectly-flat bands appear at energies above the lowest gap. Including intralayer modulation, such bands become isolated from other dispersive ones. Intriguingly, flat-band eigenstates exhibit a localization akin to wavefunctions of Kagome lattices. Flat bands could be detected via measurements of differential conductance and the inelastic electron tunneling spectrum (IETS), according to the theory for 2D-to-2D tunneling spectroscopy aided by magnetic or quantum-order excitations we have previously developed.

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Controlled transfer of a single molecule between two independent STM tips

Donato Civita, Marek Kolmer, Grant Simpson, Leonhard Grill

MC18: Developments at the Frontiers of High-resolution Scanning Probe Microscopy III, August 22, 2022, 4:30 PM - 6:00 PM

Thermally induced diffusion of atoms and molecules on a surface is typically a random process, consisting of uncorrelated hops on the atomic surface lattice [1]. In the absence of thermal motion, a scanning tunneling microscope (STM) tip can be used to induce displacement of single molecules, typically hopping from one lattice site to the next [2]. Longer distances, beyond the manipulation pathway, have been achieved with sexiphenyl molecules on Ag(111), where the molecules were initially dragged with the STM tip over the surface and then continued to move further after the tip was retracted, albeit with deflections from their original propagation path [3]. CF2 species were propelled up to ~5 nm on a corrugated Cu(110) surface, driven by excess energy from bond dissociation [4].

Here, we show how the motion of single di-bromo-ter-fluorene (DBTF) molecules on a Ag(111) surface can be controlled over large distances of more than 100 nm with sub-picometer precision [5]. Despite the flat fcc(111) surface, the molecules move strictly in one dimension across the surface, driven by an interplay of van der Waals and electrostatic interactions that are used to repel and attract the molecule. The large spatial extension of the motion, and its astonishing confinement to one atomic row of the substrate allows realization of a sender-receiver experiment where a single molecule is transferred between two independent STM tips. By measuring the tunnelling current at both tips during such an experiment, it is possible to directly measure the velocity of a single molecule.

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Unconventional charge order and superconductivity in kagome materials

Titus Neupert

MC50: Fermi Surface Topological Transitions - Effects of Interactions VII, August 24, 2022, 2:00 PM - 3:30 PM

Lattice geometry, topological electron behaviour and the competition between different possible ground states all play a role in determining the properties of materials with a kagome lattice structure. In particular, the compounds KV$_3$Sb$_5$, CsV$_3$Sb$_5$ and RbV$_3$Sb$_5$ all feature a kagome net of vanadium atoms. These materials have recently been shown to exhibit superconductivity at low temperature and an unusual charge order at high temperature, revealing a connection to the underlying topological nature of the band structure. I will discuss these discoveries, their theoretical modeling and place them in the context of wider research efforts in topological physics and superconductivity.

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Growth pathways of metal nanoparticles in the gas phase

Prof. Riccardo Ferrando

MC9: Recent Developments in Gas Phase Synthesis of Nanoparticles and Applications X, August 25, 2022, 2:00 PM - 3:30 PM

The structures of metal nanoparticles and nanoalloys are often the results of complex formation pathways which originate from the competition between kinetic trapping effects and equilibrium driving forces. The key growth mechanisms that cause the selection of the growth pathways are far from trivial and difficult to pinpoint at the atomic level by the experimental observations alone. In this regard, computer simulations can be a very useful tool, because they provide detailed physical information at the atomic level. Here we present the results of molecular dynamics simulations that aim at explaining the outcome of different growth experiments, including pure Pt [1] and pure Au [2] nanoparticles, and PtPd [3] AuPd [4] nanoalloys. In the growth of Pt and Au nanoparticles , our simulations reveal the key role of metastable defects that can cause symmetry breaking and subsequent shape changes. In Au-Pd nanoalloys, equilibrium driving forces related to surface stress relaxation cause a structural transition from fcc to icosahedral structures depending on composition.

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Structural and Optical Properties of Gold Nanosponges

Malte Grunert, Sebastian Bohm, Hauke Honig, Dr. Dong Wang, Prof. Dr. Christoph Lienau, Prof. Dr. Peter Schaaf, Prof. Dr. Erich Runge

MC13: Topological and Geometrical Effects in Complex Nanostructures II, August 22, 2022, 2:00 PM - 4:00 PM

Nanoporous gold nanosponges with dimensions of a few hundred nanometers made via alloying and dealloying of gold and silver are easily-made complex nanostructures with unique topological and geometrical properties. Obviously and trivially, using nanoporous nanoparticles instead of bulk material is technologically promising for, e.g., catalysis due to the reduced material costs and the large surface-to-volume ratio.

In contrast, the present contribution explores features resulting from the highly non-trivial topology of nanosponges. It leads to most remarkable optical properties. Most noteworthy, we showed in earlier work a strong localization of electric fields at optical frequencies [Nano Lett. 18(8):4957-4964 (2018), https://doi.org/10.1021/acs.nanolett.8b01785] and an associated strong nonlinear response [Nature Commun. 11, 32193407 (2020), https://doi.org/10.1038/s41467-020-15232-w].

We characterize the structure of typical nanoporous gold nanosponges with various geometrical parameters and compare these with computer models of nanosponges. If the structural parameters of real sponges and our best computer models agree, the experimentally observed optical spectra and those calculated with a Maxwell solver for the computer model show similar features as well. Exact agreement can, of course, not be expected because both are disordered system which qua definition differ from one nanoparticle to the next.

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Ferroelectric nematic phases and splay deformation

Alenka Mertelj, Nerea Sebastián, Luka Cmok, Matija Lovšin, Martin Čopič, Natan Osterman, Andrej Petelin, Irena Drevenšek-Olenik, Richard J. Mandle, Satoshi Aya, Mingjun Huang, Brecht Berteloot, Kristiaan Neyts

MC8: Complex Phases in Soft Matter II, August 22, 2022, 2:00 PM - 3:30 PM

I will discuss the importance of the flexoelectric coupling between splay deformation and ferroelectric order in the formation and behavior of polar nematic phases. The transition from the apolar nematic to the polar nematic phase is a ferroelectric-ferroelastic phase transition, in which due to the flexoelectric coupling simultaneously diverging behavior of electric susceptibility and instability towards splay deformation occur[1]. Below the phase transition, it is expected that first a 1D[2] or 2D[3] modulated antiferroelectric splay nematic phase (NS) appears (Fig. 1), followed by the ferroelectric nematic phase (NF) [4,5]. Experiments show, that the temperature interval in which the NS phase exists, is smaller when pretransitional softening of the splay elastic constant is more pronounced. In the end, I will demonstrate, how the coupling between splay and polarization affects the formation of the domains and topological defects in the NF phase.
Fig. 1: Schemes of isotropic (Iso), apolar nematic (N), splay nematic (NS), and ferroelectric nematic (NF) phases.

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Engineering the band structure of van der Waals materials by pressure and strain

Dr. Peter Makk

MC14: Beyond Charge Transport in Nanostructures and 2D Materials via Geometric Design VIII, August 24, 2022, 4:30 PM - 6:00 PM

Van der Waals heterostructures became the central topic of modern condensed matter physics. Their behaviour is strongly affected by the distance between the layers, the twist angle between them or strain present in the system. Here I describe two novel techniques, strain and pressure that can be used to engineer the band structure of van der Waals materials.
On the one hand, pressure can change the layer distance in van der Waals systems, that leads to changes in the coupling between the layers. I will demonstrate this effect by showing the increase of induced SOC in graphene [1,2] and the changes of single particle spectrum of twisted double bilayer graphene [3].
On the other hand strain allows to change the symmetries of the system or to introduces pseudo-magnetic fields in graphene. I will demonstrate our novel setup by showing the increase of mobility in graphene and the appearance of a scalar potential [4-6].
These techniques allow to perform transport experiments on high mobility van der Waals heterostructures and in-situ tuning of the band structure.

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Interwire Andreev reflection and Andreev molecule in double InAs nanowires

Oliver Kürtössy, Mihaly Bodocs, Zoltan Scherübl, Gergo Fülöp, Peter Makk, Thomas Kanne, Jesper Nygard, Szabolcs Csonka

MC21: Bound States in Hybrid Superconductor Nanostructures II, August 22, 2022, 2:00 PM - 3:30 PM

Double InAs nanowires grown with a a few nm spacing and connected by a common epitaxial Al shell provide a novel platform for quantum electronic devices [1]. The 1D character of the wires, presence of spin-orbit interaction and a narrow superconducting link between the semiconductors make this system attractive for Majorana box qubit, Time Reversal Invariant TOpological State (TRITOS) or Parafermions.

In this contribution we report the investigation of subgap states of such double nanowires, when quantum dots are formed in the wires. On one hand we analyze the strength of interwire Andreev reflection [2], which is essential for the realization of TRITOPS or Parafermions. We show that interwire Andreev reflection is strong thanks to the small spacing of the wires. Its interplay with interwire Coulomb repulsion is investigated in detail. We also report on the hybridization between subgap states hosted in the two nanowires [3] in DC measurements and analyze how the molecular state could be characterized by microwave techniques.

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Dark-mode based chiral resonant magnonic devices: Comparison of the backward and forward volume and Damon-Eshbach geometries

Dr Kevin Fripp, Dr Yat-Yin Au, Dr Andrei Shytov, Professor Volodymyr Kruglyak

MC44: New Perspectives in Magnonics, from 2D to 3D Systems I, August 22, 2022, 11:30 AM - 12:30 PM

The future of magnonics as a technology relies on our ability to excite short-wavelength spin waves, to control their amplitude and phase, and then to detect them, all within devices with a nanoscale footprint. A nanomagnet formed above a longitudinally magnetized magnonic waveguide (backward volume geometry) was shown to act as an efficient chiral spin wave source, trap, diode (aka valve), and phase shifter [1-3]. In such devices, the spin wave propagation along the waveguide is controlled via resonant magneto-dipolar coupling between the spin waves and the quasi-uniform mode of the nanomagnet, whose magnetization controls the coupling's strength and chirality [1-3]. Here, we use micromagnetic simulations to extend this concept in two ways. Firstly, we show that the nanomagnet's dark modes, which are insensitive to incident microwave magnetic field, may be even more suitable for creation of diodes and chiral phase shifters than the quasi-uniform mode. Secondly, we demonstrate and quantify these functionalities for the case of waveguide magnetization orthogonal to the direction of spin wave propagation, both when the magnetization is in-plane (Damon-Eshbach geometry) and when it is out-of-plane (forward volume geometry), as exemplified in Fig. 1. The quasi-uniform and dark mode resonances may have the same frequency in nanomagnets of different sizes, enabling creation of spin wave sources, gates, detectors, and complete integrated circuits driven by the same global uniform clock field without unnecessary interference effects. The use of the different spin wave geometries will be essential in designs where the ultimate chirality, bias-free operation, or propagation isotropy are required.

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Plastic Strain Induced Phase Transformations under High Pressure: Four-Scale Theory, Experiments, and Phenomena

Professor Valery Levitas

MC46: Matter Under High Pressure III, August 22, 2022, 4:30 PM - 6:00 PM

During compression in a diamond anvil cell (DAC), materials undergo large plastic deformations, which cause the growth of pressure and various phase transformations (PTs). Importantly, these PTs should be treated as strain-induced PTs under high pressure rather than pressure-induced PTs. Pressure- and stress-induced PTs occur by nucleation at the pre-existing defects (e.g., dislocations) below the yield strength. Strain-induced PTs occur by nucleation at new defects generated during plastic flow. Strain-induced PTs require completely different thermodynamic and kinetic treatment and experimental characterization [1]. Also, the superposition of plastic shear on high pressure in rotational DAC (RDAC) leads to numerous mechanochemical phenomena, including reducing PT pressure up to one to two orders of magnitude and the appearance of new phases [1]. For example, plastic shear reduced graphite-diamond PT pressure from 70 GPa under quasi-hydrostatic conditions to 0.7 GPa [2]. Here, a four-scale theory was developed, and corresponding simulations were performed [1]. Molecular dynamic [3] and first-principle [4] simulations were used to determine lattice instability conditions under all six stress tensor components. At the nanoscale and microscale, nucleation at various evolving dislocation configurations was studied utilizing developed nanoscale [5] and scale-free [6] phase-field approaches. The possibility of reducing PT pressure by more than an order of magnitude due to stress concentration at the shear-generated dislocation pileup is proven. At the microscale, a strain-controlled kinetic equation was derived and utilized in the large-strain macroscopic theory for coupled PTs and plasticity. At the macroscale, the behavior of the sample in DAC/RDAC is studied using finite element approach [7]. Various experimental effects are reproduced. In situ XRD experiments provide the evolution of pressure distributions and concentration of high-pressure phase, which are used to extract material parameters in the micro/macroscale models. The experimental calibration and confirmation of the strain-controlled kinetics were obtained for α-ω PT in Zr [8] and PT hexagonal-superhard wurtzitic BN. Some applications to geophysical problems, like strain-induced microdiamond synthesis directly in the Earth crust and new PT-based mechanisms of the deep-focus earthquakes [9], will be considered. Various new phenomena, like PT induced by rotational lattice instability, pressure self-focusing effect, self-blown-up deformation-transformation-heating process in a shear band, will be discussed. The obtained results offer a new fundamental understanding of strain-induced PTs under high pressure in DAC/RDAC and methods of controlling PTs and searching for new high-pressure phases.

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Nonlinear supratransmission in a magnetically coupled elastic rods arranged in three lines

Masayuki Kimura, Jung-Jin Lee, Alain Bertrand Togueu Motcheyo, Shinji Doi

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter XII, August 26, 2022, 9:00 AM - 10:00 AM

Nonlinear supratransmission in lattices is known as a kinetic energy transfer in which moving localized vibrations are carriers [1]. For nonlinear lattices, standing localized vibrations also exist. They are called intrinsic localized modes (ILMs) or discrete breathers (DBs) and have been widely investigated theoretically and experimentally [2].
We focus on moving/standing ILM/DB in magnetically coupled elastic rods arranged straightly which is inspired by the two-dimensionally arranged pendula with permanent magnets [3]. Each elastic rod can move not only along the axis of the array but also perpendicularly to the axis. Two types of standing ILM/DB are numerically identified. One vibrates along the axis and the other mainly vibrates transversally. The former is called longitudinal ILM (L-ILM) and the latter transverse ILM (T-ILM) in this research. It is numerically revealed that the L-ILM loses its stability when the amplitude becomes large, which is similar to the L-ILM in the flexible Fermi-Pasta-Ulam lattice [4]. The instability of L-ILM may affect the stability of moving ILM generated by the sinusoidal excitation at the end of the array. The large amplitude excitation generates moving ILMs, but they decay immediately. To suppress the instability, we added two resonators array to surround the transmitting line of moving ILMs. Although the effect of surrounding arrays is weak, it is observed that the rather large amplitude moving ILM can travel long distances without decay. Interestingly, it is found that the surrounding arrays make the T-ILM stable. We will discuss the effects of the surrounding arrays on both standing and moving ILMs.

Acknowledgments
This work is partially supported by JSPS Kakenhi No. 18K04020 and No. 21K03935.

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Ultrafast charge transfer in heterostructures of two-dimensional materials

Professor Giulio Cerullo

MC51 : Ultrafast Dynamics in Magnetic and Strongly-Correlated Materials X, August 25, 2022, 2:00 PM - 3:30 PM

Heterostructures (HS) of two-dimensional materials offer unlimited possibilities to design new materials for applications to optoelectronics and photonics. In such HS the electronic structure of the individual layers is well retained because of the weak interlayer van der Waals coupling. Nevertheless, new physical properties and functionalities arise beyond those of their constituent blocks, depending on the type and the stacking sequence of layers. In this presentation we use high time resolution ultrafast transient absorption (TA) and two-dimensional electronic spectroscopy (2DES) to resolve the interlayer charge scattering processes in HS. We first study a WSe2/MoSe2 HS, which displays type II band alignment with a staggered gap, where the valence band maximum and the conduction band minimum are in the same layer. By two-colour pump-probe spectroscopy, we selectively photogenerate intralayer excitons in MoSe2 and observe hole injection in WSe2 on the sub-picosecond timescale, leading to the formation of interlayer excitons (ILX). The temperature dependence of the build-up and decay of interlayer excitons provide insights into the layer coupling mechanisms [1]. By tuning into the ILX emission band, we observe a signal which grows in on a 400 fs timescale, significantly slower than the interlayer charge transfer process. This suggests that photoexcited carriers are not instantaneously converted into the ILX following interlayer scattering, but that rather an intermediate scattering processes take place. We then perform 2DES, a method with both high frequency and temporal resolution, on a large-area WS2/MoS2 HS where we unambiguously time resolve both interlayer hole and electron transfer with 34 ± 14 and 69 ± 9 fs time constants, respectively [2]. We simultaneously resolve additional optoelectronic processes including band gap renormalization and intralayer exciton coupling.
Finally, we investigate a graphene/WS2 HS where, for excitation well below the bandgap of WS2, we observe the characteristic signal of the A and B excitons of WS2, indicating ultrafast charge transfer from graphene to the semiconductor [3]. The nonlinear excitation fluence dependence of the TA signal reveals that the underlying mechanism is hot electron/hole transfer, whereby a tail the hot Fermi-Dirac carrier distribution in graphene tunnels through the Schottky barrier. Hot electron transfer is promising for the development of broadband and efficient low-dimensional photodetectors.

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Tuning van der Waals heterostructures by pressure

Bálint Szentpéteri, Bálint Fülöp, Albin Márffy, Simon Zihlmann, Peter Rickhaus, Folkert K. de Vries, Endre Tóvári, Christian Schönenberger, Andor Kormányos, Péter Makk, Szabolcs Csonka

MC16: Spin Control in Twisted Van Der Waals Heterostructures I, August 22, 2022, 11:30 AM - 12:30 PM

In van der Waals heterostructures the layer distance strongly affects the interaction between the layers. Therefore, pressure is an ideal tool to engineer the band structure of van der Waal materials [1].
In this talk I will show two examples for the versatility of this method. First, I will show, that in WSe2/Gr structures spin-orbit coupling can be induced in graphene using proximity effects, which can be boosted using hydrostatic pressure [2]. The enhancement is confirmed using weak anti- localization measurements. Moreover, I will also demonstrate the band structure tuning of magic-angle twisted double bilayer graphene [3]. We have performed thermal activation and magneto-transport measurements to reveal changes in the bandgaps of the system. We have observed a strong tuneability with pressure, which is confirmed by our theoretical calculations. Finally, we have also observed changes in the strength of electron-electron interactions and in the topological phases at the charge neutrality point in magnetic fields.

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Tailoring the magnetic anisotropy of mono and dinuclear lanthanide metal-organic networks by metal exchange

Sofia Parreiras, Daniel Moreno, Borja Cirera, Miguel Ángel Valbuena, José Ignacio Urgel, Beatriz Muñiz-Cano, Cristina Martín-Fuentes, Koen Lauwaet, Markos Paradinas, Mirco Panighel, Fernando Ajejas, Miguel Ángel Niño, José Maria Gallego, Manuel Valvidares, Wolfgang Kuch, José Ignacio Martínez, Aitor Mugarza, Pierluigi Gargiani, Julio Camarero, Rodolfo Miranda, Paolo Perna, David Écija

MC12 : Physics in 2D Nanoarchitectonics II, August 22, 2022, 2:00 PM - 3:30 PM

Molecular magnetism is an emerging field with potential for technological applications as high-density information storage, quantum computing and spintronics [1]. Molecular systems based on lanthanides are especially promising due to the fundamental properties of lanthanides. Their strong spin-orbit coupling can lead to a high magnetic anisotropy while the strong localization of 4f states reduces the hybridization with surfaces increasing spin lifetimes [2]. Both, a high anisotropy and a large spin lifetime, are essential to increase the magnetic stability and to develop practical applications. Some lanthanide molecular magnet systems have already been reported, as the double-decker phthalocyanine family (LnPc2) [3,4], but up to now the magnetism of lanthanides metal-organic networks remains an unexplored field.
We performed pioneering investigations in this field preparing lanthanide-direct metal-organic networks using three molecular linkers: (i) benzene-1,4-dicarboxylic acid (TPA) coordinated with Dy on Cu(111) [5]; (ii) p-terphenyl-4,4-dicarboxylic acid (TDA) coordinated with Dy and Er on Cu(111) [5]; (iii) 4,4'-Di(4-pyridyl)biphenyl (DPBP) coordinated with Dy and Er on Au(111) [6]. The structural, electronic and magnetic properties were investigated by scanning probe microscopy (STM) and spectroscopy (STS), X-ray linear dichroism (XLD) and X-ray magnetic circular dichroism (XMCD). The experimental results were complemented by density functional theory (DFT) calculations and multiplet calculations. TPA and TDA linkers coordinate with lanthanides in almost square lattices with mononuclear metallic centers, and DPBP forms rhombic binuclear lattices. In both cases the network structure is preserved when the lanthanide atom is exchanged. However, the magnetic properties are drastically altered. The orientation of the easy axis of magnetization and the intensity of the magnetic anisotropy are strongly dependent on the metallic center and the molecular linker. Our results show that it is possible to tailor the magnetic properties of lanthanides by a proper choice of molecular linkers and metallic centers.

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Microfluidic model of micro-haemodynamics

Mr Qi Chen, Dr. Naval Singh, Dr. Kerstin Schirrmann, Dr. Igor Chernyavsky, Prof. Anne Juel

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

The human placenta is an essential organ for the developing fetus, which relies on well-orchestrated haemodynamics to deliver its multiple functions. The geometrical complexity of the placenta and lack of appropriate animal models mean that biomimetic laboratory models offer a powerful tool to investigate haemodynamics and haemorheology in the human placenta and other complex biological tissues. The placental microstructure is effectively a porous medium where the particulate nature of red blood cells (RBCs) is important. However, particle transport and its influence on permeability remain unexplored.
We use droplet and capsule suspensions in planar microfluidic porous media to explore the transport of deformable particles, with the aim of characterising rheology in this setting. Droplets are the simplest RBC analogues but they lack the shear elasticity of the real RBC. In addition, undesired coalescence and breakup limit their use in experiments. A better biomimetic model of RBC is provided by polydimethylsiloxane (PDMS) capsules of adjustable diameter and wall thickness, which are microfabricated using a 3D nested glass capillary device. Their elastic modulus can be varied by an order of magnitude by adjusting the chemistry and the capsules can further be deflated by osmosis to match the area to volume ratio of real RBCs. We test the aptitude of these objects to mimic the motion and large deformations of single red blood cells and of suspensions of RBCs in straight capillaries and arrays of contractions and expansions. Planar porous media of controlled geometry, porosity and different levels of disorder are then constructed by positioning cylindrical pillars in different spatial arrangements within a Hele-Shaw channel. Suspension flows are characterised in terms of the dynamic capsule distribution, flow resistance and permeability as functions of haematocrit (concentration of capsules), capsule geometry, disorder of the medium and capillary number, which provides a measure of the importance of viscous shear forces relative to elastic forces.

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Standing and traveling discrete breathers in bcc crystals

Yusuke Doi, Akihiro Nakatani

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter XII, August 26, 2022, 9:00 AM - 10:00 AM

Discrete breathers excited by nonlinearity and discreteness are expected to be applied as atomic-scale energy localized modes in crystals. In particular, it is expected to understand and apply the phenomena as an energy transport mechanism in the lattice, which is different from phonons. In this study, we investigate the dynamics of discrete breathers in a BCC crystal model using numerical simulations based on molecular dynamics simulations.

Two types of standing DB with different spatial symmetries are found by molecular dynamics simulation and the Newton-Raphson method used as temporal evolution. We investigate not only the localized core but also the structure of the surrounding atoms, and investigate the relationship between the spatial symmetry of the crystal structure and the spatial symmetry of the vibrational displacement.

A traveling DB, which propagates at a constant velocity through the system, is also found by the Newton-Raphson method. The obtained numerical solution of the traveling DB is demonstrated to propagate stably for a certain period of time, even when used as the initial condition for larger system sizes.

Furthermore, the stability and localized energy of standing DBs are evaluated and their relationship with DB mobility is investigated. We will also investigate how to provide a perturbation to generate a mobile DB from a standing DB.

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Thermodynamic stability of quasicrystals: From fluid dynamics to soft condensed matter

Prof. Ron Lifshitz

MC8: Complex Phases in Soft Matter V, August 23, 2022, 2:00 PM - 3:30 PM

The observation of quasicrystals in soft condensed matter [1,2] has provided insight into the ongoing quest to understand their formation and thermodynamic stability. I shall explain the stability of certain quasicrystals, using surprisingly simple classical field theories [3,4], by making an analogy to Faraday waves [5]. This will provide a recipe for designing pair potentials that yield a variety of periodic and aperiodic cluster crystals with prescribed symmetry, as confirmed by molecular dynamics simulations [6,7]. I shall attempt to identify a trend that might be emerging in going from fluid dynamics to soft matter, which may (or may not) eventually lead to an understanding of the stability of quasicrystals in complex metallic alloys.

Figure shows a dodecagonal (12-fold) cluster crystal, with two types of particles, interacting via predesigned pair potentials, obtained via molecular dynamics simulation. Taken from Ref. [7].

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Dynamical and elastic properties of Cd2V2O7 under high-pressure from ab initio simulations

Dr. Plácida Rodríguez-hernández, Prof. Dr. Alfonso Muñoz

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Due to their physical and chemical properties and the wide range of applications, pyrovanadates have attracted significant attention during the last decade. We focus here on the study of the Cd2V2O7 pyrovanadate that has multiple technological uses in photocatalysis, photoluminescence, and gas sensing, among many others. To optimize these applications, an accurate study of the dynamical and mechanical properties of this material is needed. We present an ab initio Density Functional simulation study of this pyrovanadate under high pressure. We found that this compound has two pressure-driven phase transitions below 10 GPa that involve substantial changes in the polyhedral coordination of Cd and V atoms. We report the elastic constants and mechanical properties of three phases under study, their Raman and Infrared phonons, and their evolution with pressure. The dynamical and mechanical stability under hydrostatic pressure is also analyzed.

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Optimal cold atom thermometry using adaptive Bayesian strategies

Jonas Glatthard, Jesús Rubio, Rahul Sawant, Thomas Hewitt, Giovanni Barontini, Luis A. Correa

MC20: Recent Advances in Quantum Thermodynamics with a Focus on Many-body Interactions VI, August 23, 2022, 4:00 PM - 6:00 PM

Precise temperature measurements on systems of few ultracold atoms is of paramount importance in quantum technology, but can be very resource-intensive. Here, we put forward an adaptive Bayesian framework that substantially boosts the performance of cold atom temperature estimation. Specifically, we process data from release--recapture thermometry experiments on few potassium atoms cooled down to the microkelvin range in an optical tweezer. We demonstrate that adaptively choosing the release--recapture times to maximise information gain does substantially reduce the number of measurements needed for the estimate to converge to a final reading. Unlike conventional methods, our proposal systematically avoids capturing and processing uninformative measurements. Furthermore, we are able to produce much more reliable estimates, especially when the measured data are scarce and noisy. Likewise, the resulting estimates converge faster to the real temperature in the asymptotic limit. Our method can be adapted to enhance the precision and resource-efficiency of many other techniques running on different experimental setups, thus opening new avenues in quantum thermometry.

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On-chip demagnetisation cooling of electrons

Francis Bettsworth, Samuli Autti, Richard Haley, Alexander Jones, Jonathan Prance, Michael Thompson

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Cooling micro- and nanoelectronic systems to low temperatures is typically limited by weak electron-phonon coupling below 10 mK. Achieving sub-millikelvin electron temperatures would benefit research in quantum systems, allowing for further improvements in applications such as metrology and sensing, as well as aiding the search for new physical phenomena. The demagnetisation of on-chip electroplated metals, such as copper and indium, can yield effective electronic refrigeration below the base temperature of dilution refrigerators. The technique has been demonstrated by adding copper and indium nuclear refrigerant to Coulomb blockade thermometers, which allow for primary electron thermometry throughout the cooling process. Several groups have been able to record low-millikelvin and sub-millikelvin temperatures [1,2], with the current record standing at 224±7 μK [3]. We are investigating new techniques for on-chip demagnetisation cooling and thermometry of the cooled electrons. Here we report on our latest simulations and experimental results.

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Novel nonlinear phenomena driven by intense, structured femtosecond magnetic pulses

Carlos Hernández-García

MC51: Ultrafast Dynamics in Magnetic and Strongly-Correlated Materials IX, August 25, 2022, 11:30 AM - 12:45 PM

The degree of control we have achieved over the manipulation of light is truly amazing. Initiated by our Greek ancestors using mirrors to guide light, we live in a world where the most advanced laser technology allows us to create and sculpt light beams with great precision. In particular, nowadays we can create ultrashort attosecond pulses (with durations of trillionths of a second), of very high frequencies (up to the soft X-rays), and with increasingly complex spatial structures thanks to our ability to harness their angular momentum. Very interestingly, by harnessing ultrafast structured laser pulses, it has been recently proposed the possibility to generate intense, ultrafast magnetic pulses isolated from the electric field.

In this talk we will review our recent work in the generation of structured ultrashort laser pulses, and their potential to explore ultrafast magnetism. On the one side, thanks to the highly nonlinear process of high harmonic generation (HHG), we can tailor the spin and orbital angular momentum properties of extreme ultraviolet/soft x-ray laser pulses directly at their generation. In particular we have found that HHG assisted by an intense, isolated magnetic field with the proper polarization choice, results in the emission of Fourier-limited attosecond pulses in the soft X-ray regime. On the other side, we show that non-linear magnetic field effects driven by structured laser pulses provide a way to manipulate the magnetic order of ferro- and antiferromagnetic materials. We introduce a novel ferromagnetic switching scheme on femtosecond time-scales that can be achieved by purely magnetic precession of the magnetization with field amplitudes of hundreds of Tesla.

In summary, structured laser pulses offer an appealing alternative to study sub-femtosecond magnetization dynamics, where a complete understanding of the electronic and spin interactions remains unexplored.

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Structural and electronic properties of vdW-2D materials combined with organic functional groups by first principles

Dear all Abdolvahab Seif, Pier Luigi Silvestrelli

MC52: Heterostructures, Combining Organic Molecules and 2D Materials V, August 23, 2022, 2:00 PM - 3:30 PM

In recent years, heterojunction materials bonded by interlayer van der Waals (vdW) forces have grown into a very large family. Afterwards, the concept of this material extended to the integration of those materials with molecular functional groups that adhere primarily through noncovalent interactions. The carrier properties of such a system are not only determined by the host material itself, but also defined by the interlayer interactions, including charge trapping centers and stacking angles. Generally, vdW interactions can modify the interaction strength with substrates and the orientation of specific molecular groups has profound consequences on the electronic properties of the system. We address the fundamentals of design strategies toward organic molecule-combined 2D vdW heterostructures by performing first-principles simulations based on the Density Functional Theory. In particular, we show how molecular shapes at the surface of 2D materials can be tailored to achieve precise control over functional groups. We also elucidate the vital role that intermolecular interactions (e.g Hydrogen, chalcogen or pinicogen bonding, π-π staking, etc) play for building up these hetereostructures. The structural differences resulting from molecular shapes, engineered intermolecular interactions, and tunable molecule-substrate interactions can greatly alter the properties of such 2D molecular films. For instance, (see the following figures and tables) we present how some different organic molecules (e.g. Dopamine, APTS and epoxy) could affect the interactions (Fig. 1) and electronic properties (Fig. 2 and Tables 1 and 2) of the 2D h-BNNS substrate combined with the organic molecules.

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Topologically driven phi0-Josephson junctions in TBG

Miguel Alvarado, Alfredo Levy-Yeyati

MC21: Bound states in hybrid superconductor nanostructures VIII, August 24, 2022, 4:15 PM - 6:00 PM

Recent experiments in superconducting Twisted Bilayer Graphene (TBG) point towards a non-conventional superconducting order parameter [1]. We study the effect of the topological nature of normal TBG in the current phase relation of Josephson junctions. We observe non-zero valley currents at zero phase-bias that become spontaneously uncompensated when the topological nature of normal TBG is taken into consideration, giving as a result phi0-junction behavior in direct Josephson junctions only when chiral superconducting order parameters (p+ip or d+id) are considered. This result could thus be used to identify the exotic order parameter in TBG.

[1] Oh, Myungchul, et al. Nature 600.7888 (2021): 240-245.

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Photon condensation in an arbitrary gauge cavity model

Dom Rouse, Adam Stokes, Ahsan Nazir

MC25 : Emerging Trends in Many-Body Cavity Quantum Electrodynamics X, August 25, 2022, 2:00 PM - 3:30 PM

There is a long history of `no-go' and counter theorems purporting that quantum models of many charges in a cavity cannot or can support a phase transition to a photon condensate (superradiant) state. At the heart of this debate is the role of gauge-relativity. Gauge-relativity is the notion that the definitions of the light and matter subsystems, which are themselves defined by the canonical momenta, are made relative to a choice a gauge. Gauge-relativity is a symmetry of electromagnetism.

For example, the Dicke model (a single-mode cavity model) when derived in the Coulomb gauge is known to support a phase transition to a ferroelectric state and not to a photon condensate state. However, when derived in the multipolar gauge within the long wavelength approximation, this Dicke model does show a phase transition to a combined ferroelectric and photon condensate state. This difference is not a breakdown of gauge-invariance, rather it is a manifestation of the gauge symmetry: subsystem definitions are gauge-relative and therefore so are the classifications of subsystem dependent quantities like phase transitions. Crucially, the phase transition always occurs in the same parameter regime when expressed in terms of gauge invariant quantities.

Recently, a multimode cavity-jellium model was studied in the context of photon condensation. In Ref. [1] it was found that a phase transition to a photon condensate state was possible in the Coulomb gauge of the jellium model if the electromagnetic field could vary in space. The authors showed that the phase transition was caused by a magnetic instability and derived a criterion that the magnetic susceptibility of a material must satisfy for it to support a condensate state.

In this talk, we will revisit the multi-mode jellium model using an arbitrary gauge theory in which the gauge-relativity of the condensation criterion is explicit. We find that in gauges other than the Coulomb gauge a condensate is caused by a combination of magnetic and electric instabilities. The relative contributions of the instability types, and the critical value which they must exceed, are gauge-relative.

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Finite temperature chemical potential of Bose gas in harmonic trap

Kouidri Smail

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

We present our numerical results of Bose gas in harmonic trap by using both Hartree-Fock Bogoliubov Popov approximation (HFB-P) and Generalized Hartree-Fock Bogoliubov approximation (GHFB). We derive a set Bogoliubov-de-Gennes coupled equations (BdG) governing the gas static comportment at finite temperature. We focus our study to a variation of the chemical potential created by the condensate atoms, the chemical potential created by the non-condensate atoms and heat specific. We analyze its comportment in Thomas-Fermi approximation at zero and at

nite
temperature. Finally, we compare our results with various recent numerical estimates and experience.

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Exploring Applications of Graphene-Based Josephson Junctions

Emily Gamblen, Roman Gorbachev, David Perello, Jonathan Prance, Max Taylor, Michael Thompson, Wendong Wang

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Local control over the critical currents and inductances of Josephson junctions is desirable for expanding functionality beyond what is possible with oxide tunnel junctions. Junctions where monolayer or bilayer graphene acts as a bridge between two bulk superconducting electrodes have shown to exhibit Josephson effects and a critical current which can be tuned using a local gate. This has been used to build Superconducting Quantum Interference Device (SQUID) magnetometers, qubits and parametric amplifiers. This poster will describe two other applications for controllable two-dimensional material (2DM) Josephson junctions: Andreev interferometers and local magnetometry of 2DMs.

Hybrid quantum interference devices (HyQUIDs) consist of a proximitised junction in a superconducting loop with normal metal contacts to measure the junction resistance. We have fabricated HyQUIDs with graphene junctions that have controllable carrier concentration. Transport across the junction is ballistic, allowing us to observe interference between a small number of conducting channels within the graphene.

Two-dimensional crystals are subject to significant interest due to their potential uses in Van der Waals heterostructure devices. Magnetic characterisation of these materials presents several challenges due to the small signals involved and the environmental requirements of some 2DMs. We are exploring experimentally how to use graphene-based SQUIDs [1] to measure magnetic properties of 2DMs on the same chip, taking advantage of the similarities between the fabrication processes of 2DMs and graphene SQUIDs.

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Graphene Josephson junctions for microwave devices

Max Taylor, Emily Gamblen, Roman Gorbachev, Artem Mishchenko, Jonathan Prance, Wendong Wang, Michael Thompson

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Encapsulated graphene can be used to create a robust Josephson junction (JJ) with an active bridge material. The semimetal graphene becomes superconducting due to the proximity effect, similar to more conventional SNS junctions. The key difference is that graphene's charge carrier concentration can be changed through electrostatic gating, which allows the critical current of the JJ to be controlled in situ [1]. This effect also influences the more complex circuits that use graphene JJs as a building block, including superconducting interference devices (SQUIDs).
One superconducting phenomenon is the generation of single flux quantum (SFQ) pulses, which are the basis of the SFQ logic [2]. SFQ pulses are generated by briefly biasing a JJ above its critical current, so that it undergoes a 2π phase shift, producing a voltage pulse which is quantised to the magnetic flux quantum Φ_o = 2.07 ps·mV. This allows for a low power, self-timing logic basis with inherently fast clock frequencies. However, the critical current of each junction in an SFQ circuit very important for proper operation, as pulses will be used to trigger further pulses throughout the circuit. Therefore, graphene JJs could help to optimise and reconfigure the performance of these devices post-fabrication.
A test device using graphene JJs was fabricated with the potential to act as a simple SFQ circuit for signal propagation. We investigate the device's low-frequency characteristics while being driven with a microwave source so that future measurements involving the propagation of high-frequency signals in the device will be well informed.

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Quasiparticle effects in transmons with gap-asymmetric junctions

Dr. Giampiero Marchegiani, Prof. Dr. Luigi Amico, Dr. Gianluigi Catelani

MC23: Superconducting Circuits for Quantum Technologies II, August 22, 2022, 2:00 PM - 3:30 PM

Single-particle excitations, known as Bogoliubov quasiparticles, threaten the operation of superconducting qubits. In this presentation, we theoretically revisit and generalize the qubit-quasiparticle interaction, including the gap asymmetry in Josephson junctions, which naturally arise from the deposition of aluminum layers with different thicknesses. We develop a semi-phenomenological description of the qubit-quasiparticle coupling in terms of quasiparticle densities. We show how the subtle interplay of generation, tunneling and relaxation mechanisms characterizes the steady-state of nonequilibrium quasiparticles. Two substantially different regimes are identified: 1) small gap difference, where quasiparticles are located at the larger gap energy in both leads and the excited state of the qubit is depleted 2) strong gap asymmetry, similar to or higher than qubit frequency, with quasiparticles trapped in the lower gap superconductor and reduced relaxation rate. The differences between the two regimes can be explored in a split-transmon, comprising a superconducting ring interrupted by two Josephson junctions, where the qubit frequency can be modulated on-chip. Our results may be relevant to the design of qubits with improved suppression of quasiparticle poisoning.

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Electronic properties of multilayer graphene on hBN for different stacking configurations of hBN

Robin Smeyers, Dr Lucian Covaci, Dr Milorad Milosevic

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Hexagonal boron nitride (hBN) has proven to be a far superior substrate for graphene compared to more traditional materials such as SiO_2, greatly enhancing Fermi velocity and suppressing the formation of charge puddles compared to the latter. Because hBN has a similar hexagonal lattice to graphene with only a slight mismatch in the bond-length, a moiré pattern emerges when used as a substrate. Here we investigate what happens when a bilayer and trilayer graphene is sandwiched between two hBN layers which are stacked in 5 highly symmetric configurations. By using a full tight binding approach, we found that the precise placement of the hBN layers changes the symmetry of the whole system, opening bandgaps in both the primary and secondary Dirac points, resulting in some cases in flat bands and allowing for their gate-tunability. Using classical molecular dynamics the systems were relaxed by which we show that most features that were observed are robust in nature, supporting recent experimental findings of superconductivity and strongly-correlated insulating states in such heterosturctures [1,2,3].

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Twisted ground state in achiral anisotropic fluids

Dr Alberta Ferrarini, Davide Revignas

MC8: Complex Phases in Soft Matter X, August 25, 2022, 2:00 PM - 3:30 PM

The director field of liquid crystals, which describes the local average orientation of particles, either molecules or colloids, can exhibit a rich variety of structures. This feature, combined with unique properties, such as tunability and sensitivity to external stimuli and boundary conditions, that come from the simultaneous presence of order and fluidity, is of particular interest for electro-optic and photonic applications. Structures in some cases form spontaneously, whereas in other cases they are induced by confinement or by interaction with inclusions or with light. It does not come as a surprise that, if the constituent particles are chiral, twisted structures may be formed, examples of which are cholesteric [1] and blue phases [2], or skyrmion configurations [3-4]. However, twisted director configurations were recently discovered also in achiral nematic materials [4-11]. This puzzled experimentalists and theoreticians and stimulated a re-examination of classical concepts of liquid crystal physics [12-14].
This talk focuses on the microscopic origin of spontaneous breaking of mirror symmetry in nematic materials. We will discuss this phenomenon using the simple model of hard rigid particles and we will highlight the role of the molecular/colloidal symmetry [15,16]. On these grounds we will show that hard rods, which since the seminal work by Onsager [17] are a traditional paradigm of uniform nematic order, do have a spontaneous tendency towards twisted structures [18].

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Electron-phonon decoupling in two dimensions

Professor Igor Lerner, Mr George McArdle

MC40: Strongly Disordered Insulators VII, August 24, 2022, 2:00 PM - 3:30 PM

In order to observe many-body localisation in electronic systems, decoupling from the lattice phonons is required, which is possible only in out-of-equilibrium systems. We show that such an electron-phonon decoupling may happen in suspended films and it manifests itself via a bistability in the electron temperature. By studying the electron-phonon cooling rate in disordered, suspended films with two-dimensional phonons, we derive the conditions needed for such a bistability, which can be observed experimentally through hysteretic jumps of several orders of magnitude in the nonlinear current-voltage characteristics. We demonstrate that such a regime is achievable in systems with an Arrhenius form of the equilibrium conductivity, while practically unreachable in materials with the Mott or Efros-Shklovskii hopping.

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Onset of charge fluidity in two dimensions

Dr Andrey Shytov

MC14: Beyond Charge Transport in Nanostructures and 2D Materials via Geometric Design VII, August 24, 2022, 2:00 PM - 3:30 PM

In a system with momentum-conserving interparticle collisions, flows of electric charge are expected to resemble viscous flows known from fluid mechanics, rather than more conventional Ohmic flows. In the last decade, the elusive regime of e-fluidity was observed in several low-density condensed matter systems, such as graphene. The viscous drag is manifested in the non-local resistance and the (odd) Hall viscosity. These responses become the strongest at the crossover between the ballistic and hydrodynamical regimes, i.e., at the scales comparable with the collision mean-free path. Analysing such flows theoretically presents a challenge, as there is no small parameter available. We shall present an analytical treatment of the quantum Boltzmann equation that enables a detailed and quantitative insight into the onset of fluidity in a half-plane geometry. Our method allows one to make a quantitative prediction for the vicinity resistance and signatures of the odd viscosity. The approach also predicts the distributions of voltage and current near an injecting source, which can be imaged with modern scanning probes.

The research leading to these results has received funding from the EPSRC of the UK (Project EP/T001194/1).

Figure 1: a flow generated by a point current source attached to an edge of an e-fluid. The streamlines are shown in black, and the potential distribution is shown via a red-blue pseudocolor map. The negative values of the potential (blue) are due to the viscous drag. It also results in negative vicinity resistance along the edge, as shown in the bottom panel. (Distances are given in units of mean-free path, while the potentials are in a.u.)

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Signatures of Non-Equilibrium in Optically Driven Dense Colloidal Suspensions

Dr Ilya Svetlizky, Dr Maayan Levin, Dr Shlomi Reuveni, Dr Arnab Pal, Prof. Saar Rahav, Prof. Yael Roichman

MC6: Emergent Phenomena in Driven Soft, Active and Biological Matter II, August 22, 2022, 2:00 PM - 3:30 PM

We use holographic optical tweezers to drive locally a quasi-2D colloidal suspension. As a result, the colloidal suspension experiences a smooth transition from strong driving to very weak driving as the distance from the location of driving increases. At steady-state, this gives rise to a non-uniform density distribution. We find that this density profile is a result of a competition between pressure-induced by normal forces due to shear and osmotic pressure. We then use this system to study Signatures of non-equilibrium such as entropy production as a function of driving strength.

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Quantum state preparation in mechanical resonators

Yaroslav Blanter

MC17: Nanomechanical and Electromechanical Systems VII, August 24, 2022, 2:00 PM - 3:30 PM

We present several theoretical proposals to create quantum states and entanglement of mechanical resonators. Of crucial importance is both their integrability into state-of-the-art quantum platforms as well as the ability to prepare them in generic quantum states using well-controlled high-fidelity operations. One proposal is to couple one [1] and two [2] qubits via a capacitor in parallel to a superconducting quantum interference device (SQUID), which has a suspended mechanical beam embedded in one of its arms. Using state-of-the-art parameters and qubit operations at single-excitation levels, we numerically demonstrate the possibility of ground-state cooling as well as high-fidelity preparation of mechanical quantum states and qubit-phonon entanglement. In a second proposal, following our work on cavity magnonics [3], we show how one can entangle two mechanical resonators or a magnon mode with a mechanical resonator using a superconducting qubit.

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Microfluidic flow of vesicle prototissues as a model for cellular tissues

Majid LAYACHI, Laura CASAS-FERRER, Gladys MASSIERA, Laura CASANELLAS

MC3: Tissue Dynamics, From in Vivo Experiments to in Silico Modelling XI, August 25, 2022, 4:30 PM - 6:00 PM

To circumvent the barriers to the comprehension of cellular behavior and its contribution to biological processes, the emergence of biomimetic tissue engineering has proved to be a valuable ally. Following this bottom-up approach, it has become possible to design model tissues. By isolating specific physical or chemical mechanisms, the complexity of biological processes such as morphogenesis can be broken down. Here, we focus on the mechanical characterization of such prototissues, specifically in flow conditions, based on a microfluidic approach.

Starting with the synthesis of custom Giant Unilamellar Vesicles (GUV), we proceed to assemble them through Streptavidin-Biotin based adhesion to obtain spheroidal prototissues. These prototissues show tunable vesicle-vesicle adhesion and size. Moreover, the latter can be comparable to the one of embryonic tissues. The assembled prototissues are then mechanically probed in a "pipette-aspiration" inspired microfluidic chip, coupled with epifluorescence microscopy, under controlled flow and pressure conditions.

We quantify the rheological response of the prototissue to a creep experiment and we describe the viscoelastic behavior observed with a modified Maxwell model. Moreover, flow velocimetry and fluorescence quantification provides the monitoring of phenomena happening at the meso scale such as tissue reorganization and vesicle-vesicle rearrangement.

This rheological tool allows the simultaneous study at two different length scales making a bridge between the global viscoelastic response of the whole prototissue and the adhesion properties between the individual vesicles. Designed for vesicle prototissue assays, it can be translated to the study of embryonic tissues, thus allowing a deeper comprehension by comparing the two tissular systems. This parallel can help giving valuable insights into the complex phenomena at the tissue scale observed during morphogenesis.

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Assessing, Predicting, and Validating Metastable Phase Formation via Irradiation

Vancho Kocevski, Ghanshyam Pilania, Benjamin Derby, James Valdez, Yongqiang Wang, Blas Uberuaga

MC38: Controlled irradiation Disorder in Model Systems: Organisation, Dynamics, and Transformations VII, August 24, 2022, 2:00 PM - 3:30 PM

Metastable phases – phases away from thermodynamic equilibrium – form when excess energy is present in the material. Irradiation naturally introduces stored energy into the system, often inducing phase transformations. However, it isn't always obvious what phases might form. Here, we use density functional theory to construct so-called metastable phase diagrams – phase diagrams that describe what phases will become favorable as more stored energy is introduced into a material. We examine the Ln2O3 series of compounds, important in their own right as dielectric materials, scintillators, and as neutron absorbers in fuels, as a case study. We predict a series of metastable phases with increasing stored energy that varies with the nature of the Ln ion. To validate the theoretical results, we perform ion beam irradiations of Lu2O3. We observe, as a function of fluence, a series of phase transformations directly corresponding to the predictions, not only validating the theoretical approach but also demonstrating that we can systematically explore the metastable phase diagram with irradiation. To the best of our knowledge, this is the first time that multiple crystalline-to-crystalline phase transformations have been observed in an irradiated oxide.

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Non-Markovian Dynamics of Decoherence in Bio-molecular Chromophores

Adam Burgess

MC20: Recent Advances in Quantum Thermodynamics with a Focus on Many-body Interactions VI, August 23, 2022, 4:00 PM - 6:00 PM

By utilising a spin-boson model, we study the dynamical decoherence of a Green-Fluorescent protein (GFP) due to being within a finite-temperature solvent environment. This is undertaken by deploying the Hierarchical Equations of Motion (HEOM) allowing for us to capture non-perturbative and non-Markovian characteristics of the system. We study both the monomeric form of GFPs as well as try to understand the anomalously long decoherence time for coherent energy transfer in the homo-dimer of GFPs. We derive spectral densities using the Fluctuation-Dissipation Theorem and a Debye dielectric model for the solvent environment. Having studied different system architectures, we see some very interesting properties of the evolution. The specific architecture of the GFP appears well suited to preserving the coherences in the homo-dimer system. We also find a dynamical correlation between the coherent energy transfer of these systems and the entropy production, even leading to transient reductions in entropy, a distinct feature of the non-Markovian approach. We also find that when accounting for different timescales of the environmental relaxation the system reduces to a free system Gibbs state appropriate for a weak coupling regime. However, by introducing additional rapid timescales the system diverges from this Gibbs state showing a transition away from weak coupling regimes.

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Wetting at the nanoscale: molecular desorption induced by a moving contact line

Thierry Ondarçuhu

MC7: Exploring Liquid Properties in Confined Geometry (Up To Mesoscopic Scales) VII, August 24, 2022, 2:00 PM - 3:30 PM

It is well established that the wetting properties of a surface by a given liquid largely depend on the topographic and chemical nature of the substrate, down to the nanometer scale. The coupling with the liquid can also trigger a modification of the substrate properties leading to complex situations of adaptative wetting [1]. In this context, the interplay between the substrate modification by the liquid and the dynamics of the drop is an open question in wetting science, which requires new specific experiments at the molecular scale.
Atomic force microscopy (AFM) is a unique tool to study the dynamics of contact line or nanomeniscus at the nanometer scale [2,3]. The monitoring of the capillary force exerted by the liquid on a nanoneedle carved at the apex of the AFM tip allows one to distinguish the effects of topographical and chemical defects and to monitor minute changes of the needle surface properties. In recent studies [4,5], we evidenced a change of wettability when the tip is continuously dipped in and withdrawn from the liquid a large number of times. We demonstrate that this leads to a decrease of the contact angle down to a constant value while keeping the topography intact. Interestingly, the initial surface properties can be recovered when leaving the tip in air. We interpret these results as the result of an adsorption of airborne contaminants on the tip surface and their desorption by the liquid. Using specific experiments, we unambiguously demonstrate that the desorption mechanism is induced at the contact line, as a result of the capillary force on the molecules, as already observed on particles [6]. Using a large range of liquids, tips and velocities, we present a comprehensive study of this effect and show its applications for monitoring molecules adsorption and desorption with a subsecond time resolution or for cleaning of surfaces.

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Molecular-substrate systems studied by scanning tunnelling microscopy: Spatial, energetic, and temporal resolution

Dr Alex Saywell, Mr Matthew Edmondson, Dr Eleanor S. Frampton, Dr Chris J. Judd, Professor Neil R. Champness, Professor Robert G. Jones, Professor Elena Besley, Professor Harry Anderson

MC18: Developments at the Frontiers of High-resolution Scanning Probe Microscopy I, August 22, 2022, 11:30 AM - 12:30 PM

The self-assembly and on-surface reactivity of molecular species is central to the concept of devices which incorporate the functionality of molecular components. [1] Materials with specific catalytic, electronic, optical, and/or magnetic properties can, in principle, be realised by an appropriate choice of molecular-substrate systems. However, the preparation of such materials requires an understanding of the processes which give rise to ordered molecular arrays and, in the case of covalently organic frameworks (COFs), the mechanics underlying the observed on-surface chemistry. [2] Ultra-high vacuum (UHV) scanning probe microscopy (SPM) approaches allow on-surface processes to be studied on the single-molecule and single atom level, [3] and in combination with photoemission spectroscopies can provided detailed structural and chemical characterisation. [4,5]

Here we present details of our recent work where scanning tunnelling microscopy (STM) techniques have allowed detailed characterisation of the energetic, and spatial, distribution of the electronic states within cyclic porphyrin polymers. [6] The high lateral resolution of STM, combined with the electronic characterisation offered by differential conduction maps, provides unique information on these materials. A similar approach can be taken to characterise single molecular species (Br functionalised porphyrins) and we demonstrate how single-point scanning tunnelling spectroscopy (STS) measurements, and differential conductance maps corresponding to specific electronic states, provide information which can allow the identification of chemical groups within single molecules and extended molecular structures. Additionally, we can make use of temperature-dependant SPM measurements to obtain information on the dynamics and energetics of on-surface diffusion of porphyrins, and the use of synchrotron-based photoelectron spectroscopies (e.g. XPS and NEXAFS) provides a route to quantify the chemical changes within on-surface reaction processes (e.g. self-metalation of porphyrins [7]).

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Topological Physics in Finite Graphene Structures: Theory and Experiment

Ms Maxine McCarthy, Professor David Whittaker

MC41: Real Space Simulations of Topological Matter and Disordered Materials III, August 22, 2022, 4:30 PM - 6:00 PM

The ideal graphene Hamiltonian, with only nearest neighbour interactions, has chiral (sublattice) symmetry. In two dimensions this symmetry does not lead to distinct topological phases; all Hamiltonians are topologically equivalent [1]. However, any real graphene structure will necessarily be finite: a ribbon, or a nanotube, or possibly a more complex connectivity. Hence a full understanding of the topology of graphene requires a treatment of these finite structures. For instance, finite graphene ribbons have been shown to host non-trivial topological states [2].

We present a topological classification of finite chiral structures based on the eigenvalues of the transfer matrix, evaluated at zero energy, which takes a state around a loop in the structure. The chiral symmetry means that these eigenvalues occur in mutually reciprocal pairs. Starting from a finite rectangular sheet of graphene and forming a loop by connecting opposite edges, a pair of unit eigenvalues for the loop transfer matrix corresponds to a pair of zero energy eigenstates of the Hamiltonian, demonstrating that the structure is topologically marginal. Thus the number of transfer matrix eigenvalues less than (or greater than) unity is a topological invariant. Different topological phases can be obtained by changing the strength of the hopping terms, either periodically or randomly.

There are many ways in which edges can be joined, potentially including twists to form a Möbius strip or Klein bottle geometry. We investigate the topological classification of these structures, and show that there are cases, such as a looped ribbon, where the transfer matrix eigenvalues are necessarily real, so distinct topological phases can be found. However, for others, including tori, the eigenvalues can be complex, so we can move anywhere in the complex plane by changing the hopping terms, avoiding passing through unity. This means that there are no topological phase boundaries.

Real graphene does not have exact chiral symmetry, due to next nearest neighbour hopping It cannot be fabricated into arbitrary structures and it is difficult to locally vary the strength of the hopping terms. Hence, in order to investigate experimentally the topological properties, we make use of a mapping from transmission line networks to tight binding Hamiltonians. A network made from sections of coaxial cable can, provided that the transmission time in each cable is the same, be described by a 'Hamiltonian' with nearest neighbour hopping's between nodes determined by the impedances of the corresponding cables [3]. Thus we can make a network model of an arbitrary graphene structure, with controlled nearest neighbour hopping terms, and by measuring the transmission between nodes, study the properties of the electronic states in graphene.

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Ultrafast electronic cooling in graphene/hBN van der Waals heterostructures using time-resolved photocurrent microscopy

Dr Jake Dudley Mehew, Dr Alexander Block, Jaime Díez Mérida, Rafael Luque Merino, Dr Dmitri K. Efetov, Dr Klaas-Jan Tielrooij

MC51: Ultrafast Dynamics in Magnetic and Strongly-Correlated Materials XI, August 25, 2022, 4:30 PM - 6:00 PM

Van der Waals heterostructures allow for the layer-by-layer design of complex material systems in which new physics and novel device properties can be studied. For instance, twistronics is a developing field in which topological and correlated phases of matter emerge in systems where individual layers are rotated with respect to their neighbours. It is of great importance to understand electron dynamics in such systems, particularly given the implications for electronic and optoelectronic applications.

Ultrafast time-resolved photocurrent microscopy enables the study of hot electron cooling at sub-picosecond timescales in nanoscale systems such as graphene. [1,2,3] In this pump-probe technique, the time-dependent photocurrent represents the temporal dynamics of the electron temperature.

Here, we investigate hot electron cooling dynamics in heterostructures of mono- and bi-layer graphene encapsulated in hexagonal boron nitride (hBN). We find that the cooling time constant varies from 1 to 100´s picoseconds as we vary the number of graphene layers, Fermi level, and electron and lattice temperatures.

These results are particularly relevant to fundamental studies of emergent quantum effects, including the Dirac fluid regime, [4] as well as more broadly for applications in high-speed electronics and optoelectronics.

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Fig. 1. Schematic of experimental setup. Graphene top gates (VA and VB) define the pn-junction in hBN encapsulated bilayer graphene. Ultrafast pulses illuminate the nanoscale junction generating a photocurrent.

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Polarisation of water under thermal fields: the effect of

the molecular dipole and quadrupole moments

Aidan Chapman, Professor Fernando Bresme

MC7: Exploring Liquid Properties in Confined Geometry (up to mesoscopic scales) X, August 25, 2022, 2:00 PM - 3:30 PM

Thermal gradients induce a wide range of powerful non-equilibrium coupling effects, such as the Ludwig-Soret and the Seebeck effects. These effects now have important applications in biomolecule sensing and nanoscale waste heat collectors, respectively. A more recently discovered coupling effect is thermopolarisation (TP) [1]. The application of thermal gradients gives rise to molecular orientation and subsequently electric fields, in polar fluids. Both water [1–3] and acetonitrile [4] have both been shown to exhibit this effect in simulations. The importance of thermopolarisation has been discussed in applications such as optothermoelectrics, mechanisms for sonoluminescence, in the study of bioelectric effects, and the microwave drying of materials.

In this work [5], we have used non-equilibrium molecular dynamics (NEMD) simulations to investigate thermopolarisation for four popular rigid water models (OPC, TIP3P, TIP4P/2005 and SPC/E). The effect is quantified by the thermopolarisation coefficient, S_TP, which is the ratio between the induced electric field and the applied thermal gradient. Near ambient temperatures this coefficient has a magnitude on the order of 0.1-1 mV/K [2,5] for all four models. Below an inversion temperature the coefficient is positive [3,5], but above which the coefficient changes sign and the field changes direction. We have precisely determined the temperatures of inversion for each model by applying thermal gradients that covers the temperatures of inversion. Clear lines of inversion can be seen on the density-temperature phase diagrams of all four water models investigated, due to changes in the inversion temperature with pressure.

The electrostatic potential in water can be expanded into multipole moments, with the dipolar and quadrupolar contributions dominating. This has allowed us to define an alternative criterion for the inversion in S_TP as the point where the dipolar and quadrupolar contribtutions to the field are equal and opposite. Furthermore, considering just these two terms, we have derived an expression for the thermopolarisation coefficient in terms of the molecular multipole moments, the average molecular orientation, and the thermal expansion coefficient.

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Predicting the emergent density profile in a stationary nonequilibrium population of polarising and migrating cells

Christophe Deroulers

MC6: Emergent Phenomena in Driven Soft, Active and Biological Matter I, August 22, 2022, 11:30 AM - 12:30 PM

Since the spreading of cancer cells in diffuse glioma (a type of brain cancer) seems to be one of the main reasons which make this disease almost impossible to cure in the long term, we try to build mathematical models of the collective invasion of healthy brain by these cells, at the scale of the organ, based on cellular automata formulated at the scale of cells.

Real cells exhibit, at least in vitro, a sequence of the following events: polarisation (with spatial extension) in some random direction, migration in this roughly constant direction, depolarisation (with spatial compaction), rest --- we neglect cell division by simplicity. Therefore we chose these rules (together with exclusion, a.k.a. hardcore repulsion) for our lattice-based models of cells (on square lattice and honeycomb lattice).

Extensive simulations in an out-of-equilibrium stationary situation between a source and a sink of cells show surprising emergent behaviour, as compared to linear diffusion or to cells which do not extend-and-retract when polarising and depolarising. Namely, there is a phase with nontrivial density close to the source, where diffusion is governed by the hopping of holes. This region is crucial for the whole emergent spatial pattern insofar as it governs the total flux of cells. We managed to get analytic predictions about it which are exact in the limit of infinitely large systems.

Further away from the source, where the density of cells is lower, we predict the spatial density profile thanks to an approximate nonlinear diffusion equation. We derived it from the rules of motion at the microscopic scale, neglecting high-order correlations. A full prediction (without fitting parameter) of the whole profile between source and sink is possible only thanks to the analytic formulas we got before about the flux in the high density region.

These results are robust vs. the lattice type and should also give hints about the non-stationary situation found in brain, namely invasion of space from a source without sink and with proliferation of individual cells. In the long term, this could help to cure the disease by testing and optimising numerically treatment strategies before choosing the most promising one. More generally, the same techniques can be applied readily to the many situations when living cells invade space by migration, being it other tumours, development of the embryo, or wound healing.

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Surface Incompressibility effect on Brownian Dynamics near a real Air-Water Interface

Stefano Villa, Christophe Blanc, Antonio Stocco, Maurizio Nobili

The presence of a confining interface breaks spatial symmetry of a fluid. Consequently, the dynamics of objects within the fluid in the boundary vicinity experiences an anisotropic and space dependent drag which depends on the boundary conditions at the interface.
While the mobility in the vicinity of a solid boundary, where no-slip or partial-slip BCs applies, has been widely experimentally characterized in the past, the dynamics of colloids close to a slip interface has received less attention and only few experimental results, mainly for gap distances larger than particle size, can be found [1]. At the same time, given the ubiquitous presence of air-water interface in many biological phenomena [2,3] and industrial processes [4,5], filling the gap between the dynamics in bulk water and at its interface with air is of a paramount interest.
To this aim, we systematically studied the 3D dynamics of both isotropic and anisotropic colloidal particles close to air-water interface until gap distances 1-2 orders of magnitude smaller than their size, where dynamics is more sensitive to BCs. A Dual Wave Reflection Interference Microscope has been specifically developed for this geometry [6]. Combining imaging and interferometry, it enables the tracking degrees of freedom both parallel and orthogonal to the interface. We then compared experimental results with theoretical predictions and simulations for both full-slip and no-slip BCs.
Intriguingly, while the dynamics of translational and rotational degrees of freedom parallel to the interface approaches more full-slip BCs expectations, the out of plane dynamics is compatible with no-slip BCs predictions. Such a puzzling result has been rationalized considering recent models of interfacial surface incompressibility BCs, resulting from the unavoidable presence of surfactants at water surface. Apart for the fundamental interest, practical relevance of such findings is straightforward as the present condition approaches much more than the classic free interface predictions real natural systems like swimming bacteria [3].
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Flows induced by a capsule of microalgae

Gabriel Amselem

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

When active particles are encapsulated in a droplet, the droplet exhibits a random motion. To rectify this random motion and obtain a directional trajectory of the droplet, the only current means is to place the droplet in an anisotropic solution of liquid crystals. Here, we encapsulate the microalgae Chlamydomonas reinhardtii in aqueous droplets and place them in oil. The oil is seeded with microparticles, enabling to track the oil flow induced by the encapsulated microalgae. The oil flow is tracked under different conditions: random swimming of microlgae in the droplet, directed swimming of microalgae in response to a light stimulus, and in the presence of photobioconvection patterns. The dependence of flow on algae concentration is studied, as is the flow asymmetry between two halves of a droplet. Our results will help understand under which condition it is possible to make move directionally a droplet filled with microalgae, and how to steer it with light.

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Quantum noise in cavity Bose-Hubbard systems

David Nagy

MC25: Emerging Trends in Many-Body Cavity Quantum Electrodynamics IX, August 25, 2022, 11:30 AM - 12:30 PM

We investigate the quantum measurement noise effects on the dynamics of an atomic Bose lattice gas inside an optical resonator [1]. The system is described by means of a hybrid model consisting of a Bose-Hubbard Hamiltonian for the atoms and a Heisenberg-Langevin equation for the lossy cavity-field mode. We assume that the atoms are prepared initially in the ground state of the lattice Hamiltonian and then start to interact with the cavity mode. We show that the cavity-field fluctuations originating from the dissipative outcoupling of photons from the resonator lead to vastly different effects in the different possible ground-state phases, i.e., the superfluid, the supersolid, the Mott and charge-density-wave phases. In the former two phases with the presence of a superfluid wavefunction, the quantum measurement noise appears as a driving term leading to depletion of the ground state [2]. For the latter two incompressible phases, the quantum noise results in the fluctuation of the chemical potential. We derive an analytical expression for the corresponding broadening of the quasiparticle resonances.

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Velocities of nanoparticles exiting the gas aggregation source through different orifices

Kateřina Škorvánková, Pavel Solař, Anna Kuzminova, Jaroslav Kousal, Ondřej Kylián

MC9: Recent Developments in Gas Phase Synthesis of Nanoparticles and Applications IX, August 25, 2022, 11:30 AM - 12:30 PM

Gas aggregation sources (GAS) are among the most common means used for the physical production of nanoparticles (NPs). In the GAS systems, the NPs are formed in high pressure (tens of Pa) aggregation chamber and subsequently ejected into low-pressure deposition chamber through an orifice installed at the end of the aggregation chamber. Naturally, the pressure conditions and orifice geometry may influence the velocity of the exiting NPs. The velocity is, in turn, an important parameter during the interaction of the NPs with their surroundings, e.g., in the case of in-flight modification / coating of NPs or during their landing onto a substrate. To control the speed of nanoparticles, it is necessary to find out the relationship between the velocities of nanoparticles and process parameters. These parameters include the pressure in the aggregation chamber, the length and the diameter of the orifice through which nanoparticles get from the aggregation chamber to the deposition chamber and the pressure in the deposition chamber.
A mechanical time-of-flight filter has been developed to measure nanoparticle velocities regardless of their size and charge. The dependence of velocities of nanoparticles on the pressure in the aggregation chamber and the pressure in the deposition chamber is presented alongside with the relationship between the nanoparticle velocity and the orifice geometry.

Acknowledgments
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Radiative heat transfer with a cylindrical waveguide decays logarithmically slow

Kiryl Asheichyk, Matthias Krüger

MC19: Advances in the Casimir Force and Heat Transfer Phenomena V, August 23, 2022, 2:00 PM - 3:30 PM

We show that radiative heat transfer between two far-field-separated nanoparticles placed close to a perfectly conducting nanowire decays logarithmically slow with the interparticle distance. This makes a cylinder an excellent waveguide which can transfer thermal electromagnetic energy to arbitrary large distances with almost no loss. It leads to a dramatic increase of the heat transfer, so that, for almost any (large) separation, the transferred energy can be as large as for isolated particles separated by a few hundred nanometers.

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Cryogenic CMOS Voltage Amplifier with variable power consumption for Quantum Transport applications

Mr George Ridgard, Dr Jonathan Prance, Professor Richard Haley, Dr Michael Thompson, Dr Viktor Tsepelin

MC24: Quantum Electronics at Ultra-low Temperatures XII, August 26, 2022, 9:00 AM - 10:00 AM

Research in Low Temperature Physics and Quantum Technology applications fundamentally require measurements of small electronic signals below 1 kelvin. Quantum Transport experiments are common in Condensed Matter Physics. These experiments are important for an array of immerging and established fields, such as graphene, 2D materials and topological insulators. The electronic signals are inherently tiny due to the energy scales involved at Low Temperature and are typically in the frequency range from DC to ~MHz. Cryogenic amplifiers are desirable or sometimes required to improve sensitivity. Amplifying the signal close to a sample at low temperature [1,2] can improve the signal-to-noise ratio and bandwidth. Commonly used and commercially available low temperature amplifiers are often based upon HEMT technology and have excellent noise characteristics and bandwidths [3,4]. Typically, these amplifiers have power consumptions on the order of 100 µW exceeding by one or two orders of magnitude the cooling power of commercial dilution fridges base plate temperatures around ~10 mK.
Here we report on a prototype of a DC-coupled cryogenic voltage amplifier with a tunable power consumption and a bandwidth in the range of 100kHz. We also present characterization measurements of the n-MOSFET used in the amplifier. The low threshold of the FET allows the power consumption of the amplifier to be tuned in-situ over a wide range, increasing the potential use cases.

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Interplay of Kondo, RKKY and frustrations: 2-impurity spin liquid and lattice perspective

Dr Krzysztof Wójcik, prof. Johann Kroha

MC50: Fermi Surface Topological Transitions - Effects of Interactions VIII, August 24, 2022, 4:30 PM - 6:00 PM

The phase diagram of the conventional 2-impurity Kondo model and its relevance to correlated lattice models have been a subject of a long debate. It features Jones-Varma quantum phase transition (QPT) between the Kondo and the RKKY phase, which is unstable against particle-hole asymmetry in the presence of inter-impurity charge transfer. I will present results obtained for a modified 2-impurity model, where each of the impurities is coupled to a different host, and the hosts (not impurities) are directly coupled by spin-spin exchange. The model exhibits Jones-Varma QPT even away from the particle-hole symmetry point. Even more importantly, a second QPT occurs upon tuning the same inter-host coupling to even higher values, where the system forms 2-impurity version of a Kondo-stabilized spin-liquid, a state with large, but not complete spin-spin correlations and non-universal impurity spectral density. At high Kondo couplings the Kondo and the spin liquid phase are connected by a continuous crossover.
Further evolution of the phase diagram in the presence of frustration shall be explained. This includes emergence of the phase exhibiting ferromagnetic correlations and stability of the spin-liquid regime. I will also discuss the possibilities for direct realization of these scenarios in quantum-dot structures and their relevance for heavy-fermion materials. The latter may be valid for the materials close to the spin density wave instability.

*This work was supported by the Alexander von Humboldt Foundation.
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Optomechanical nonreciprocal stabilization

Laure Mercier De Lépinay, Caspar Ockeloen-Korppi, Daniel Malz, Clara Wanjura, Matteo Brunelli, Andreas Nunnenkamp, Mika Sillanpää

MC17: Nanomechanical and Electromechanical Systems X, August 25, 2022, 2:00 PM - 3:30 PM

Cavity optomechanics has successfully proposed inventive cooling techniques for mechanical oscillators, allowing to bring phononic occupations of macroscopic motion modes below unity. On the other hand, in the past few years, mechanically-mediated, nonreciprocal coupling of electromagnetic cavities has been extensively studied as a means to engineer directional propagation of signal and noise. Interestingly, the directional exchange of noise between mechanical oscillators can be expected to propose a novel stabilization mechanism based on nonreciprocal coupling of mechanical oscillators. Ref. [1] demonstrates an experimental study of the impact of nonreciprocal coupling of a pair of membrane modes on their phononic occupancies. We propose interpretations of the observed signatures. We show that different simultaneous stabilization mechanisms coexist. Among these we show that one can indeed be identified as nonreciprocal cooling. Its impact must however be carefully distinguished from the other cooling mechanisms', for which we propose an experimental method. This method is carried out experimentally on a pair of drum resonators in optomechanical coupling with a microwave cavity. We show that a quantum limit exists to this reduction of fluctuations, which emerges in our experimental setup thanks to operation at low phonon numbers.

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In-situ Electrochemistry Applied to Electrochromic Materials

Florian Gillissen, Brandon Faceira, Abdelfattah Mahmoud, Aline Rougier, Rudi Cloots, Anthony Maho

MC48: Multi-modal Characterisation of Thin Film Optoelectronics for Energy Applications IV, August 23, 2022, 11:30 AM - 12:30 PM

In-situ electrochemistry represents a broad field of research and developments in which liquid- or solid-state electrochemistry setups are coupled with other analytical, spectroscopic methods so to better understand (opto-)electronic processes taking place in given materials, interfaces and devices. Over the years, numerous physico-chemical techniques have been adapted to be coupled with electrochemistry, and specifically UV-Vis-NIR spectrophotometry in so-called spectroelectrochemical (SEC) setups. The first demonstration of an SEC experiment was presented by Kuwana et al. in 1964 (Kuwana T., Analytical Chemistry 1964), with Sb-doped SnO2 glass being used as a transparent conductive electrode substrate to monitor the color evolution of an indicator during its oxidation. SEC therefore presents great interest to study the dynamics and kinetics of the different reactive mechanisms being induced by the application of the electrochemical bias, to identify species formed as intermediates during physico-chemical reactions taking place in the materials, etc.

This presentation will focus on the use of SEC methods to study the opto-electronic behavior and performances of electrochromic thin films and devices. Electrochromism is defined as the ability of a material to reversibly switch between different optical states upon the application of an electrochemical bias. In the case of transition metal oxides (WO3, NiO, V2O5), the modification in the optical properties arises from the insertion/extraction of cations (H+, Li+, Al3+, …) and electrons into the crystal lattice of the active species, ensuing the reduction/oxidation of the metallic ions (Wang Y., Annu. Rev. Chem. Biomol. Eng. 2016). Given this context, SEC methodologies, and especially the coupling of electrochemistry with UV-Vis-NIR spectrophotometry, allows a comprehensive study of the behavior of electrochromic materials submitted to different bias conditions. Most of the significant information on the electrochromic processes, such as the contrast in transmittance between optical states, the kinetics of coloration and bleaching, the amount of inserted/extracted charges as well as the efficiency of these electrochromic system, can be retrieved from SEC analyses (Denayer J., Appl. Surf. Sci. 2014; Chatzikyriakou D., Microporous Mesoporous Mater. 2017; Maho A., Sol. Energy Mater. Sol. Cells 2019)

Other techniques such as Fourier transform infrared (FT-IR), Raman spectroscopy, electron paramagnetic resonance (EPR) and nuclear magnetic resonance (NMR) can also be coupled with electrochemistry (Zhai Y., Nanoscale 2018). When coupled with X-ray diffraction (XRD) for Operando analyses, in-situ electrochemistry can be further exploited to monitor the evolution of the crystallographic properties of a material as a function of the potential being applied during the charge/discharge processes. The presentation will further highlight on-going work being conducted by our teams to successfully use this advanced technique with electrochromic materials, based on previous developments conducted in-house on battery-related powders and thin layers (Mahmoud A., Appl. Mater. Interfaces 2018; Jungers T., J. Mater. Chem. A 2019).

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Vibrational and optical properties of a non-ideal MoSSe Janus monolayer from first-principles calculations

Mr. Hamid Mehdipour, Mr. Peter Kratzer

MC52: Heterostructures, Combining Organic Molecules and 2D Materials V, August 23, 2022, 2:00 PM - 3:30 PM

Advanced synthesis techniques have made it possible to fabricate MoSSe monolayers with different 'upper' and 'lower' sides consisting exclusively of sulfur or selenium atoms, respectively. In addition to the well-known unique optical properties of transition metal dichalcogenide monolayers, such as a direct band gap, the MoSSe layer offers an intrinsic electrical dipole moment that could facilitate the adsorption of organic or water molecules. However, the complex preparation procedure inevitably leads to defects in the MoSeS layer. Aiming at a better understanding of their role, we carried out a first-principles study using a 3x3 or 4x4 supercell addressing the properties of a real, defective MoSSe layer. The enthalpies of formation calculated within density functional theory indicate that substitutional defects at the anion sites, S_Se and Se_S, are energetically most favorable, followed in stability by the single-atom vacancies V_Se and V_S. We study the defect-induced electronic gap states associated with these point defects. Besides these common defects that have a singlet ground state, our calculations predict triplet states for some energetically high-lying substitutional defects, e.g. MoSe and SeMo that may be detectable in electronic spin resonance spectroscopy. Moreover, the influence of point defects on optical absorption properties is addressed via calculation of the imaginary part of the dielectric function within the random-phase approximation, and the calculated results are compared to experimental data. Due to the different ionic character of Se and S, the vibrational spectrum of MoSSe is predicted to show a large gap between acoustic and optical phonons from 290 to 330 cm^-1. From our calculations, we observe that defected MoSSe shows characteristic localized modes of the defects energetically located inside this gap. Thus, they are expected to give rise to sharp features in infrared spectra that can be used as an experimental fingerprint for the type and concentration of point defects. In summary, our first-principles calculations aid the characterization of non-ideal MoSSe monolayers and will thus help to make this material a more wide-spread and usable choice for applications in which an intrinsic dipole moment and a fine-tuning of the band gap are desired.

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The structural, vibrational and mechanical properties in jammed packings of deformable particles

Dong Wang, John Treado, Arman Boromand, Michael Murrell, Mark Shattuck, Corey O'Hern

MC3: Tissue Dynamics: From In Vivo Experiments to In Silico Modelling X, August 25, 2022, 2:00 PM - 3:30 PM

Soft particulate materials, e.g. emulsions, colloids, cellular packings and tissues, are composed of discrete particles that can change their shapes when subjected to applied forces. Previous numerical models of these materials have employed either fixed-shaped particles or tessellations for confluent systems. In this talk, we will show models of particles with explicit deformability over a wide range of packing fractions in two (2D) and three (3D) dimensions. We have found that the jamming onset packing fraction for deformable particles depends on the particle asphericity and particle rigidity (i.e., particles with or without bending energy). Studies of the vibrational modes reveal a large number of low-frequency, quartic modes in jammed packings of deformable particles without bending energy. The number of quartic modes decreases with increasing asphericity and matches the number of missing contacts relative to the isostatic value for particles without bending energy, while the number of quartice modes is zero for particle packings with nonzero bending energy. We also find that the ensemble-averaged shear modulus scales as a power-law with pressure with a smaller exponent for particle packings with nonzero bending energy than those with zero bending energy. These findings underscore the importance of incorporating particle shape change when modeling soft particle systems. Further, our findings provide insight into many biological systems and processes, such as tumor invasion and morphogenesis.

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Stretching magnetic cells: from myoblasts to muscle differentiation

Irène Nagle, Nathalie Luciani, Claire Wilhelm, Myriam Reffay

MC3: Tissue Dynamics, From in Vivo Experiments to in Silico Modelling XI, August 25, 2022, 4:30 PM - 6:00 PM

Tissue mechanics drives growing interest in tissue engineering as mechanobiology represent an appealing way to produce differentiated tissue with specific function. The idea that forces drive cell fate arise an interest on mechanobiology. In contrast, translating this exciting approach to tissue engineering is not trivial. It implies to develop new approaches to control tissue formation and to stimulate them at will.

Skeletal muscle is a remarkable tissue with a multi-scale structure. It consists of aligned bundles of muscle fibers that originate from the fusion of hundreds of muscle precursor cells, the myoblasts. Creating in vitro models of skeletal muscle for the development of new drugs or gene therapies, reproducing both its architecture and its function represents a challenge for mechanobiology as it implies device to create large multicellular aggregates in 3D purely cellular elongated structures.
We manage to create muscle tissues models without support matrix by using magnetic muscle cells via the incorporation of biocompatible superparamagnetic nanoparticles. Magnetic labelling enables both the manipulation of cells at distance to create purely cellular aggregates of controlled shapes and millimeter size and the application of forces to organize them, measure their mechanical properties (biorxiv, 2021, DOI : 10.1101/2021.12.18.473332) or drive their differentiation.

We develop a magnetic stretcher (Du et al. Nat. Comm (2017)) by trapping a magnetic multicellular aggregate between two micro-magnets. This device allows to align cells, fuse them and to stimulate them to drive their differentiation to early muscle tissue. Influences of both the stimulation and the dimensionality were considered and compared on muscle differentiation looking at cell organization and biological markers.

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A tunable fiber Fabry-Perot cavity for hybrid optomechanics stabilized at 4K

Dr. Francesco Fogliano, Thibaud Ruelle, David Jaeger, Floris Braakman, Martino Poggio

MC17: Nanomechanical and Electromechanical Systems X, August 25, 2022, 2:00 PM - 3:30 PM

Hybrid optomechanical systems, which combine the capabilities of cavity optomechanics (COM) with cavity quantumelectrodynamics (CQED) promise increased optomechanical coupling, quantum control of mechanical resonators, quantum technology applications, and access to the physics of a fully coupled tripartite system.
Fiber Fabry-Perot cavities are an ideal platform for the realization of hybrid optomechanical system in the optical domain, making use of a mechanical resonator in an object-in-the-middle configuration. However, conflicting requirements for high finesse and small mode volume make their implementation challenging. We discuss here the implementation of an experimental platform based on high-finesse, micrometer-scale fiber Fabry-Perot cavity, which can be widely tuned using piezo-electric positioners. The combination of a stiff mechanical design, passive vibration isolation, and active stabilization using the Pound-Drever-Hall (PDH) technique combined with a digital filter, results in a mechanical stability of a few pm over many hours both at room temperature and at 4K.
Preliminary results of the mechanical properties of hBN drum resonators, positioned within the cavity mode volume by a second set of piezo positioners, will be discussed.

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Medial molecular motifs in tubular soft matter crystals:

Revisiting packing frustration and strong-segregation stability of block copolymer gyroids

Gregory Grason

MC8: Complex Phases in Soft Matter X, August 25, 2022, 2:00 PM - 3:30 PM

Supramolecular soft crystals are periodic structures formed by the hierarchical assembly of macromolecular constituents and occur in a broad variety of soft matter systems, from polymers and liquid crystals to biological matter. The building blocks soft crystals -- “mesoatomic” molecular groups -- are readily reconfigurable individually and collectively at the sub-unit cell scale, strongly coupling to periodic symmetries at supra-unit cell scale. In this talk I describe structure formation of soft crystals deriving from the assembly block copolymer (BCP) melts, a prototype for a broader class of supramolecular materials. While supramolecular crystals are observed to form crystal symmetries whose complex symmetries rival their hard atomic counterparts, rational frameworks for understanding and guiding these complex symmetry based on properties of the molecular constituents lag far behind. I will describe theoretical models that map thermodynamics of soft crystal formation in BCP onto geometric models which encode two competing tendencies. On one end, generically repulsive interactions favors minimal area of the inter-material dividing surface between unlike chemistries with mesoatomic domains. At the same time, the entropic cost of extending polymeric blocks to fill space evenly in these domains tends for favor uniformity in domain “thickness”.

We exploit this theoretical perspective to revisit long-held views of "packing frustration" in complex, supramolecular BCP crystals, which refers to the thermodynamics cost of "fitting in" to a domain that requires BCP chains to adopt variable extensions and shapes. Here, the particular focus will be on the bicontinous network phases, such as double gyroid (DG) and double diamond (DD), where it has been long held that packing in the intercatenated tubular domains plays a critical role in their stability. I describe the how the medial decomposition, a method developed in the field of computational geometry and recently extended to molecular assemblies, provides a natural means of measuring packing frustration in BCP domains. The medial set, which is the set of points equidistance to multiple points on a bounding surfaces, provides a purely geometric and fully general definition of the "mid-point" within BCP domains, and framework for quantifying the variable chain extension (or packing) within a domain of arbitrary shape and topology. In the context of the network phases, I show how the medial set of the tubular domain is in fact as 2D surface as opposed to a 1D skeleton, suggesting that previous heuristic notions of packing frustration have grossly overestimated the entropic cost of this domains. I describe a new strong-segregation theory calculation that incorporates a medial construction of intra-domain packing yields markedly lower free energy bounds on the DG and DD phases, to the point where it revises previous conclusions about their equilibrium stability in the infinite segregation limit for both linear diblocks and a larger family of elasitically asymmetric BCPs. Finally, I discuss the application of the medial analyses to directly quantify inhomogeneous packing from experimental BCP, and further how this analysis can be applied to address open questions in the BCP domain shapes in complex sphere phases (e.g. the Frank Kasper lattices).

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Evidence for coexistence of charge and antiferromagnetic orders in a high Tc superconductor

Cyril Proust

MC31: The Physics of Cuprates X, August 25, 2022, 2:00 PM - 3:30 PM

Multilayered cuprates possess not only the highest superconducting temperature transition but also offer a unique platform to study disorder-free CuO_2 planes and the interplay between competing orders with superconductivity [1]. After a short introduction on multi-layered cuprate superconductors, I'll present a recent study of quantum oscillation and Hall effect in magnetic field up to 88 T in the underdoped trilayer cuprate $HgBa_2Ca_2Cu_3O_8$. A careful analysis of the complex spectra of quantum oscillations strongly supports the coexistence of multiple competing orders [2]. In particular, our interpretation implies that a metallic antiferromagnetic state extends deep inside the superconducting phase, a key ingredient that supports magnetically mediated pairing interaction in cuprates [3].

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Subgap resonances in monolayer semiconductors with superconducting contacts

Ian Correa Sampaio, Mehdi Ramezani, Kenji Watanabe, Takashi Taniguchi, Zakhar R. Kudrynskyi, Amalia Patanè, Christian Schönenberger, Andreas Baumgartner

MC21: Bound States in Hybrid Superconductor Nanostructures III, August 22, 2022, 4:30 PM - 6:00 PM

Superconductor-semiconductor hybrid devices have attracted large interest, for example as potential hosts of topological quantum states [1], or as a source of spin-entangled electron pairs [2]. Many of these systems rely on essentially one dimensional nanowire crystals, with the corresponding limitations in device design and material choices. Here, we report experiments on superconducting hybrid devices based on single layers of the semiconducting transition metal dichalcogenide (TMDC) MoS_2, itself a promising candidate material for spin- and valleytronics applications [3]. In a first step, we introduce and characterize superconducting vertical interconnect access (VIA) contacts [4], with MoRe as the superconductor to contact fully boron nitride encapsulated MoS_2. The magnetic field and temperature dependence of the observed transport gap is consistent with the bulk value of MoRe, and possibly with a superconducting proximity region around the contacts. In a second step, we compare regular quantum interference resonances below and above the gap, suggestive of Andreev reflection at low energies. In addition, we present preliminary data on a «minigap» found at very low bias voltages, with a zero-bias peak forming at large magnetic fields, which we tentatively attribute to Andreev bound states forming in two dimensions, with characteristics determined by disorder near the contacts. Our experiments provide the first steps towards an ultimately thin semiconductor-superconductor hybrid material platform, using a technology that can be applied to a large variety of other layered, twisted and stacked materials.

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Why is the high-pressure 4-fold to 6-fold transition correlated to softening of zone-edge TA phonons?

Dr. B. A. Weinstein

MC46: Matter Under High Pressure III, August 22, 2022, 4:30 PM - 6:00 PM

Based on early pressure-Raman experiments on tetrahedral crystals to ~25GPa, a linear correlation was proposed between the threshold PT for transition from 4-fold to 6-fold bonding and the pressure-softening of zone-edge(ze) TA phonons.[1] The pressure range of this correlation has been tested repeatedly with inconclusive results. In fact, for crystals that transform at higher pressures the compression-induced frequency shifts of the TA(ze) phonons become progressively less negative, and even turn positive for AlN, BP, BeO and diamond, making a linear correlation with PT no longer possible. The reason is the competing contributions to the phonon frequency shifts from central bond-forces and non-central angular forces. Under compression, the former act to decrease, but the latter act to increase, the TA(ze) frequencies. Hence, a valid test for correlation between PT and the tendency for pressure to soften the TA(ze) frequencies should include only the central-force term that actually causes softening. To that end, an effective phonon pressure shift is computed using simple tight binding arguments to remove the non-central angular force contribution from the measured pressure shift. Even when the measured shifts are positive this effective shift remains negative. We test for a correlation of PT with the inverse of the effective pressure shift, also incorporating the ratio of shear-to-bulk moduli as a factor to account for shear rigidity. The test is performed for 25 zincblende and wurtzite materials.[2] A strong linear correlation (adj. R-square = 0.993) is found in all cases except for AlN. This correlation holds to at least 160GPa, the range of the BeO and BP transitions. Estimates at much higher pressure indicate that diamond also may be an exception. The obtained linear correlation has near unity slope, a fortuitous result that, along with the causes for the two exception materials, bears further study. The correlation has the following physical basis. In tetrahedral solids the pressure-softening of zone-edge TA modes is driven by the negative tension produced in the bonds by compression. This is just the central-force contribution to the pressure shift. The negative tension arises from increased electron overlap repulsion. This tends to redistribute the valence electron charge density, modifying the metallic and ionic character of the bonding to different degrees depending on ionicity. The resulting variation in interatomic forces eventually lowers the binding energy of the 4-fold phase below that of the 6-fold phase, which benefits from its two additional bonds. This qualitative physical picture, based on conventional bonding ideas, is sufficient to justify the strong correlation found between the softening of zone-edge TA modes and the threshold PT of the 4-fold to 6-fold transition. Compression-induced increase in electron overlap repulsion is the underlying cause of both phenomena.

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Dispersion of plasmons in 3D BCS Superconductors

Thomas Repplinger, Hadrien Kurkjian, Serghei Klimin, Jacques Tempere, Mathieu Gélédan

MC35: Collective Effects and Non-Equilibrium Phenomena in Quantum Gases and Superconductors VII,
August 24, 2022, 2:00 PM - 3:30 PM

Superconducting plasmons are interesting both from a fundamental point of view (the opening of a plasma gap in the Goldstone branch of a fermionic condensate is analoguous to the mechanism of mass-acquisition in high-energy physics [1]) and for practical applications, as they reveal the microscopic structure of superconducting materials like cuprate, where the existence of such low-energy plasmons was cited as a possible explanation of the critical temperature increase
in cuprates [2]. We make the link between 2 regimes, where the plasma frequency is bigger or smaller than 2Δ and we study the plasma branch (dispersion and lifetime of plasmons) when the plasma gap (corresponding to the plasma frequency) is close the pair-breaking continuum 2Δ. The dispersion of plasmons is pushed back when the plasma frequency is between 1.7Δ and 2Δ. We also show the coexistance of a broadened peak above the pair breaking continuum and an undamped peak inside the band gap.

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Oxygen related defects on silicon and their nanostructuring

Kieran Spruce, Dr Taylor Stock, Dr Tassem El-Sayed, Dr Steven Schofield, Prof Neil Curson

MC12: Physics in 2D Nanoarchitectonics III, August 22, 2022, 4:30 PM - 6:00 PM

The fabrication of atomic scale quantum devices is crucial for the progression of solid-state quantum computing technologies. Fabrication techniques are continuously improving towards this goal, including utilising scanning tunnelling microscopy and hydrogen desorption lithography to pattern 2D dopant-in-silicon device structures. Since the behaviour of devices made in this way critically depends on their atomic-scale environment, a complete understanding of all surface defects is required.

The most regularly reoccurring defects on hydrogen-terminated silicon, such as dangling bonds and dimer vacancies, are well characterised and understood, however the less common 'split dimer' (SD) defect is still the subject of debate. This defect has been previously described as a bridge bonded, non-monoatomic hydrogen atom in the dimer row [E. J. Buehler and J. J. Boland, 1999]. The contrasting view is that the defect is an oxygen atom in the same bridge bonded location - a siloxane defect [B. R. Trenhaile, A. Agrawal, and J. H. Weaver, 2006]. Here we characterise the SD defect by studying the relationship between the defect density and partial pressure of water during the hydrogen termination process. We also monitor the defect density as a function of time in ultra-high vacuum, over the period of 24 months, and assess the stability of the defect to hydrogen desorption lithography. The conclusion we draw from these experiments is that the atomic composition of the SD defect is oxygen-based i.e. the siloxane defect.

Finally, we present a method of reliably creating a high density of SD defects. At the highest defect densities, ordered arrangements of the defects can be seen, which agree with thermodynamic calculations for an oxygen-based defect. This order consists of repeating base units, with clusters of up to 6 defects. These results raise the intriguing possibility of precisely controlled atomic-scale oxidation for future device technologies.

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Synthetic morphogenesis driven by conditional gene activation in a human pluripotent embryonic stem cell population

Manon Valet, Ali Brivanlou, Eric Siggia

MC3: Tissue Dynamics, From in Vivo Experiments to in Silico Modelling XI, August 25, 2022, 4:30 PM - 6:00 PM

In vitro platforms are convenient tools to study spatialization and temporality of the signals triggering developmental events. The use of human pluripotent cells, representative of the earliest stages of human embryos, has opened an avenue to study embryonic and extra-embryonic lineage specification, using optogenetics or bio-engineered platforms to deliver biochemical programs in a restricted and controlled manner.
We present here a novel method to study lineage specification in human embryonic stem cells, whereby a gene representative of an extra-embryonic module - in this case GATA6, a key regulator of the primitive endoderm lineage - is activated in a salt-and-pepper manner. In absence of external signal, we solely rely on the interactions between the two emergent cell types to instruct a morphogenetic program downstream. The resulting patterning is thus fundamentally different from the one induced by position-based information in a morphogen gradient. We show that following this randomized gene induction, cells remodel their adhesions to segregate, forming two distinct compartments that subsequently undergo morphogenesis. We separately label and track both populations to investigate the dynamical properties induced by the expression of the master gene.
We envision that this methodology can be used to test functionally lineage markers identified through genomic studies, as well as to direct morphogenesis when the specific pathways responsible for embryonic boundaries constitution are unknown.

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Summary and prospects for curcuminoids in electronic devices and as 2D materials

Núria Aliaga-alcalde

MC12: Physics in 2D Nanoarchitectonics I, August 22, 2022, 11:30 AM - 12:30 PM

Curcuminoids (CCMoids) are a family of molecules, that includes curcumin, whose origin can be natural as well as synthetic. These molecular systems are well known in the field of biomedicine for their anti-inflammatory and antioxidant applications, with additional studies on their potential uses, among others, as antifungal and anticarcinogen agents.[1]
Apart from their potential in this area, there is a growing interest in the use of such units in other fields within Nanoscience and Nanotechnology. One of the reasons for this interest lies in the inherent and general nature of such molecules, being linear conjugated, and including a central -diketone group as well as aromatic units at the ends. Another advantage is that the CCMoid backbond can be fully modified; and many CCMoids can be obtained in one-pot reactions, with high purity and yields, with the possibility of scaling up the processes. This facilitates the creation of new generations of CCMoids, optimizing the molecular design and exploring new properties (colorimetric, sensing, optical and electronic, among others). My group, along with others, has been pioneer of these studies, initially with the use of CCMoids as chelates, in the creation of single-molecule magnets;[2] also as electron transporting materials in perovskite devices for photovoltaic cells;[3] as linkers, in the creation of 2D coordination polymers and MOFs,[4] and above all, as nanowires connecting graphene and gold electrodes in the study of two/three-terminal devices.[5]
Here, I will present CCMoids from a chemical point of view, emphasizing the structural peculiarities and the motivation for their study in the above mentioned fields, besides proposing new ideas and emphasizing the projection of CCMoids as active components on substrates.

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Bloch Oscillations in Disordered Mesoscopic Devices

J. M. Alendouro Pinho, S. M. João, J. P. Santos Pires, B. Amorim, J. M. Viana Parente Lopes

MC41: Real Space Simulations of Topological Matter and Disordered Materials III, August 22, 2022, 4:30 PM - 6:00 PM

Cold electrons in crystals can have their quantum nature unveiled as an oscillatory behaviour driven by uniform fields. Oscillating currents are well-known to appear as steady-state transport regimes of electrons that move across periodic lattices in the presence of static electric fields. Moreover, the eigenstates of such a system (Wannier-Stark states) are well localized in a region of space inversely proportional to the electric field strength. Previous work has further demonstrated this oscillatory behavior to be present in the propagation of single-electron (gaussian) wave-packets in one-dimensional tight-binding models biased by a sufficiently strong potential ramp, causing the wave-packet's motion to be oscillatory with a frequency proportional to the electric field strength [1]. In contrast, if the system has nearby bands that can be coupled by the potential ramp, through a spectral gap, the effects of Bloch-Zener tunnelling lead to an altered regime of Bloch oscillations that now develop two π-shifted periodic components [2]. These Bloch Oscillations are also spotted on mesoscopic transport systems, such as the partition-free Landauer setup [3], for high potential biases, and are responsible for trapping states inside the sample, resulting in a halt of current transmission between the leads. Conversely, a correspondence with the Landauer formula is expected for small biases [3].
In this work, the aforementioned results are re-analysed by numerically propagating the electron wave-packets in real-space using a Chebyshev method [4]. We perform a systematic analysis of a single-band, as well as a gapped two-band (ABAB-lattice) tight-binding model with and without disorder. In the context of mesoscopic transport, the current response to an electric bias in one- and two-dimensional tight-binding samples coupled to finite leads with open boundaries is analysed. For high applied voltages, we observe an emergent oscillating current and a proper connection to the localization of the Wannier-Stark states of the potential ramp is drawn. A steady-state local current response inside one of the leads is obtained and benchmarked against the Landauer
formula, with the equilibration time being estimated from the escaping rate of the states inside the sample. We also performed a similar study in a square sample connected as a Hall device in presence of an applied magnetic field. The measurement of the transversal current also shows an oscillating behavior for high longitudinal voltages. Finally, a possible connection of these effects to the emergence of a diffusive transport regime in 2D systems is exploited.

Acknowledgements
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Topological and optical solitons in frustrated chiral nematics

Professor Slobodan Zumer

MC8: Complex Phases in Soft Matter V, August 23, 2022, 2:00 PM - 3:30 PM

Topological and optical solitons in frustrated chiral nematics

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Frustrated chiral nematics are known for supporting a variety of metastable topological defect and solitonic structures controlled by confining geometry and anchoring conditions. Here we use modeling and simulation approaches to explain recent findings. First we focus to topological solitons characterized by topologically protected deformations of order parameter fields that are relevant in various fields of physics ranging from condensed matter to cosmology [1]. The interaction of light with selected topological solitons like torons [2] and twist walls [3] appearing in unwounded chiral nematics will be illustrated [4]. Further we focus to optical solitons where nonlinear media compensates diffraction spreading of light beams. We illustrate bouncing optical solitons in frustrated chiral nematics where self-focusing is strongly induced by chirality [5]. Interactions of both kind of solitons is expected to be interesting for applications to soft photonics [6].

Work was done in collaboration with Guilhem Poy, Ivan Smalyukh, and Andrew Hess.

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Integrating Ccmoids based wires and 2D COF in silicon for opto electronic applications

Dr Rossella Zaffino, Dr Raphael Pfattner, Mr Daniel Riba, Mrs Teresa Cardona, Dr Daniel Herrera, Dr Laura Rodriguez, Mr Marc Suros, Dr Arantzantzu Gonzales-Campo, Prof Herre van der Zant, Prof Nuria Aliaga-Alcalde

MC12: Physics in 2D Nanoarchitectonics III, August 22, 2022, 4:30 PM - 6:00 PM

Silicon will continue to play the central role in electronic devices and especially in high dense integrated circuits. Here, the incorporation of emergent 2D materials is expected to improve the performance of existing architectures beyond the limits of Moore law[1].
In this work, we analyze the integration of curcumin derivate wires into graphene nano-gap electrode devices toward the establishment of robust molecular transistors. We will present, moreover, the optimization of the delivery of novel Ccmoids 2D COF materials [2] on silicon/SiO2 substrates as the first step to studying their electrical behaviour aiming toward CMOS compatible devices.

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This work was supported by the project PID2019-108794GB-I00 (AEI/FEDER, UE) and the European Research Council Consolidator Grant Tmol4TRANS (ERC 724981). AGC and RP acknowledge the Ramon y Cajal fellowships program RyC 2017-229210 and RyC 2019-028474I.

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Decoupling nanoporous graphene from the metallic catalytic template by intercalation of self-assembled monolayers in ultra-high vacuum

Serni Toda Cosi, Markos Paradinas, Dominik Volavka, Jose Ramón Durán, M. Vilas-Varela, D. Peña, Aitor Mugarza

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Atomically precise nanoporous graphene nanoarchitectures can be synthesized by following a sequential reaction scheme that starts from specifically designed precursor monomers to obtain polymers, then nanoribbons, and finally the 2D nanoporous structure (1). This approach requires a metallic catalytic template, in our case Au(111). After its synthesis, the significant interaction between the NPG and the underlying Au substrate impedes its direct transfer to other substrates, or the analysis of its pristine electronic properties. Ohtomo et al. reported a procedure consisting on the intercalation of a self-assembled monolayer (SAM) comprised of 1-octanethiol that effectively decouple graphene nanoribbons and enable their transfer by means of mechanical (dry) methods (2). Alkanethiol SAMs are used to this aim because the Sulphur-gold bond that forms is quite strong, they form a crystalline structure, and the aliphatic chain acts as an isolating layer. However, this approach requires the immersion of the sample in a solution in ambient conditions, which can degrade the properties of pristine NPG. Here we demonstrate the intercalation of alkanethiol SAMs at the NPG/Au interface under ultra-high vacuum conditions. By optimizing the dose and thermal annealing parameters, we obtain SAMs of 1-octanethiol uniformly covering the macroscopic Au(111) surface. A structural Scanning Tunneling Microscopy (STM)study carried out at room temperature resolves different structural phases of the SAM intercalating under the pre-synthesized NPG. The decoupling of NPGs achieved in ultra-high vacuum can enable a clean, dry transfer of NPGs onto dielectric substrates, and also the in-situ study of their pristine (electronic, magnetic, optical) properties.

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Cylindrical Core-shell nanostructures of Mn-V oxides
obtained by electro-spray deposition on graphite

Mr Roberto Gunnella, Dr Rahul Parmar, Dr Sayad Rezvani, Prof Mauricio Rosolen

MC9: Recent Developments in Gas Phase Synthesis of Nanoparticles and Applications XI, August 25, 2022, 4:30 PM - 6:00 PM

Heterostructure based on metal sulfoxides nanomaterials can be relevant to the charge storage devices and also in many other processes using smart catalysts. Here, we show that Mn(CH3COO)2·4H2O and VOSO4·xH2O, by a scalable method with low-cost reagents employed, can react in ethanol/water droplets
generated by an electric field assisted spray system, so that MnSx-VSx/MnzV2O5 heterostructures in the shape of nanometric cylindrical particles can be deposited on a graphite foil substrate [1]. The composite material phases were analysed by spectromicroscopy tools, i.e., micro-Raman and scanning X-ray photoemission microscopy. The nanometric cylindrical particles were relatively homogenously distributed throughout the film covering the graphite foil. Film thickness modulation on surface was calculated between 100 and 300 nm range.
which is the optimized thickness for batteries and supercapacitor industries. We show that the segregation of MnV-O and MnV-S relative abundance in the internal and external volume of the cylindrical nanoparticles respectively, can be exploited during faradaic and non-faradaic processes in charge/discharge. Additionally, the MnSx-VSx/MnzV2O5/graphite electrode was subjected to Li ions intercalation for demonstrating its potential application in energy storage devices. Similar procedures have been considered for development of binder-free electrodes of high interest to electrochemical devices on carbon papers and felts instead of graphite. Moreover, electric-field assisted spray technique could be applied for further development of this emergent class of binder-free electrodes. These inputs will be the incipit to discuss the physico-chemical mechanisms of the growth and the parameter of optimization.
[1] Journal of Alloys and Compounds
Volume 888, 25 December 2021, 161483

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Porous silicon nanowires phase transformations at high temperatures and pressures

Javad Rezvani

MC46: Structure, Dynamics and States in Matter Under High Pressure IV, August 23, 2022, 11:30 AM - 12:30 PM

Porous silicon nanowires (NWs) with homogenous lateral dimensions of 90 nm are investigated by Raman scattering experiments along isothermal pressure cycles in a diamond anvil cell. Experiments were performed at variable temperatures up to 400 °C for maximal pressures of about 30 GPa comparing directly with transformations in bulk Si and porous NWs. Scanning electron microscopy demonstrates the persistence of one-dimensional morphology after high pressure investigation. The diamond phase in porous nanowires persists upon compression up to around 20 GPa at room temperature (25 °C) and to about 14 GPa at 200 °C and 400 °C. However, the β−Sn high pressure phase is seen to coexist with the diamond phase above 12 GPa at 25 °C and above 6 GPa at 200 °C and 400 °C. The coexistence region of the two phases is found to be considerably enlarged as compared with crystal silicon at each temperature. Upon decompression from 30 GPa, nucleation to the β−Sn, followed by formation of amorphous structures, is observed for porous NWs. Returning to ambient pressure and temperature, amorphous silicon is the dominant form with a residual contribution of β−Sn. At higher temperatures, nucleation back to the diamond structure is triggered although coexistence of amorphous and crystalline phases is observed up to 400 °C.

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Exploring the Phase Behaviour of Hard-Sphere Dimers

Mr Omar-farouk Adesida, Dr Livia Bartok-Partay, Dr David Quigley

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Hard sphere potentials are of particular interest due to their ability to express complex behaviour while being relatively cheap. Studies have explored the phase spaces of hard sphere dimers with varying bond lengths, L[1][2]. The phase behaviour of these regions is not trivial to decipher without prior information on the stable and metastable phases being known beforehand, hence, this project demonstrates the use of the Nested Sampling(NS) algorithm as a technique which better explore the phase space of hard-sphere dimers, sampling over different values of L and pressure. NS is a technique developed in 2004[3] which is able to sample configurations from regions which occupy a particularly small phase volume, and can locate and characterise the phase transitions and crystal structures present in this regime without any specific knowledge of the system[4].

For L values between 0.1 to 0.3, rotator phases - where dimers occupied lattice sites but were still free to rotate - were detected at lower pressures, whereas at higher pressures a close-packed crystal phase was observed. Meanwhile for L values of 0.9 to 1.0, at high pressures an aperiodic crystal phase was observed, where individual hard-spheres occupied lattice sites within the crystal, but the bond-order was found to be random[5]. At L values of 0.5 to 0.8, the stability of the crystal becomes more difficult to elucidate, which suggests that significant portions of the phase volume in this region are occupied by amorphous states, hence estimating properties of the system at this point may require higher resolution sampling.
To aid our understanding of the characteristic behaviour of this system, experiments studying similar systems with softer potentials and less rigid bonds, such as LJ potentials with harmonic bonds can provide a useful insight into how to to explore the phase space of more complex molecular systems effectively.

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Scanning Probe Microscopy Studies of Ion-Patterned FeRh

Adrian Peasey, William Griggs, Rantej Bali, Thomas Thomson

Antiferromagnetic (AF) spintronic devices are an active area of study at present, and FeRh is one of the most promising materials for these devices. There is a need for stable, non-volatile devices to provide room temperature storage, and metamagnetic phase change materials present a possible solution in the form of antiferromagnetic anisotropic magnetoresistance (AF-AMR) memory[1]. The AF state produces no stray magnetic fields and is itself insensitive to externally applied fields, however in the ferromagnetic (FM) state the electron spins can be aligned by an external field due to the presence of a net magnetic moment in the lattice[1].

Materials such as FeRh are able to be reversibly and reliably transitioned between the AF and FM states using controlled temperature changes[2]. Equiatomic FeRh is an antiferromagnet at room temperature and transitions to a ferromagnet at around 370K, with the transition temperature approximately 10K higher during heating than cooling[3]. The phase does not change uniformly, with the FM state forming nucleations which expand to cover the whole device as it is heated, and these may be characterised using magnetic force microscopy[4].

The room temperature magnetic ordering may be manipulated by irradiating the surface with light noble gas ions, which introduce lattice disorder leading to ferromagnetic regions[5]. Lithography may be coupled with this technique to produce magnetic patterns without significantly altering the topography, allowing such films to be used in devices such as multilayer stacks. This work provides nanoscale characterisation of patterned FeRh through scanning probe microscopy techniques.

The first aspect of the work uses magnetic force microscopy to observe the effect of thermally cycling a patterned device, and demonstrates the persistence of the ferromagnetic structures over multiple cycles. The second makes use of the secondary effect that the electrical resistivity of FeRh films is significantly different between the two states[6], allowing the local magnetic configuration to be measured via electrical measurements. The metallic conduction required the development of bespoke conductive microscopy techniques, which have been used to probe the local resistivity of this sample.

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Multi-class classification of crystal lattice waves

Jānis Bajārs, Filips Kozirevs

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter X, August 25, 2022, 2:00 PM - 3:30 PM

Recently in [1] we proposed data-driven machine learning algorithms for classification and detection of lattice waves in one-dimensional crystal lattice models. Linear and nonlinear kernel Support Vector Machine classifiers (SVCs) [2, 3] were trained to differentiate between linear phonon and nonlinear localized waves, also known as intrinsic localized modes (ILMs) or discrete breathers (DBs), based on locally sampled data of particle displacements, momentum and energy density values. Efficiency of classification algorithms was further improved by two dimensionality reduction techniques, i.e., principal component analysis (PCA) and locally linear embedding (LLE) [2]. Motivation of this work stems from the open and challenging problem of study and detection of localized energy transport by lattice excitations in numerical simulations of muscovite mica crystal models [4, 5, 6]. Such phenomenon is also supported by laboratory experiments [7]. Proposed methods were analyzed and successfully applied to multiple discrete breather simulations to detect localization regions. Machine learning algorithms were able to detect ILMs in crystal lattice simulations. In general, developed methodology extends to any one-dimensional crystal lattice model which supports localized wave solutions. In this work we have extended SVCs to multi-class problem where we are able to differentiate between linear phonon waves, stationary and propagating DBs. We explored dimensionality reduction techniques PCA and LLE and observed that it is not sufficient in multi-class problem to reduce data dimensionality to two dimensions, therefore, classification algorithms such as linear and nonlinear kernel SVCs should be trained in high dimensional spaces. Trained multi-class classifiers in combination with sliding window object detection method are applied to discrete breather collision numerical simulations. Not only the localization regions are detected, but the particular type of localized waves is identified as well.

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Control-based exploration of bubbles in Hele-Shaw channels.

Sammy Ayoubi

The non-linearity of multiphase flows is primarily due the deformation of the interface between two fluids. Analytical solutions of these systems are not always available, while numerical simulations can be very computationally expensive. Stable steady-state solutions are usually easy to observe experimentally, however it is practically impossible to observe unstable-steady states. Control-based continuation is a recently developed experimental technique which explores unstable steady-state solution branches, without the need of a mathematical model or a priori information of the system. The unstable steady-states are detected by performing a parameter sweep, controlling the free-surface to a steady-state, then measuring the final states of the control inputs. Controlled steady-states which do not need invasive control, indicate steady-state solutions of the uncontrolled system. As well as a solution-finding method, control-based continuation has the potential to control free-surface unstable-steady states, which has many applications in microfluidics. Control-based continuation has been applied to simple mechanical problems such as oscillating springs and bending beams but has yet to be applied to a complex problem such as free-surface fluid flow. We apply control-based continuation to search for steady-state solutions of a dynamical system, in which an initially stationary air bubble positioned in the centre of a Hele-Shaw channel, filled with silicone oil, is perturbed by a constant pressure from each side of the channel walls next to the bubble. In the uncontrolled version of this system, the bubble deforms to become elongated for low perturbing pressures, while deforming to a dumbbell shape for high perturbing pressures, and in both cases quickly translates sideways away from the perturbing force. Numerical simulations predict that only one stable steady-solution exists, which is when the perturbing pressure is trivially zero. The simulations further predict the existence of two unstable steady-state solution branches, in which the deformed elongated and dumbbell bubbles do not move sideways when being perturbed. In practise these unstable steady-state solution branches can not be observed experimentally, so we apply control-based continuation to experimentally find and observe them. Four actuators are placed in a rectangular array around the centre of the channel, when the bubble moves sideways the appropriate actuators inject fluid into the channel to push the bubble back towards the centre of the channel. Once a steady-state is achieved, the final amplitudes of the actuators are recorded. In this poster we present preliminary results of the experiment, which show that control-based continuation can control unstable steady-state bubbles in Hele-Shaw channels, while also being used as a tool to compute bifurcation diagrams without the need for a mathematical model.

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Engineering electrical lattices to support resonant, gap, or edge localized modes

Lars English

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter IX, August 25, 2022, 11:30 AM - 12:30 PM

The unit cell properties, crystal structure, and coupling characteristics of electrical lattices can be tailored to make them hosts for a variety of nonlinear localized excitations. Here we explore three examples through experimental measurements and numerical simulations: (a) resonant localized modes in a lattice with second-neighbor interactions exhibiting oscillatory wings, (b) bright and dark localized modes in the bandgap of a diatomic lattice, and (c) edge localized modes in a finite two-dimensional honeycomb lattice near the Dirac points in frequency.

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Liquid-infused stainless steel and different types of polymer surfaces.

Thanaphun Jitniyom

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Slippery liquid-infused porous surfaces (SLIPS) consist of a micro-nano-porous substrate infused with an inert, water insoluble, non-toxic liquid lubricant that forms a slippery overlayer on the top. Recent studies have shown that SLIPS can be used to repel various liquids and microorganisms, exhibiting huge potential for applications in both engineering and biomedical industries. In order to achieve sustainable slippery properties, the micro-nano and porous structures will need to confine and stabilise the infused lubricant layer. In this work, by using femtosecond laser ablation, we fabricate micro-nano and micro-nano-porous surface structures inspired by pitcher plants that can accommodate slippery lubricant. This occurs on various polymeric and metallic materials including: poly (ethylene terephthalate) (PET), poly (methyl methacrylate) (PMMA), polyamide (PA), polycarbonate (PC), polyethylene (PE), High-density polyethlene (HDPE), polypropylene (PP) and stainless steel. Silicone oil has been applied onto the micro-nano-porous network substrates to generate a slippery surface following the pitcher plant idea. This poster demonstrates the experiment results and detailed investigation of a single droplet on various nano-micro and porous network structures. Our results show that droplets of water exhibit low contact angle hysteresis between the advancing and receding contact angles on the lubricant-infused surfaces. These results will be used to guide further design of SLIPS with low adhesion properties and long-term sustainability.

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Collective modes as precusors of the phase transition in superfluid Fermi gases

Hadrien Kurkjian, Jacques Tempere, Serghei Klimin

MC35: Collective Effects and Non-Equilibrium Phenomena in Quantum Gases and Superconductors IV, August 23, 2022, 11:30 AM - 12:30 PM

I will discuss the collective excitation spectrum of a superfluid Fermi gases at and around the critical temperature. In this regime, the response of the system to a driving pairing field is dominated by a collective mode with a quadratic dispersion.
Still visible above Tc, this mode acts as a precursor of the phase transition. It evolves from a relaxation mode (of pure imaginary frequency) to a propagating mode as a function of the interaction strength, and it can be observed by coupling the gas to a reservoir of Cooper pairs.

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Determination of sub-ps lattice dynamics in FeRh thin films

Michael Grimes, Professor Thomas Thomson

MC51: Ultrafast Dynamics in Magnetic and Strongly-Correlated Materials IX, August 25, 2022, 11:30 AM - 12:45 PM

FeRh is an archetypal system for the investigation of ultrafast behaviour in coupled transitions due to its meta-magnetic phase transition occurring around 380 K [1]. In this coupled phase transition, the electronic structure transforms lowering the resistivity by ≈ 33%, the lattice expands isotropically with a volumetric expansion of ≈ 1%, and the magnetic order changes from a G-type antiferromagnet (AF) to a ferromagnet (FM) [1], [2]. Previous x-ray diffraction (XRD) studies have indicated that the lattice expands with first-order dynamics within 10-30 ps [3], with long-range AF order throughout the transition [4]. The sub-ps capabilities of the SACLA free-electron laser allowed for investigation of the ultrafast behaviour of the FeRh lattice upon laser excitation. This shows new dynamics at high fluences which were compared to the quasi-static behaviour of the Bragg peaks as measured using heated XRD. We describe the lattice temperature (see Fig. 1a) and expansion as a function of pump-probe delay. We have observed a perturbation to the expected dynamics above fluences of 5 mJ cm-2 where the lattice initially contracts before finally expanding as predicted. We demonstrate that a model (see Fig. 1b) using a transient lattice state [5] can explain the observed behaviour. Our model suggests that the transient state is paramagnetic, reached by a subset of the phonon bands which are preferentially coupled to the electronic system [6]. A complete description of the FeRh structural dynamics requires consideration of coupling strength variation across the phonon frequencies.

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Analysis of Theoretical and Experimental Performance of Travelling Wave JPA's in the Three Wave Mixing Regime with Considerations of Fabrication Tolerances

Mr Searbhán Ó Peatáin, Mr Tom Dixon, Dr Jonathan Williams, Dr Phil Meeson, Dr Sergey Kafanov, Prof Yuri Pashkin

MC23: Superconducting Circuits for Quantum Technologies V, August 23, 2022, 2:00 PM - 3:30 PM

The ability for high amplification with quantum limited noise have made Josephson Parametric Amplifiers (JPA's) a vital device for many highly sensitive metrology experiments. Although, due to the resonant structure in these devices they suffer from an inherent gain-bandwidth trade-off which limits their use in experiments over a large frequency range such as qubit read out or axion detection.

This requirement can be met by re-engineering of the Josephson element into a travelling wave structure, such as a transmission line, thus removing the bandwidth limitation while still allowing for large gain. These Travelling Wave JPA's (TWJPA's) have been shown to work in two regimes, three or four wave mixing, with varying degrees of success. The three wave mixing regime promises larger dynamic range and easier separation of signal tone from pump and parasitic tones than four wave mixing [1,2]. Experimental results have, unfortunately, not yet managed to replicate the promises of theory leading to proposals for novel amplifier designs and technologies [3].

We present here our recent simulation results of TWJPA schemes completed in open-source WRspice along with Coupled Mode Equation solutions. These results are then compared with experimental results and the discrepancies discussed, with special attention given to the importance of impedance matching and other factors towards a successful device [4].

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SWAP gate between a Majorana qubit and a parity-protected superconducting qubit

Luca Chirolli

MC21: Bound States in Hybrid Superconductor Nanostructures V, August 23, 2022, 2:00 PM - 3:30 PM

High fidelity quantum information processing requires a combination of fast gates and long-lived quantum memories. In this work, we propose a hybrid architecture, where a parity-protected super- conducting qubit is directly coupled to a Majorana qubit, which plays the role of a quantum memory. The superconducting qubit is based upon a π-periodic Josephson junction realized with gate-tunable semiconducting wires, where the tunneling of individual Cooper pairs is suppressed. One of the wires additionally contains four Majorana zero modes that define a qubit. We demonstrate that this en- ables the implementation of a SWAP gate, allowing for the transduction of quantum information between the topological and conventional qubit. This architecture combines fast gates, which can be realized with the superconducting qubit, with a topologically protected Majorana memory.

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QED fluctuation phenomena for non-reciprocal media in and out of equilibrium

Matthias Kruger

MC19: Advances in the Casimir Force and Heat Transfer Phenomena II, August 22, 2022, 2:00 PM - 3:30 PM

Casimir forces and heat transfer have been found to show a variety of interesting phenomena which are specific to nonreciprocal media, such as persistent heat flow in thermal equilibrium [1], repulsive forces [2], or propulsion forces out of equilibrium [3]. In this contribution, we discuss general properties possibilities of fluctuation phenomena involving non-reciprocal media [4], such as the question of stability, ruled out for reciprocal media [5], and the question of existence of a multi-body Casimir potential in situations involving persistent heat currents.

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Collective dynamics of self-propelled camphor rotors

Dr. Jyoti Sharma, Mr. Ishant Tiwari, Professor Dibyendu Das, Professor Veronique Pimienta, Professor V. S Akella, Professor M. Rivera, Professor Punit Parmananda

MC6: Emergent Phenomena in Driven Soft, Active and Biological Matter VI, August 23, 2022, 4:30 PM - 5:30 PM

Collective dynamics, being one of the most common and spectacular portrayals of coordinated behaviour of autonomous units, is ubiquitous in nature. On a daily basis, we witness many cases of collective motion in living objects such as humans, birds, ants and non-living objects such as cars, etc. Recently, there has been an increasing interest in the investigation of collective dynamics of artificial self-propelling objects. The aim of such studies is to understand and explore the underline dynamics in the complex biological entities, however, in an easy to control and establish lab setup.
To this end, we present experiments on pinned self-propelled camphor rotors. Camphor particles are a well-known example of artificial interfacial swimmers. A camphor rotor(ribbon)is a rectangular paper with camphor infused in its' matrix. This rotor performs self-motion at the air-water interface due to Marangoni forces induced by the surface tension gradient around it. Two coupled camphor rotors showed rotational synchronization on the fluidic surface[1]. Rotors experience chemical coupling via the camphor layer on the water's surface. Synchronization was observed at a pivot to pivot distance less than twice the length of a single rotor. Furthermore, we found that multiple such pinned rotors placed in different geometries also show the synchronised dynamics [2]. The number of synchrony modes depends upon the number of ribbons used and the geometry of ribbon placement.
Apart from synchronisation, we have investigated yet another interesting collective behaviour of rotors-Chimera-like states. These states emerged in three homogeneously coupled camphor ribbons placed on triangular geometry [3]. They are characterised by the coexistence of one synchronised and two unsynchronised groups of camphor rotors. Our findings demonstrate a chimera-like state with a minimum network of active rotors.
Recently, we reported aperiodic bursting dynamics of a camphor rotor [4]. Aperiodic bursting is specified by an irregularly repeated run (motion) and halt (stop) of a rotor. Subsequently, the aperiodic rotor was entrained with external periodic forcing. Moreover, synchronised bursting of two aperiodic-coupled rotors was observed.
We rationalise the mechanism via a numerical model, incorporating the Yukawa type interaction between the point particles constrained to move a circle[1] [2] [3]. This minimalist model qualitatively reproduced the synchronised and chimera-like states observed in the experiments

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Designing and Characterising Magnetic Superstructures in Vacuum Deposited Phthalocyanine Thin Films

Mr Harry Demetriou

MC48: Multi-modal Characterisation of Thin Film Optoelectronics for Energy Applications VI, August 23, 2022, 4:15 PM - 5:45 PM

Phthalocyanines are a class of polyaromatic molecules presenting favourable optical, physical and electronic properties for a plethora of technological applications. This includes optoelectronics, spintronics, as well as quantum information processing. Production of phthalocyanines as molecular thin films is a novel approach toward such applications with greater device compatibility, where further development and understanding of interactions between deposited molecules and at the substrate interface are developed through multi-modal characterisation.

Crystallisation of planar phthalocyanines occurs into columnar stacks with a characteristic tilt angle, via π-π interactions, with adjacent stacks interacting through van der Waals forces. Their macrocyclic structure allows the coordination of core nitrogen atoms to a wide range of transition metal ions or functional groups. This has a significant effect on physical properties, altering charge transfer, as well as influencing magnetic properties of the molecule and film ensemble. Mixed film phthalocyanines have been investigated in literature, where stronger electrostatic interactions between the two components facilitate increased structural order and charge transfer, improving properties for prospective optoelectronics and spintronic applications.

In this work, vacuum deposition is employed to reliably deposit high purity mixed thin films of non-planar vanadyl phthalocyanine (VOPc) and planar iron or zinc phthalocyanine (FePc/ZnPc). By selectively utilising combinations of spin-active and diamagnetic phthalocyanines in a controlled stoichiometry, regimes with favourable magnetic and conductive properties for magneto-optical, spintronic and quantum information processing applications can be obtained. Co-deposition is explored on a range of weakly interacting substrates, as well as utilising a templating layer of perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA) to effectively control phthalocyanine molecular orientation. Composition and molecular orientation are varied, where superstructures of alternating or isolated spin-active phthalocyanines occur depending on the stoichiometry. Coordination of metal ions with the oxide moiety of VOPc is used as a potential driving force for ordering between the two species and formation of superstructures.

Electron paramagnetic resonance (EPR) spectroscopy is utilised to investigate spin-properties of the ordered films. The orientation-dependence of the signal, supported by detailed simulations, provides information about the spread of molecule-substrate angles. Grazing-incidence wide angle x-ray scattering (GIWAXS) measurements are further used to provide a complementary detailed texture analysis. Synchrotron-based diffraction measurements are also used in combination with UV-Vis spectroscopy, among other spectroscopic techniques, to characterise molecular mixing and morphological properties. Orientation-dependent magnetic exchange interactions are studied through superconducting quantum interference device (SQUID) magnetometry, providing further multi-modal characterisation of mixed thin film structures. Choice of different transition metal ions within a controlled structure provides the opportunity to help build methodology for creating structural regimes with new optoelectronic and magnetic properties.

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Hubbard Model for Quasicrystalline Potentials

Emmanuel Gottlob, Ulrich Schneider

MC41: Real Space Simulations of Topological Matter and Disordered Materials II, August 22, 2022, 2:00 PM - 3:30 PM

Quasicrystals represent a middle ground between periodic and disordered materials. They possess perfect long-range correlation, yet they are not periodic, thereby giving rise to novel physics. This offers an exciting challenge for condensed matter physics, as we cannot resort to the usual toolbox based on Bloch's theorem. In our group, we have recently realised a 2D optical quasicrystal, i.e. an eighfold rotational symmetric optical lattice potential, for ultracold atoms [1,2].

In this talk, we will present a numerical method for constructing the Hubbard Hamiltonian of non-periodic potentials and illustrate it in the case of the above quasicrystal. We will show how to construct quasicrystalline Wannier Functions without resorting to Bloch's theorem and use them to extract the on-site energies, tunneling amplitudes and on-site interaction energies.

Finally, we will show how re-expressing the quasicrystalline lattice sites in a suitable configuration space – where sites are ordered in terms of shape and local environment – provides us with a description of the infinite-size quasicrystal.

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“Total” Ion Beam analysis and 3D imaging of thin films using MeV ion beams technique: latest development at Surrey Ion Beam Centre to characterise material composition

Pierre Couture, Matthew K Sharpe, Jeevan Dulai, Callum Mcaleese, Geoff W Grimes, Vladimir Palitsin, Jonathan England

“Total” ion beam analysis (IBA) is a characterisation technique combining multiple individual IBA techniques i.e., Rutherford backscattering (RBS), elastic recoil detection (ERD), particle induced x-ray emission (PIXE) [1]. Total IBA technique provide more information than the sum of the individual techniques [2]. Total IBA bring the advantages of each technique used while reducing each individual technique limitation [1]. X-ray analysis techniques are not depth sensitive, thus PIXE will be used to analyse elemental composition of the entire structure the incident beam encounter. While RBS and ERD are depth sensitive, light element samples on heavy substrate are better characterised with ERD and heavy element samples on light substrate are better characterised by RBS [3]. The advantageous setup combining RBS and PIXE is common in some laboratories like in Surrey to improve the elemental mapping and depth profiling of samples [4]. The addition of the ERD for light element detection provides access to new fields of research i.e., analysis of organic semi-conductors, oxide thin films and hydrogenated steels [5]. RBS uses the backscattered incident ion beam after interaction with the sample while ERD used the recoil of the sample’s light elements.

At the Surrey Ion Beam Centre, we have a 2MeV Tandetron accelerator with an analysing chamber containing 2 RBS detectors for 3D metrology analysis, 1 PIXE detector and 1 classical ERD detector. The goniometer inside the chamber allows for classical IBA and channelling IBA. Channelling techniques are often used to characterise crystalline materials (when aligned to the channel, the backscattering yield and x-ray counts decrease; the amount of decrease can be used to assess crystal quality, damage or doping). We are improving our total IBA offering with the latest addition of a time-of-flight elastic-recoil-detection system (TOF-ERD). TOF-ERD increases the accuracy analysis compared to conventional ERD and combines the ERD and RBS analysis simultaneously. Also, TOF-ERD can analyse every element lighter than silicon individually without overlapping signal.

We will present the latest achievement at the Surrey Ion Beam Centre in terms of total IBA using examples of our work on silicon carbide which is an example of material being research for electronic applications.

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Interactions of solitons with a localized impurity in Schrödinger lattices with saturable nonlinearity

Joël François Tsoplefack, Jesus Cuevas-Maraver, Faustino Palmero Acebedo, Astero Provata, Dimitri Frantzeskakis

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter XIII, August 26, 2022, 10:00 AM - 11:00 AM

We study the interactions of moving discrete solitons with a localized impurity in periodic systems described by the discrete nonlinear Schrödinger equation. The localized impurity is modeled by the delta function. Numerical simulations of collisions between moving solitons and the impurity show that the soliton can be transmitted, reflected, trapped or scattered by the imputity during the interaction, depending on the velocity of the incoming soliton and the impurity strength. The trapping of soliton is explained by resonance between the soliton and the nonlinear impurity mode. For different values of the soliton frequency ranging from \omega = 0.1 (high amplitude) to \omega=0.9 (small amplitude), we elucidate in details as a function of impurity strength and soliton initial velocity, the different regimes of soliton-impurity interaction (pure trapping, pure transmission, pure reflection, reflection and transmission, trapping and transmission, trapping and reflection, and trapping with reflection and transmission). We observe that as the soliton frequency increases towards 0.5, the trapping region becomes larger, and becomes narrower when it increases from 0.5 to 0.9. We determine specific values of impurity strength and soliton initial velocity for which the incoming soliton is split equally into a reflected and transmitted parts (for \omega=0.7 and \omega=0.9), and for which we observe the phenomenon of "double" trapping and "simple" transmission followed by "simple" trapping and "double" transmission (for \omega=0.3).

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Oxygen driven spreading and microphase separation of eukaryotic cells

Jean-paul Rieu, Adrien Carrère, Olivier Cochet-Escartin, Christophe Anjard, François Detcheverry, Mete Demircigil, Vincent Calvez

MC3: Tissue Dynamics, From in Vivo Experiments to in Silico Modelling XI, August 25, 2022, 4:30 PM - 6:00 PM

Cells exhibit multiple responses to environmental stresses. A state of low oxygen (O2) occurs frequently in soil, water and multicellular tissues and has played a pivotal evolutionary role in shaping multicellularity. We study the mechanisms of a novel behavior in the amoeba Dictyostelium discoideum (Dd) in which cells collectively regulate their motility and adhesion in response to self-generated hypoxia.

Below a millimetric culture medium film, Dd cells grow until some critical density. Then they stop to grow, and assemble in compact domain with a characteristic size of typically 100µm surrounded by a dense cellular gas phase. These domains stay mobile and stable in size during several days. Moreover, if one changes the O2 atmospheric level or the height of the medium, aggregate will quickly equilibrate with a new characteristic size and spacing (Fig. A-B). Vertically confining a not too dense micro-colony of Dd cells in a growth medium with a non-gas permeable coverglass triggers cells to move quickly outward of the self-generated central hypoxia area and thus form an expanding ring propagating for days (Figure C, [1]).

These observations as well as microfluidic experiments with imposed O2 gradients highlight the importance of oxygen regulation and self-generated gradients as an emergent organizing principle for biological matter. The variety of cell behaviors are modeled using both mean field PDE models and Monte-Carlo Lattice models with a few measurable parameters: cell division rate, motility (diffusion constant), aerotactic speed, oxygen modulated cell-cell adhesion and consumption [1]. In particular, the new dynamical microphase separation of Dd results from a balance between a long-range repulsion, trough self-generated O2 gradients due to O2 consumption, and a short-range attraction due to cell-cell adhesion.

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Figure: (A) Dd aggregates under a culture medium layer of varying height, with the height profile from the dish wall (left) drawn above. (B) Zoom on one aggregate surrounded by a cellular gas phase (arrows point to the first layer of cell flattened on the surface). (C) Spreading of a Dd covered spot of cells with a ring formation moving outwardly toward free O2.

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Finding higher order Van Hove singularities in practice: a method for detailed multi-band models with applications to Sr_2RuO_4

Dr Anirudh Chandrasekaran, Joseph Betouras, Claudio Chamon

MC50: Fermi Surface Topological Transitions - Effects of Interactions V, August 23, 2022, 2:00 PM - 3:30 PM

Recent angle resolved photoemission spectroscopy (ARPES) and tunneling conductivity measurements have led to the discovery of higher order Van Hove singularities (HOVHS) near the Fermi level in quite a few materials. Nevertheless, a conclusive theoretical diagnosis of HOVHS in real materials is often difficult to obtain since real materials may not always be amenable to simple and analytically tractable tight-binding treatment where only a few bands are taken into account. In this presentation, we will outline a method that we recently developed, based on a generalization of the Feynman-Hellmann theorem, that allows us to directly extract the Taylor expansion of the energy dispersion of bands at arbitrary k points in large and detailed multi-band models. As an illustration of its application, we will use it to resolve the long standing question of the existence of an ‘extended’ Van Hove singularity in Sr_2RuO_4.

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Blood memory effect in 3D microconfined structure

Amirreza Gholivand, Prof. Minne Paul Lettinga

MC7: Exploring liquid properties in confined geometry (up to mesoscopic scales) VIII, August 24, 2022, 4:30 PM - 6:00 PM

The significance of healthy blood vessels and blood flow for proper brain functioning is becoming more recognized as the involvement of brain vasculature in the development of human neurodegenerative disorders, notably Alzheimer's disease, is increasingly recognized [1]. Therefore, it is of interest to develop a platform to investigate blood flow and blood cells behavior through brain vasculature. The field got a boost with the introduction of microfluidics, which allowed to study the effects of morphological parameters systematically, mostly using 2D channels with rectangular cross section. The main drawback of this approach is that the 2D micro-channels are inherently different from the physiological vessels [2].
Here we present model 3-D microfluidic channels to study the RBCs flow through different vessels geometry and their flow dynamics. RBCs in microcirculation and at bifurcation may attain different memory effect this effect is studied systematically varying the interaction strength between the red blood cells and the complexity of flow geometries. To this end, we make use of a novel technique, Selective Laser-induced Etching (SLE), which can produce 3D structures in glass with any desirable shape [3]. To study the shape memory of the vessels the second generation of the bifurcation has been implemented with a parallel and perpendicular orientation relative to the first bifurcation, see Figure 1a. Using ultra-fast microscopy in combination velocimetry analysis we identify a new memory effect, where there is a shift in the maximum velocity, depending on the orientation of the downstream bifurcation, see Figure 1b.

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Geometric anomalies in non-relativistic topological matter

Jaakko Nissinen

MC13: Topological and Geometrical Effects in Complex Nanostructures II, August 22, 2022, 2:00 PM - 4:00 PM

I discuss geometric anomalies in topological matter that extend the definition of topological and geometric phases in terms of field theoretic anomalies and bulk-boundary correspondences to situations where non-relativistic geometry and symmetries, in addition to topology, play a key role. Such anomalies can be understood based on chiral gravitational anomalies with torsion, controversial in relativistic field theory, and their suitable generalizations to non-relativistic systems.

As examples I discuss anomalous chiral hydrodynamics and torsional anomalies in chiral Weyl superfluids, superconductors and semimetals, as well as topological-geometric ``translational" responses in crystalline insulators and semimetals, including subsystem and higher-order multipole insulators.

In contrast to usual relativistic anomalies, the discussed geometric anomalies are "unquantized" and feature properties of the momentum space geometry and Fermi surfaces in terms of UV-IR dependencies but nevertheless define phases of matter via the associated responses.

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Quasi-particle excitations and nonlinear dynamics in an attractive Bose-Bose mixture

I-Kang (Gary) Liu, Nick Proukakis

MC35: Collective Effects and Non-Equilibrium Phenomena in Quantum Gases and Superconductors VII,
August 24, 2022, 2:00 PM - 3:30 PM

We study the quasi-particle excitations in an attractive Bose-Bose mixture: the presence of attractive interactions leads to a drastic decay in the excited dipole mode and localized excitations in the density overlapped region, as already characterized in joint experimental-theoretical work [Phys. Rev. Research 3, 033096 (2021)]. The fully 3D Bogoliubov-de-Gennes approach for highly anisotropically harmonic traps allows us to investigate the complex couplings for different types of excitations with huge particle number imbalance. We introduce a systematic way to define, characterize and focus on the important modes, of which the excited component in the experiment are found to be coupled to the transverse multi-pole and longitudinal surface modes for the other, and the nonlinear mode mixings are measured in the basis of the quasi-particle modes. The complete knowledge of the quasi-particle excitation profiles can also be implemented to engineer shapes of external potentials to excite specific types of motions.

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Nonlinear quantum optics with Josephson meta-materials

Arpit Ranadive, Martina Esposito, Luca Planat, Giulio Cappelli, Gwenael Legal, Sebastien Leger, Dorian Fraudet, Vincent Jouanny, Edgar Bonet, Cécile Naud, Olivier Buisson, Wiebke Guichard, Jose Aumentado, Florent Lecocq, Nicolas Roch

MC23: Superconducting Circuits for Quantum Technologies V, August 23, 2022, 2:00 PM - 3:30 PM

Josephson meta-materials have recently emerged as very promising platform for novel quantum optics experiments in microwave domain. Engineering them at sub-wavelength scales can allow complete control over wave dispersion and non-linear interactions.

We will discuss experimental realization of a broadband non-linear Josephson meta-material composed of an array of superconducting non-linear asymmetric inductive elements (SNAILs). The asymmetry in the SNAILs allows tuning and sign reversal of the Kerr and second order non-linearity by applying an external magnetic flux. The sign reversal of non-linearities at sub wavelength scales can also be utilized for their suppression.

We will present use case of such meta-material as a near quantum limited broadband amplifier, a key pillar for rising quantum technologies and in general for applications that rely on the low noise readout of weak microwave signals [1].

The range of applications of these nonlinear meta-materials is not limited to amplification. They are also promising candidates for multi-mode entanglement generation to realize quantum optics experiments in the microwave regime. We will present the experimental operation of the broadband meta-materials as a source of two-mode squeezed microwave radiation, demonstrating broadband entanglement generation and discuss the perspectives of these results [2].

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Charge transport in materials by mobile nonlinear inter-atomic interactions called quodons.

Dr Francis Russell

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter X, August 25, 2022, 2:00 PM - 3:30 PM

The transmission of charge by mobile, highly-localized, nonlinear lattice excitations through various materials including polymers and metals is reported. The excitations, called quodons, are created by collisions of swift particles with a material. Filters made of PTFE allow separation of conduction-currents from quodon-currents. This allows study of the existence and propagation of quodons in metals and semiconductors. Demonstration of ability of quodons to propagate across interfaces of different materials revealed their pervasiveness. This suggested the structure and stability of a quodon is not critically dependent on the structure of the material. The cause and sources of free-charges in a material that are trapped by quodons are revealed in time-resolved spectra of the quodon-currents. It was found that significant fractions of quodon-currents can be short-circuited or blead to ground by insulators used in coaxial cables and connectors. This can result in complete loss of quodon-current to ground by even a short length of coaxial cable connecting to a current meter. This loss can be minimized by use of magnetic levitation or vertical hanging of samples from a current-meter. However, this does not eliminate loss to ground potential by insulating material used in the input connector of a current meter. These losses pose a serious problem in exploiting the exceptional properties of quodons for practical applications to power transmission systems. So far, transmission of quodons can only be stopped by inserting in a circuit, or a supporting structure, a gap containing a gas or vacuum. This limitation is not surprising as quodons are similar to phonons as both involve inter-atomic interactions. This suggests the possibility of using multiple layers of materials of very different density and atomic mass to impede quodons. Nevertheless, it is possible to construct a practical source of quodons to exploit their ability to anneal defects or, at higher intensities, cause structural damage to organic materials such as DNA. One such device is described. Finally, it is expected that quodons will be created copiously in devices involving swift ions, such as potential fusion reactors.

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The nanostructured MoO3 films prepared by electrospray: A new way for technologial devices

Maryam Azizinia, Javad Rezvani, Francesco Paparoni, Roberto Gunnella

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

In this research work, nanostructured MoO3 thin films by the electrospray deposition method has been investigated. To this purpose, a Molybdenum trioxide aqueous solution sprayed on both metallic and non-metallic substrates. In each individual experiment the process was done while applying a positive voltage, and a fixed gas fellow. The topic is of interest because in the recent past the electrospray deposition method, as a novel coating process for thin-film devices, has gained a great attention. Furthermore, MoO3 as a transition metal oxide is an absorbing subject for both fundamental and technological issues and for several applications, including microelectronic devices, sensors, and etc. due to its properties and the multiple valence states of Molybdenum. In the present work, the synthesized samples have been characterized using atomic force microscopy, scanning electron microscopy, X-ray florescence, Raman spectroscopy and optical microscopy analysis techniques.
the results obtained from different substrate materials have been confronted, and it will be shown whether the use of metallic and non-metallic substrates can effect on the MoO3 structure, thickness and characteristics or not. Finally, the outcome will compare with the available previous results.

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Signatures of Vacancy-Induced Nodal States in T -Symmetric Three-Dimensional Weyl Electrons

Mr. João Pedro Santos Pires, Mr. Simão Meneses João, Dr. Aires Ferreira, Dr. Bruno Amorim, Dr. João Manuel Viana Parente Lopes

MC41: Real Space Simulations of Topological Matter and Disordered Materials II, August 22, 2022, 2:00 PM - 3:30 PM

In spite of the peculiarities of crystalline Weyl semimetals (WSMs), once the system is allowed to be disordered a plethora of new and interesting phenomena emerges. For instance, if disorder is modeled as a random on-site potential,a mean-field calculation entails a semimetal-to-metal quantum critical point with the mean nodal density of states (DoS) behaving as an order parameter [1]. Vacancies are another common set of lattice defects that have so far been overlooked in theoretical studies of dirty WSMs. In fact, vacancies generically appear as natural by-products of any crystal growth process [2], but may also be purposely introduced [3] by light-ion irradiation of crystalline samples in a controlled manner [4].
In this contribution[5], we demonstrate that an isolated vacancy is enough to trap zero energy Weyl electrons as localized states with wavefunctions that decay as r^-2. Moreover, as long as these defects exist in finite concentrations, the nodal states lead to an enhanced nodal mean density of states (DoS) that is further broadened, by inter-vacancy hybridization, into a finite width peak flanked by subsidiary resonances. This particle-hole symmetric structure of resonances clearly sets these 3D WSMs apart from its two-dimensional counterpart (e.g. grafene). Despite the quantum interference, both the nodal peak and the subsidiary resonances are shown to retain a (quasi-)localized nature that manifests as a low spectral sensitivity to applied magnetic fields and a suppressed quantum diffusivity around the node. The latter affects the longitudinal dc-conductivity, which is shown to yield reduced values whenever a subsidiary resonance lies at the Fermi level. Finally, a clear signature of vacancy-induced states is also found in the linear optical response of WSMs, which provides a way to unambiguously detect them with no need to tune the bulk Fermi energy. Simulations were performed using the efficient QuantumKITE [6] Implementation of the Kernel Polynomial Method.

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Acknowledgements: Work supported by the Portuguese Foundation (FCT) within the Strategic Funding UIDB/04650/2020 and through projects POCI-01-0145-FEDER-028887 and CEECIND/02936/2017 (B.A.). J.P.S.P. and S.M.J are funded by FCT grants No. PD/BD/142774/2018 and PD/BD/142798/2018, respectively. A.F. acknowledges support from the Royal Society through a Royal Society University Research Fellowship.

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Phase transitions in cell tissues

Prof. Dr. Roberto Cerbino

MC6: Emergent Phenomena in Driven Soft, Active and Biological Matter I, August 22, 2022, 11:30 AM - 12:30 PM

Cell collectives adapt their structural, dynamical and rheological properties by triggering phase transitions from solid-like to liquid-like states, and viceversa. Intriguingly, these phase transitions are emergent traits caused by biochemical and/or biophysical changes that do not affect the behaviour of the same cells in isolation, but rather depend on the interplay between the properties of individual cells and the interactions between cells. Phase transitions in cell collectives are used to perform key biological processes, such as embryogenesis and organogenesis, but they are also exploited by cancer as a gateway to invasion and metastasis. In this talk, I will describe the main ingredients involved in the cellular jamming and unjamming phase transitions, by focusing mostly on their possible role in cancer. Results obtained with a variety of two-dimensional and three-dimensional cell collectives show that a rich phase diagram exists, and small biochemical changes can easily drive the tissue from one state to another one, by altering the biomechanical properties of the tissue and causing coordinated motion characterised by long-ranged cell alignment, and large density fluctuations, whose persistence leads to nuclei rupture and consequent pro-inflammatory transcriptional changes.

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Dynamic Build-Up of Mesoscopic Quantum Entanglement by Quantum Spin-Transfer Torque Effect

Rafael D. Soares, P Mondal, A Suresh, João P. Santos Pires, Adrian E. Feiguin, João M. Viana Parente Lopes, Aires Ferreira, P Plecáč, Branislav K. Nikolić

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

In the last twenty years, quantum information theory has provided a whole new set of tools for the investigation of condensed matter systems. In particular, the study of various entanglement measurements has produced a new perspective that is helping to unveil and characterize exotic quantum phases of matter, especially strongly-correlated systems that can have their Hilbert space ergodicity broken by many-body localization [1] and often feature long-range entanglement [2] in space. Entanglement has been seen as a common property of the microscopic quantum systems which is washed out by thermal fluctuations in macroscopic systems at room temperature. However, over the years several experiments [3-4] have shown the possibility to entangle macroscopic systems at long distances [5].
In this contribution, we present early simulation results that demonstrate the arisal of quantum entanglement between two mesoscopic large spin-½ Heisenberg ferromagnetic chains that are mutually coupled by a local interaction with the spin of a spin-unpolarized single-electron pulse propagating across a longer one-dimensional tight-binding chain [6]. This effect is driven by a quantum spin-transfer torque effect [6-7] in which flowing electronic spins can exchange angular momentum with localized quantum spins of a magnetic material even when they are collinear but antiparallel. The results were obtained using an efficient and heavily parallelized implementation of the Chebyshev expansion for the time-evolution operator [8], which is then used to evolve the reduced density matrix of the two spin chains in time, as the electron pulse travels between them. Finally, through quantum tomography of the reduced density matrix, we are able to compute the time-dependent entanglement negativity between pairs of spins belonging to the distinct ferromagnetic layers and, thus evaluate the build-up of long range entanglement.

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Influence of quantum dots on the optical properties of a room temperature cholesteric liquid crystal

Marouen Chemingui, Donghao Yang, Yu Wang, Irena Drevensek-Olenik, Xinzheng Zhang

MC8: Complex Phases in Soft Matter V, August 23, 2022, 2:00 PM - 3:30 PM

Liquid crystals (LCs)-nanoparticles (NPs) composites usually have many excellent properties and potential applications. On one hand, the doped LCs can integrate the advantages of NPs. On the other hand, the properties of LCs can be modulated by different NPs. Here we focus on the influence of optical properties of Cholesteric LC (CLC) by Cu-In-Zn-Se quantum dots (QDs). More specifically, we study optical properties (transmission, absorbance (A), and photoluminescence (PL)) of CLC-QDs composites that were prepared with different QDs concentrations. The homogeneity of mixtures and QDs dispersion in the CLC medium are also investigated by using polarising optical microscopic textural studies. The locally formed QDs clusters may distort the CLC to induce an imperfect planar texture and cause slight broadening of CLC's photonic band gap. With the increase of the QDs concentration, both the PL and A of the composites are enhanced. The optical band gap obtained by the Tauc plot method suggests that the observed optical band gap narrows after the dispersion of QDs into the CLC.

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Gate tunable anomalous Hall effect as a probe of Berry curvature in oxide interfaces

Roberta Citro, Mr. Mattia Trama, Prof. Francesco Romeo, Prof. Carmine Perroni, Prof. Vittorio Cataudella

MC14: Beyond Charge Transport in Nanostructures and 2D Materials via Geometric Design IX, August 25, 2022, 11:30 AM - 12:45 PM

We present the theoretical prediction of a gate tunable anomalous Hall effect (AHE) in an oxide interface as a hallmark of spin-orbit coupling. The observed AHE at low-temperatures in the presence of an external magnetic field emerges from a complex structure of the Berry curvature of the electrons on the Fermi surface and strongly depends on the orbital character of the occupied bands. A detailed picture of the results comes from a multiband low-energy model with a generalized Rashba interaction that supports characteristic out-of-plane spin and orbital textures. We discuss strategies for optimizing the intrinsic AHE in (111) SrTiO3 heterostructure interfaces.

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Giant Shear Displacement by Light-Induced Raman Force in Bilayer Graphene

Habib Rostami

MC52: Heterostructures, Combining Organic Molecules and 2D Materials VI, August 23, 2022, 4:30 PM - 6:00 PM

Light-induced structural manipulation is a non-destructive method to control the electronic and optical properties of the system. Collective macroscopic oscillation of atoms in a solid, i.e., coherent phonons, facilitates reaching this aim. Coherent phonons can be excited by irradiating an ultrashort optical pulse and detected using transient optical transmission or reflection measurements using pump-probe spectroscopy. Recently, there has been significant interest in photo-induced structural transition between crystalline layered MoTe2 using ultrafast pump-probe and time-resolved second-harmonic-generation spectroscopy. A displacive coherent excitation of Raman-active shear phonon in MoTe2 causes a first-order phase transition from inversion symmetric 1T' structure to non-centrosymmetric 1Td phase [1,2]. Similarly, it has been experimentally proven a switch from an ABA structural phase to ABC one by laser irradiation in trilayer graphene [3]. The other scenario is the laser-induced heating effect that can provide activation energy for the phase transition. However, it is unclear which of the two mechanisms are more relevant in different laser power and frequency and electron doping in the layered materials. In this work [4], I develop a systematic theory to investigate displacive excitation of coherent shear phonon in a bilayer system using a diagrammatic formalism. Using a Raman force mechanism, I predict a highly controllable relative lateral shift of layers depending on the laser power and frequency in different electronic doping (see Fig. 1) . My theoretical finding is consistent with available experiments and can be examined in other layered 2D materials.

Caption for Fig. 1. Light-induced shear displacement in bilayer graphene versus chemical potential for realistic experimental values of frequency ω , electric field strength E0, electron scattering rate Te and electronic temperature Te [4].

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Theory of glasses in infinite dimensions

Pierfrancesco Urbani

MC38: Controlled irradiation Disorder in Model Systems: Organisation, Dynamics, and Transformations IX,
August 25, 2022, 11:30 AM - 12:30 PM

In recent years there has been a huge progress in building a first principle theory of glasses. This has been achieved in the limit of infinite spatial dimensions.
In this talk I will review these progresses and discuss the overall emerging picture. In particular I will focus on what happens when glasses are forced to be at the bottom of their free energy landscape which happens either at low temperature or, for colloidal systems, at large pressure. In this case I will review the appearance of the Gardner and jamming transitions and their critical properties. I will show what are the predictions that have been extracted from the theory and how they compare with observations.

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Impact of microstructure on crystallinity driven singlet fission efficiency in diF-TES-ADT

Hoyeon Choi, Patrick Parkinson

MC48: Multi-modal Characterisation of Thin Film Optoelectronics for Energy Applications IV, August 23, 2022, 11:30 AM - 12:30 PM

Singlet fission (SF) is a promising phenomenon describing the creation of a pair of excitons from a single photon which has been observed in a group of organic materials based on conjugated molecules.[1-4] Despite the significant interest focussed upon this process, the link between microstructure, temperature and SF efficiency remains ambiguous, not least because a series of energetic steps with diverse timescales determine SF efficiency.[1,5] Notably, primary singlet fission (PSF) is the initial step of the SF process in which the exciton created by the absorption of a photon takes on the character of an entangled pair of triplet excitons while conserving the spin momentum.[1-5]

By using cryogenic hyperspectral emission microscopy, we are able to link PSF with local film morphology in a prototypical anthradithiophene (diF-TES-ADT) thin film. This material has been previously reported as a high efficiency SF film at intermediate temperature, as well as that shows an emissive triplet state by Herzberg-Teller intensity borrowing mechanism, thereby it is possible to quantify the PSF efficiency.[1, 6] The hyperspectral microscopy imaging allows to obtain the both the absorption and emission map with sub-microscale spatial resolution. This approach offers significant advantageous over traditional spectroscopy, providing 8 times faster acquisition speeds, the removal of raster-scanning associated noise and artefacts and limiting photo degradation due to the prolonged exposure of the focused laser beam. Our results demonstrate inhomogeneous PSF efficiency, which is significantly correlated to the morphological features in the film. By studying these correlations, we observe the temperature dependent Franck-Condon progression, and the absorption characteristics, which suggest that the local crystallinity of the molecules is closely related to the PSF efficiency variance in the film. The temperature dependent interferometric time correlated single photon counting (i-TCSPC) reveals that the enhanced PSF efficiency in the high crystallinity regions is due to the endothermic energy alignment of the CT state which facilitates the initial singlet state converts into entangled triplets.[5, 6]

Our findings demonstrate that the local molecular crystallinity plays a key role in governing the efficiency of the PSF process, with variation in the efficiency as large as factor of 3 dependent on the local crystallinity. This insight may provide the pathway toward the creation of highly efficient SF films that can be integrated into highly efficient energy harvest systems.

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Simulating Mesoscopic Transport on Finite Systems with Space-Modulating Hoppings

Henrique P. Veiga, João M. Alendouro Pinho, Simão M. João, João P. Santos Pires, João M. Viana Parente Lopes

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

H. P. Veiga[1], J. M. Alendouro Pinho[1], S. M. João[1], J. P. Santos Pires[1] and J. M. Viana Parente Lopes[1]
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Abstract:

Closed quantum systems have a unitary time-evolution, which imply a finite recursion time to its initial quantum state, provided the Hilbert space is finite. In contrast, in an electrically biased 1D sample sandwiched between two semi-infinite leads, the electrons are naturally driven towards a state of dynamical equilibrium, in which a stationary particle current traverses the sample with a value given by the Landauer-Büttiker formula. This quantum equilibration is made possible by the infinite size of the entire system (leads+sample), and was shown to have an asymptotic Markovian character, with the independent electrons losing memory of the many-particle state in which they were initially prepared [1], [2]. Recently, some of us have analyzed how this Markovian time-evolution emerges in a disordered tight-binding system with finite “leads”, as their size gets larger [3]. While a convergence towards the aforementioned results was verified by increasing the leads’ size, several new finite-size effects were unveiled and shown to be controlled by the Fermi velocity inside the leads alone. In this work, we extend the previous study by numerically simulating a similar setup with finite leads that feature hopping strengths that slowly decrease away from the mesoscopic sample. If done smoothly [4], this alteration is expected to slowly modulate the Fermi velocity and speed-up the convergence towards the limit of semi-infinite leads without changing the current that flows through the central sample. For this contribution, we present some preliminary results on quantum transport studied in an one-dimensional tight-binding chain. Such a study is a sandbox to create new and more controlled methods for real-space simulations of coherent mesoscopic transport in higher-dimensional setups based upon O(N) spectral expansions with hermitian hamiltonians [4].

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Investigating the templating effect of patterned ferroelectric substrates on molecular semiconductor growth using PFM and KPFM

Emma Bryan

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Piezoelectric force microscopy (PFM) can be used to both image and pattern ferroelectric domains in electroactive polymer thin films such as polyvinylidene fluoride (PVDF). In this work, we use PVDF prepared via a range of techniques to control the growth of organic semiconductor molecules and define local electronic properties. PVDF films prepared by spin-coating and Langmuir Schaefer deposition have been optimized by solvent selection and control of evaporation rate to give a high ferroelectric beta phase content. Self-assembled PVDF molecular orientation has been investigated, and polarization lifetime and hysteresis properties have been characterized by voltage cycling using scanning spectroscopic PFM. We then combine the use of PFM with Kelvin probe force microscopy (KPFM) to investigate the correlation between PVDF poling and the electronic properties of the semiconductor molecules deposited on it. We further use a range of diffraction and spectroscopic techniques to gain further insights into the molecular film structure. The application of patterned ferroelectric polymers in devices to control the orientation of semiconductor molecules is discussed.

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Exploring the disorder self-energy with KITE: from the Gade singularity in graphene to disorder-enhanced superconductivity

Simão Meneses João, João Viana Parente Lopes, Aires Ferreira

MC41: Real Space Simulations of Topological Matter and Disordered Materials III, August 22, 2022, 4:30 PM - 6:00 PM

The accurate simulation of quantum systems is a critical component in the search for new exotic materials. Recent advancements in numerical methods, software development and computational power, in tandem with the increasing accessibility and ease of use of these tools have brought quantum transport simulations to a broader public [1,2]. The introduction of spectral methods [3] to electronic structure and quantum transport simulations has produced a significant leap in the kind of systems that are able to be studied.

KITE [4] represents yet another step forward in the development of these real-space numerical tools, combining the efficiency of iterative spectral methods with a user-friendly interface, a memory-efficient implementation of the Chebyshev recursion tailored to short-range real-space Hamiltonians and a HPC-enabled multi-domain parallelization scheme. This is an open-source project which has already been used to simulate systems with unprecedented sizes (10^{10} atoms) and energy resolutions (sub-meV). KITE is tailor-made for systems with disorder, where the reciprocal-space approaches are of limited application.

In this talk, I will demonstrate how spectral methods can be used to calculate the disorder self-energy operator in the lattice in a numerically exact fashion based on its most recent application to the Gade singularity problem in graphene. This new method challenges the current diagrammatic paradigm and is capable of capturing previously unreachable features of the self-energy operator. In the same line, I will showcase a modified version of the Chebyshev-Bogoliubov-de Gennes formalism which provides a good compromise between resolution and system size, enabling the self-consistent simulation of disordered superconducting systems with 10^6 lattice sites. This allows us to see a disorder-mediated phase transition in plasmon-mediated metal-coated superconducting graphene [6,7]

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What's in a single-cycle light pulse?

Helder Crespo

MC51 : Ultrafast Dynamics in Magnetic and Strongly-Correlated Materials X, August 25, 2022, 2:00 PM - 3:30 PM

The answer to the title of this talk could jokingly be “Not much, really”. In fact, and as the name implies, a single-cycle light pulse contains only a single oscillation of the electric field inside its temporal envelope. However, if such a pulse lies in the near infrared spectral region (800 nm), its duration is only around 2.7 femtoseconds and its spectral bandwidth is extremely broad, extending well into the visible range and making it look like white light to the naked eye.

Intense pulses in the few-cycle regime (~5-10 fs) have been around for 25 years now and are behind the emergence and enormous advances in experimental attosecond science, but it took some 15 years since then for intense single-cycle pulses to become a practical reality.

At first sight, going from 5 fs (approximately 2 optical cycles) to 2.7 fs may seem somewhat incremental and of limited impact. However, and apart from the obvious gain in temporal resolution compared to longer pulses, there are fundamental differences in the way light interacts with matter in the single-cycle limit, which makes single-cycle pulses highly desirable in various fields of ultrafast science. Strong-field ionisation dynamics are very different from multi-cycle pulses, and single-cycle light pulses show promise for generating isolated attosecond pulses more directly and efficiently than multi-cycle pulses. Single-cycle pulses also enable exposing wide-bandgap dielectric materials to unprecedentedly strong fields of several volts per angstrom without damage, making them important drivers for attosecond science in solids and petahertz electronics.

Like the few-cycle pulses that preceded them, single-cycle pulses are usually produced by post-compression of longer pulses from ultrafast laser amplifiers, but the degree of precision with which this compression must be performed requires sophisticated optical elements at the edge of present-day capabilities and, very importantly, a temporal measurement technique capable of dealing with the extremely short pulse durations and associated large spectral bandwidths. Despite their strong potential, these difficulties have hampered the widespread use of single-cycle pulses.

The dispersion-scan (d-scan) technique for pulse measurement and control has greatly simplified the notoriously difficult task of measuring and compressing few-cycle light pulses, enabling the generation of high-quality intense pulses down to the single-cycle limit. In this talk I will review key aspects of the technique and show how d-scan-enabled single-cycle sources are now behind a variety of high-impact results and applications.

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Direct-write nanofabrication of novel SQUIDs for quantum sensing

Dr. Kaveh Lahabi, Matthijs Rog, Tycho Blom, Julian Linek, Prof. Dieter Kölle

MC22: Nanoscale Fabrication of Superconducting Devices and their Applications X1, August 25, 2022, 4:30 PM - 6:00 PM

Josephson devices, such as SQUIDs, represent the most sensitive electronic tools used in quantum sensing. However, the practices involved in the preparation of such sensors put unavoidable restraints on their applications. For instance, the lithographic processes used in conventional SQUID fabrication, are incompatible with the sharp tips needed for ultra-high-resolution scanning probe microscopy. To overcome this challenge, my team and I apply direct-write nanofabrication techniques, such as electron beam-induced deposition (EBID) and focused ion beam (FIB) milling.

In this talk, I will describe our newly-developed EBID approach, where a scanning electron microscope can be used to print functional SQUIDs on almost any given structure [1]. Furthermore, I will present our efforts toward developing FIB-structured MoGe nanoSQUIDs, which can be integrated into sharp microscopy probes for magnetic and thermal imaging.

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Packings in cylinders: columnar crystals, helical viruses and hysteresis

Adil Mughal

That nature creates forms and structures of great diversity according to the requirements of simple physical laws is a subject of endless fascination. The possible ways in which atoms, spheres or cells fit together into alternative structures depends on both symmetry and the nature of the physical forces involved. While these physical interactions maybe simple, nevertheless the high pressures encountered in strongly confined systems can compel molecules to adopt complex yet ordered arrangements. In such systems there exists an intimate connection between morphology and the precise shape of the container. An example of this is the dense packing of idealised particles inside narrow channels. Extensive results from simulations and experiments (over the last thirty years) have shown that in such systems the particles form extended helical or chiral structures - of the type usually associated with various biological microstructures (e.g. flagella, the morphology of the tobacco virus and microtubules). Such one-dimensional structures are the focus of considerable scientific attention because of their potential utilisation as functionalized devices. This presentation will give a broad historical overview of columnar crystals, the progress that has been made in rationalising, review some relevant experiments and show that these results generalise to cylinders packed with soft (deformable) spheres

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Modular assembly driven by external electric fields.

Mr. Tanuku Venkata Manikantha Sai Ganesh, Mr. Nädir Müller, Prof.Dr. Thomas Palberg

External electric fields show the advantage in the construction of stable cargo swimmers with on/off functionality and better controllability of cargo particles. In the present work, we introduce and study ion-exchange-based modular micro-swimmers in presence of an alternating electric field (Ac). The modular swimmers in a low-frequency Ac field assemble into self-propelling complexes transporting cargo with speeds of several microns per second over extended distances and times. We systematically quantify the assembly shape and speed of the complexes by varying the strength of the electric field. The swimming speed of the assembly shows a stepwise increase as a function of the applied field strength. We could in general able to build a stable cargo that shows a promising pick and drop mechanism. The high level of control on cargo pick-up, transport, and release leads to a powerful delivery tool, which could eventually be used in microactuators or microfluidics.

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Discovering dynamic laws from observations: the case of self-propelled, interacting colloids

Dr. Miguel Ruiz-García, Mr. C. Miguel Barriuso Gutierrez, Dr. Lachlan Alexander, Prof. Dirk Aarts, Dr. Luca Ghiringhelli, Prof. Chantal Valeriani

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Active matter spans a wide range of time and length scales, from groups of cells and synthetic self-propelled particles to schools of fish, flocks of birds, or even human crowds. The theoretical framework describing these systems has shown tremendous success at finding universal phenomenology. However, further progress is often burdened by the difficulty of determining the forces that control the dynamics of the individual elements within each system. Accessing this local information is key to understanding the physics dominating the system and to create the models that can explain the observed collective phenomena.

In this work, we present a machine-learning model, a graph neural network based on [1], that uses the collective movement of the system to learn the active and two-body forces controlling the individual dynamics of the particles. We verify our approach using numerical simulations of active brownian particles, considering different interaction potentials and levels of activity. Finally, we apply our model to experiments of electrophoretic Janus particles, extracting the active and two-body forces that control the dynamics of the colloids. Due to this, we can uncover the physics dominating the behavior of the system. We extract an active force that depends on the electric field and also area fraction. We also discover a dependence of the two-body interaction with the electric field that leads us to propose that the dominant force between these colloids is a screened electrostatic interaction with a constant length scale. We expect that this methodology can open a new avenue for the study and modeling of experimental systems of active particles.

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Superconductivity-Lattice Coupling in Maximally Overdoped Cuprates: The Structure of [p=1/Tc=92 K] YBa2Cu3O8 Prepared with High Pressure Oxygen

Dr. Steven Conradson

MC38: Controlled irradiation Disorder in Model Systems: Organisation, Dynamics, and Transformations VIII,
August 24, 2022, 4:30 PM - 6:00 PM

Approaching forty years after the original discovery of superconductivity in cuprates its mechanism remains unknown. A contributing factor to this problem is that the well known, “universal” quantum phase diagram of cuprates that shows the superconductivity of all three structure classes – single layer La2CuO4, YBa2Cu3O7 with CuO3 chains as the charge reservoir, and the variable layered Bi, Hg, and Tl-based compounds – confined within the same narrow dome. In doing so it overlooks numerous materials of the first two structure families whose superconductivity extends to much higher doping levels1. Aggressive neglect by the community has inhibited research and even knowledge of these compounds whose properties challenge much of the conventional wisdom on high temperature superconductivity. Using High Pressure Oxygen (HPO) methods, we have very recently prepared YBa2Cu3O≥7.8 with doping value, p, close to the maximal value of 1. Remarkably, it retains its Tc of 92 K and its superfluid density over the full range of oxygen stoichiometry. Using a combination of x-ray diffraction and EXAFS we have determined that the excess oxygen is located in the sites between the Cu1 atoms of the Cu-O chains of the charge reservoir layer, explaining its tetragonal structure. We have similar results for two related compounds, YSr2Cu2.75Mo0.25O7.54 (Tc=85 K) and CuBa2Ca3Cu4O11+δ (Tc=115 K). In contrast, Sr2CuO3.3 (Tc=95 K) is highly disordered. Far from being an essential and therefore common property of high temperature superconductivity, the “dome” is optional. Specific kinds of ordering cause it to occur whereas others obviate it. Insofar as the dome is an essential factor is virtually all of the theories developed for HTSC these results demonstrate the catastrophic result of by ignoring these HPO compounds. As an alternative we utilize two other properties of cuprates. The numerous ones we have studied with EXAFS show changes in their spectra in proximity to their superconducting transitions, demonstrating strong coupling of their dynamic structure to their superconductivity. These changes in particular oxygen positions are assigned to the internal dynamics of the charge inhomogeneities in these systems, thus Internal Quantum Tunneling Polarons (IQTPs). The second result is that with our access to the full range of p values we find that the superconductivity saturates, with additional carriers shunted to the Fermi liquid phase. This would be consistent with condensation of the IQTPs into the superfluid, with the limiting factor therefore being the structure of the condensate that is coupled to the crystal lattice.

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Magnetic-field control of the electronic structure of Sr3Ru2O7

Professor Peter Wahl

MC50: Fermi Surface Topological Transitions - Effects of Interactions V, August 23, 2022, 2:00 PM - 3:30 PM

The phenomenology and radical changes seen in materials properties traversing a quantum phase transition has captivated condensed matter research over past decades. Strong electronic correlations lead to novel ground states, including magnetic order, nematicity and unconventional superconductivity. To provide a microscopic model for these requires knowledge of the electronic structure in the vicinity of the Fermi energy, promising a complete understanding of the physics of the quantum critical point. The strontrium ruthenates provide an ideal material system to explore this physics using spectroscopic techniques, providing high-quality atomically-flat surfaces. It has recently been shown that a number of phenomena in Sr3Ru2O7 can be understood as originating from a Lifshitz transition in the electronic structure[1]. Spectroscopic confirmation of the energy and field-dependence of the electronic structure would allow verification of this scenario, as well as assessing the role of quantum fluctuations. Here, we demonstrate such a measurement at using ultra-low temperature scanning tunneling microscopy at temperatures below 100mK.[2]

Our results show that even in zero field the surface electronic structure of Sr3Ru2O7 is strongly C2 symmetric and that an out-of-plane magnetic-field drives both a Lifshitz transition and induces a charge-stripe order, suggesting that as in Sr2RuO4,[3] the surface exhibits subtle differences in its properties compared to the bulk. Our results provide a microscopic picture of the field-induced changes of the electronic structure across the Lifshitz transition from quasi-particle interference imaging.

Intriguingly, the C2 symmetry breaking of the low energy electronic structure can be manipulated by an in-plane magnetic field. This finding suggests an important role of spin-orbit coupling in the field-induced nematic state of Sr3Ru2O7. Our results demonstrate compass-like control over a materials electronic structure. I will discuss the relation of these findings to the nematic state found in the bulk of the material,[4] and the magnetic-field controlled spin-density wave phases seen there[5].

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Towards the multicritical Lifshitz point in Sr3Ru2O7

Dr Andreas W Rost, Maximillian Pelly, Caitlin O'Neil, Dr Craig V. Topping, Dr Robin S. Perry, Dr Alexandra S. Gibbs

MC50: Fermi Surface Topological Transitions - Effects of Interactions VII, August 24, 2022, 2:00 PM - 3:30 PM

Strongly correlated Sr3Ru2O7 displays phenomena associated with a metamagnetic quantum critical end point and the formation of complex electronic phases [1,2]. The physics of this material is associated with a Van Hove singularity (VHs) in the electronic band structure [3] close to an unusual multicritical Lifshitz transition [4]. Tuning the properties of Sr3Ru2O7 has been pursued through a number of strategies including magnetic field, pressure, uniaxial strain and doping.

Here we present results from both an isovalent Ba doping study and high resolution dilatometry measurements in order to explore the detailed interplay of structure-property relationships that control the Van Hove singularity and hence metamagnetism and phase formation in Sr3Ru2O7.

Sr substitution by Ba can in principle be understood as a chemical pathway to expand the lattice via the larger ionic radius of Ba. The increase of the effective tolerance factor drives the system closer to the tetragonal aristotype structure. At the same time Ba has minimal effect on the orbital character of the band structure at the Fermi energy which is dominated by Ru and O. We present high resolution neutron diffraction, magnetisation and specific heat measurements of the series (Sr1-xBax)3Ru2O7. Our data show a clear shift of the Van Hove singularity towards the Fermi energy, crossing it at approximately x = 0.08, with a subsequent sharp decrease in the density of states. The results allow us to determine the evolution of the VHs within the multicritical Lifshitz point's phase diagram [4] with Ba doping.

In addition, recent high resolution dilatometry measurements resolved quantum oscillations in the length of Sr3Ru2O7 approaching the quantum critical end point. The significance of these measurements lies in the sensitivity to those Fermi surfaces that most strongly change under uniaxial stress. In combination with thermodynamic data this enables in principle the identification of the Fermi surface pockets driving metamagnetism in this material and deduce the evolution of the band structure under c-axis stress.

We will discuss the details of the structural distortions occurring both in the case of Ba doping and c-axis uniaxial stress and how they impact on the microscopic details of the Van Hove singularity in Sr3Ru2O7 and by extension other members of the Ruddlesden-Popper ruthenates in general [4].

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Fluoroarenes in On-Surface Synthesis and Organic/TMDC Hybrid Interfaces

Prof. Dr. Michael Gottfried

MC52: Heterostructures, Combining Organic Molecules and 2D Materials IV, August 23, 2022, 11:30 AM - 12:30 PM

This talk addresses the roles of fluoroarenes in hybrid interfaces and the formation of new two-dimensional (2D) materials. Hybrid systems of 2D materials such as transition metal dichalcogenides (TMDCs) and organic semiconductors (OSCs) have become subject of great interest for future device architectures. Although OSC-TMDC hybrid systems have been used in first device demonstrations, the precise preparation of ultra-thin OSC films on TMDCs has not been addressed. Due to the weak van der Waals interaction between TMDCs and OSCs, this requires precise knowledge of the thermodynamics at hand. Here, we use temperature-programmed desorption (TPD) to characterize the desorption kinetics of pentacene (PEN) and perfluoropentacene (PFP) on MoS_2 as a model system for OSCs on TMDCs. We show that the monolayers of PEN and PFP are thermally stabilized compared to their multilayers, which allows to prepare nominal monolayers by selective desorption of multilayers. This stabilization is, however, caused by entropy due to a high molecular mobility rather than an enhanced molecule-substrate bond. Consequently, the nominal monolayers are not densely packed films. Molecular mobility can be suppressed in mixed monolayers of PEN and PFP that, due to intermolecular attraction, form highly ordered films. Although this reduces the entropic stabilization, the intermolecular attraction further stabilizes mixed films. The second part focusses on the on-surface synthesis of biphenylene network, a new carbon allotrope, from a partially fluorinated terphenyl. The quest for planar sp^2-hybridized carbon allotropes other than graphene, such as phagraphene, graphenylene, and biphenylene network, has stimulated substantial research efforts because of the materials' predicted unique mechanical, electronic, and transport properties. However, their syntheses remain challenging due to the lack of reliable protocols for generating non-hexagonal rings during the in-plane tiling of carbon atoms. We have developed an on-surface synthesis strategy by which we first generate straight polymer chains, which then link to form the non-benzenoid graphene isomers. Using this approach, we achieved the bottom-up growth of biphenylene network with periodically arranged four-, six-, and eight-membered rings of sp^2-hybridized carbon atoms, through on-surface inter-polymer dehydrofluorination (HF-zipping) reaction. Apart from graphene, biphenylene network is the only experimentally known planar sp^2 carbon so far. Its characterization by scanning probe methods confirms the non-benzenoid nature and reveals that it is metallic rather than a dielectric already at very small dimensions.

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Quantum linear magnetoresistance from the classical point of view

Alexander Kazantsev

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

We give the semiclassical derivation of Abrikosov's quantum linear magnetoresistance. This gives a clear physical picture of the cause of the linear magnetoresistance and hints at a general semiclassical mechanism of linear magnetoresistance in semimetals.

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Experimental and numerical study on excitation and interaction of nonlinear localized oscillations in a mass-spring chain

Dr. Yosuke Watanabe, Dr. Yusuke Doi

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter XII, August 26, 2022, 9:00 AM - 10:00 AM

Nonlinear localized oscillations excited and propagated in a mass-spring chain are studied. Letting the mass at one end of the chain driven sinusoidally at high frequency and large amplitude, localized oscillations can be excited intermittently near the end and propagated down the chain one after another at a constant speed. This phenomenon is known as supratransmission [R. Khomeriki, et al., Phys. Rev. E 70 (2004) 066626; F. Geniet and J. Leon, Phys. Rev. Lett. 89(13) (2002) 134102]. We have experimentally observed the supratransmission by a mechanical mass-spring chain which emulates the Fermi-Pasta-Ulam (FPU) one of beta type [Y. Watanabe, et al, Phys. Lett. A 382 (2018) 1957-1961]. At one end of the chain the device to drive the end sinusoidally in the direction of the array is attached and at the other end the chain is simply fixed. Keeping driving the end at a high frequency, we can observe that the localized oscillations excited at intervals propagate down the chain one after another and reflect at the fixed end. Our experimental results show that, the higher the driving frequency is, the longer the time intervals of excitations of localized oscillations become. (In the case that driving frequency is higher than threshold, no localized oscillations are excited.) When taken the value of driving frequency near the threshold, it may be possible for us to observe the collisions or interactions between two independent localized oscillations. In this study, we consider the behavior of the collisions and compare the experimental results with the numerical ones.

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Microwave spectroscopy of Andreev bound states in a magnetic field using superconducting circuitry

Jaap J Wesdorp, Arjen Vaartjes, Lukas Grunhaupt, Sebastiaan Roelofs, Lukas Splitthoff, Marta Pita Vidal, Arno Bargerbos, Leo Kouwenhoven, Bernard Van Heck, Gijs De Lange

Microwave spectroscopy of Andreev bound states (ABS) using hybrid superconducting circuit-QED techniques has so far been limited to magnetic fields of a few tens of mT. In contrast to ABS transitions involving pairs of quasiparticles, i.e. in the even-parity manifold, transitions involving a single spin-carrying quasiparticle to higher lying ABS manifolds have been observed and manipulated recently. Here, we expand on these results by performing microwave spectroscopy of a gate-tunable InAs-Al hybrid Josephson junction in the presence of spin-orbit coupling and Zeeman fields. In parallel magnetic fields up to a quarter Tesla we track both the even and odd parity branches of the spectrum. Additionally, in nanowires with broken chiral and time-reversal symmetry, through spin-orbit coupling and magnetic field respectively, one expects an anomalous Josephson current to appear. In contrast to measurements of this aggregate effect, we show a field induced anomalous phase shift involving transitions between the individual Andreev bound state levels as a function of gate.

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Thermometric protocol for ultraprecise thermometry in many-body systems at low temperatures

Karen Hovhannisyan, Ivan Henao, Raam Uzdin

MC20: Recent Advances in Quantum Thermodynamics with a Focus on Many-body Interactions VI, August 23, 2022, 4:00 PM - 6:00 PM

Low-temperature thermometry through equilibrium probes is exponentially inefficient — thermal states of small systems are exponentially hard to distinguish at low temperatures. Nonequilibrium probes can deliver qualitatively more information about the temperature, albeit at the cost of undergoing fine-tuned, high-complexity joint evolution with the macroscopic sample. In this work, we leverage this tradeoff by presenting a low-complexity thermometric scheme that is nonetheless capable of delivering enough information about the temperature to overcome the exponential inefficiency of equilibrium schemes. This is made possible thanks to a suitable interaction that couples the probe to the sample, and to an auxiliary thermal bath known to be at a higher temperature. We show that, for many-body samples described by gapped frustration-free Hamiltonians, our scheme is capable of achieving signal-to-noise ratios that diverge polynomially with the temperature.

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Probing light-driven superconductors with ultrafast resonant inelastic x-ray scattering

Prof. Matteo Mitrano

MC47: X-ray FreeElectron Lasers for Condensed Matter & Materials Physics (XFELs for CMMP) I, August 22, 2022, 11:30 AM - 12:30 PM

Ultrafast optical excitation, especially when resonant to specific lattice modes, has recently emerged as a powerful means to control and induce new functionalities in quantum materials. One of the most ambitious goals is to selectively drive structural or electronic degrees of freedom to bring about nonequilibrium superconductivity at temperatures far above the equilibrium critical temperature Tc. While this phenomenon has been observed in a variety of systems ranging from copper oxides to organic molecular metals, the microscopic physics of these dynamics is still largely unexplored. By focusing on the paradigmatic example of light-driven La2-xBaxCuO4, I will show how the newly developed technique of time-resolved resonant inelastic X-rays scattering (trRIXS) provides an unprecedented route to probe the finite-momentum excitation spectrum of these transient phases (see Fig. 1) [1,2,3]. Furthermore, I will discuss how intense fields are conducive to a dynamical renormalization of the Hubbard U in the CuO2 plane [4] and how these electronic changes can affect the finite-momentum spin fluctuation spectrum detected in trRIXS experiments [5].

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From chiral squeezing to nonlinear topology in optomechanics

Javier Del Pino, Jesse J. Slim, Ewold Verhagen, Jan Košata, Toni Heugel, Oded Zilberberg

MC17: Nanomechanical and Electromechanical Systems VIII, August 24, 2022, 4:30 PM - 6:00 PM

Synthetic gauge fields can be harnessed to engineer unconventional transport and localization of bosonic states by breaking time-reversal symmetry and mimic the behavior of electrons in electromagnetic fields. Optomechanical systems allow addressing optically mechanical modes via modulated radiation pressure, enabling spring constant tuning and strong mechanical interactions that imprint nonreciprocal Peierls phases – akin to the Aharonov-Bohm effect for electrons 1.

Here we demonstrate how optomechanical cavities unlock the synthesis of pseudo magnetic fields for many-mode nanomechanical networks, offering a route towards acoustic chirality and non-Hermitian topological states 2 . Our ideas are tested within state-of-the-art optomechanical nanobeam photonic crystals that support localized optical resonances at telecom frequencies coupled to multiple, highly coherent (Q-factors > 500), mechanical overtones at MHz frequencies. Phase control of intensity-modulated driving lasers in a single cavity then unlocks a versatile, optically-tunable nanomechanical network, featuring arbitrary-range interactions spanned along a synthetic dimension. In our study, we analyze the emergence of chiral phononic propagation in single mechanical loops with nonreciprocal link phases, and Aharonov-Bohm interference between multiple loops. In addition, we show that inhomogeneous mechanical damping rates allows a pseudo-magnetic-dependent cooling of mechanical resonators. Finally, we demonstrate radiation-pressure-induced parametric interactions and consider the resulting interplay of gain and loss, yielding non-Hermitian physics, including exceptional points and non-reciprocal phononic amplification.

Our findings open new prospects for thermal transport and non-Hermitian topological phases for mechanical modes at the nanoscale. They ultimately illustrate the potential of optomechanical systems towards quantum chiral acoustic networks orchestrated by optical fields.

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Exploiting the chemistry of liquid metallic hydrogen in mixtures with other elements

Dominik Kraus

MC38: Controlled irradiation Disorder in Model Systems: Organisation, Dynamics, and Transformations VIII, August 24, 2022, 4:30 PM - 6:00 PM

High energy densities can significantly alter the electronic structure of materials. The pressure-induced insulator-metal transition of hydrogen is a model case that has been subject of theoretical and experimental studies for many decades. Here we present evidence for the creation of liquid metallic hydrogen in C-H mixtures shock-compressed by laser-irradiation to pressures around ~150 GPa and temperatures of ~5000 K, which were probed by different in situ X-ray methods at X-ray free electron lasers. Our observations suggest new ways to study the chemical properties of this exotic state in mixtures with other elements, which is highly relevant for a better understanding for the interiors of giant planets. Moreover, exploting liquid metallic hydrogen chemistry may allow to realize the synthesis of highly interesting materials such as tailored nanodiamonds with specific color centers, new ultrahard forms of carbon or hydride-based compounds possibly providing room-temperature superconductivity.

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Nanoporous Graphene Field Effect Transistors and Short Channel Effects

José Ramón Durán Retamal, Markos Paradinas, Nicolau Molina Bom, Aitor Mugarza

MC12: Physics in 2D Nanoarchitectonics III, August 22, 2022, 4:30 PM - 6:00 PM

Atomically precise graphene nanoribbons (GNRs) grown by on-surface synthesis have raised a great interest due to their versatility to tune graphene bandgap in a bottom-up controlled fashion. Consequently, the semiconductor properties of GNRs and the capability of realizing short-channel FETs with them could enable their operation as field effect transistors and even tunneling-FETs with subthreshold slopes steeper than the thermionic limit of 60 meV/dec. Short-channel FETs where GNRs are connected to the two electrodes exhibit large on/off ratios up to 105 (1, 2). However, the non-linear ID-VD curves in these devices still show that these devices are affected by the length of the channel and the active layer. Indeed, the average length of individual GNRs, below 50 nm, limits severely the contact area to few nanometers and the channel length to few tens of nanometer for contacting individual GNRs. As a consequence, only few studies with sub 30-nm channels have rendered on/off current ratios higher than four orders of magnitude. On the other hand, larger channel FETs fabricated with two-dimensional films based on GNR networks typically exhibit low on/off current ratios, non-linear transport, low and field dependent mobilities, and hysteresis, despite the high-quality of as-grown single GNRs (3). Accordingly, in these devices the transport mechanism is mostly dominated by the disorder introduced by the GNRs-network and the large presence of defects as well as surface and interface states, which is similar to disordered semiconducting organic 3D matrix in organic transistors. In such scenario, we propose nanoporous graphene (NPG), a 2D matrix of covalently bonded parallel array of GNRs, to minimize disorder. The microscopic structure of polycrystalline NPG is characterized by covalently bonded, 50-100 nm scale single crystal domains oriented in 3 azimuthal domains. We tested several arrays of interdigitated gratings with electrode interspaces ranging from 50 nm to 600 nm. The results show a consistent non-linear behavior in the output characteristics and almost 3 order of magnitude on/off current ratio in the transfer characteristics. Furthermore, we also find ambipolar behavior which open new venues to exploit them as building blocks for logic operation and optoelectronic applications.

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Doped Nanoporous graphene as a new material for ultrasharp superlattice heterojunctions

Dr. María Tenorio, Dr. César Moreno, Pol Febrer, Dr. Jesús Castro-Esteban, Pablo Ordejón, Prof. Diego Peña, Dr. Miguel Pruneda, ICREA Prof. Aitor Mugarza

MC12 : Physics in 2D Nanoarchitectonics II, August 22, 2022, 2:00 PM - 3:30 PM

Bottom-up synthesis has shown to be a very efficient method to build graphene nanoarchitectures with atomic precision. The most illustrative example is the plethora of graphene nanoribbons (GNR) that have been created practically à la carte. Despite such impressive advances in 1D homostructures, going beyond in structural complexity has turned to be a tough challenge. In particular, the synthesis of heterostructures has been limited to 1D, with no control on size and distribution of fusing components [1]. Here we report a novel synthetic strategy to fabricate atomically precise, lateral superlattice heterojunctions built in a Nitrogen-doped nanoporous graphene structure. For that we harness our ability to create parallely-aligned graphene nanoribbons superlattices [2] in order to guide the synthesis of a second GNR component, in this case an N-doped isostructural counterpart, within the empty channels of the superlattice. The final step consists on fusing laterally [3] the components alternatively into a hybrid nanoporous graphene (h-NPG). The electronic structure is that of a superlattice of type-II heterojunctions whose atomically sharp stepped potential, at the ultimate limit of a single carbon-carbon bond unveils the presence of in-gap tunnelling states and interface quantum dipoles. We envision that our fabrication scheme will facilitate a new class of atomically precise hybrid nanomaterials with high flexibility on structural composition and functionality, unfolding their impact in the fields of (opto)electronics, catalysis, and bio-chemistry.

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Nonlinear and active rheology of cell tissues

Charlie Duclut, Joris Paijmans, Mandar Inamdar, Carl Modes, Frank Jülicher

Tissues are assemblies of large numbers of cells which form a soft active material. In amorphous solids as in tissues, neighbour exchanges (or T1 transitions) can relax local stresses and allow the material to flow. In tissues, in addition to these passive events, energy consumption at the microscopic level allows cells to perform active neighbour exchanges that can shape the tissue into a prescribed geometry.

In my talk, I will consider an anisotropic vertex model to study T1 rearrangements in polygonal cellular networks. I will consider two different physical realizations of the active anisotropic stresses, that can be both observed in experiments: (i) anisotropic bond tension and (ii) anisotropic cell stress. Interestingly, the two types of active stress lead to patterns of relative orientation of T1 transitions and cell elongation that are different. Using the lens of a continuum description of the tissue as an anisotropic active material, I will discuss the energetics of the dynamic tissue and express the energy balance in terms of internal elastic energy, mechanical work, chemical work and heat. This allows us to define active T1 transitions that can perform mechanical work while consuming chemical energy.

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First principles calculations of current flow and control in 2D molecular networks

Prof Mads Brandbyge

MC12 : Physics in 2D Nanoarchitectonics II, August 22, 2022, 2:00 PM - 3:30 PM

The strong progress in two-dimensional(2D) materials holds a great promise for new science and technology, not least for electronic applications. To this end, first principles calculations and simulations play an important role in order to explore the many possibilities of novel electronic devices both in terms of 2D materials and device principles. I will present the methods we have developed based on density functional theory in combination with non-equilibrium Greens functions (DFT-NEGF), allowing for multiscale device simulations of 2D nano-electronic devices beyond 100 nm in size.
I will discuss applications to graphene-based 2D molecular networks where current-injection from a point source (STM tip) give rise to different large-scale current patterns featuring anisotropic spreading. In particular, we study how the current spreading may be controlled in various ways, e.g. by electrostatic gating or molecular conformations, and using quantum interference.

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Out-of-plane nano-magnonics

Andrii Chumak

MC44: New Perspectives in Magnonics, from 2D to 3D Systems I, August 22, 2022, 11:30 AM - 12:30 PM

Magnonics addresses the physical properties of spin waves and utilizes them for data processing [1]. Nano-magnonics addresses the investigation of spin waves in magnetic nanostructures of minimal sizes of a few hundred nanometers or less. Previously, only the in-plane magnetized nanostructures were investigated: A single-mode spin-wave propagation with 1.8 µm propagation length was observed in the 50 nm-wide yttrium iron garnet (YIG) waveguides magnetized along [2]. The longer propagation length of 8 µm and the phenomenon of the edge modes merging was observed in the same nano-waveguides magnetized in-plane transversally [3]. The out-of-plane investigation of spin waves in YIG nano-waveguides was beyond the state-of-the-art since the scattering cross-section in the Brillouin Light Scattering (BLS) spectroscopy was expected to be zero in the small precession angle regime [4].

In the talk, I will present a set of experimental and numerical results on the investigation of spin waves in out-of-plane magnetized YIG nano-waveguides. This configuration offered a set of conceptual advantages compared to the in-plane configurations:

- The BLS signal of excited spin waves for out-of-plane configuration appeared to be compa-rable to that of in-plane magnetization for the same applied microwave power.
- The out-of-plane magnetization allowed for the excitation of extensive precession angles of up to ~50° without triggering parasitic multi-magnon scattering phenomena responsible for the loss of coherent information carried by spin waves.
- A “controllable” nonlinear shift of the dispersion curve up to 2 GHz was observed experi-mentally and used successfully for the excitation of short-wavelength exchange spin waves. The mechanism of the wavelength transformation down to 200 nm wavelength. This phe-nomenon allowed for the efficient detection of spin waves at distances of at least 35 µm from the antenna.
- The out-of-plane magnetization allows for the isotropic spin-wave transport in 2D magnonic circuits, one of the critical challenges for the in-plane magnetized networks, and is an ideal configu-ration for the inverse-design magnonics [5].

On the other hand, out-of-plane magnetization requires the application of relatively large external magnetic fields to overcome the demagnetization. However, the use of nanostructures automatically reduces the magnitude of the required fields, and the novel out-of-plane easy-axis material, like partially compensated Ga:YIG [6], is another step towards application-relevant devices [1].

Acknowledgments: This research has been funded by the Austrian Science Fund (FWF) through Project No. I 4696-N.

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Driving quantum many-body scars

Dr Ana Hudomal, Mr Jean-Yves Desaules, Dr Bhaskar Mukherjee, Mr Guo-Xian Su, Dr Jad Halimeh, Dr Zlatko Papic

MC42: Broken Ergodicity and Localisation in Quantum Many-body Systems VI, August 23, 2022, 4:15 PM - 5:30 PM

Periodic driving has been established as a powerful technique for engineering novel phases of matter and intrinsically out-of-equilibrium phenomena such as time crystals. Recent experiments have demonstrated that periodic driving can also lead to a significant enhancement of quantum many-body scarring, whereby certain non-integrable systems can display persistent quantum revivals from special initial states. Nevertheless, the mechanisms behind driving-induced scar enhancement remain poorly understood. Here we report a detailed study of the effect of periodic driving on the PXP model describing Rydberg atoms in the presence of a strong Rydberg blockade - the canonical static model of quantum many-body scarring. We show that periodic modulation of the chemical potential gives rise to a rich phase diagram, with at least two distinct types of scarring regimes that we distinguish by examining their Floquet spectra. We formulate a toy model, based on a sequence of square pulses, that accurately captures the details of the scarred dynamics and allows for analytical treatment in the large-amplitude and high-frequency driving regimes. Finally, we point out that driving with a spatially inhomogeneous chemical potential allows to stabilize quantum revivals from arbitrary initial states in the PXP model, via a mechanism similar to prethermalization.

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Fddd - A liquid crystal phase of rotating quadrupoles

Kutlwano Gabana

MC8: Complex Phases in Soft Matter X, August 25, 2022, 2:00 PM - 3:30 PM

The search for chiral liquid crystals made from achiral mesogens, not chiral, continues to be an exciting yet difficult task in the soft matter community, especially within columnar liquid crystals. Some of the proposed candidates have either turned out to have too high an order for liquid crystals or not having long range chirality with respect to the columns and being prone to chiral reversals. This was true at least until a report of the observation of a chiral columnar phase, Fddd, in compounds that were made from achiral polycatenars [1]. The phase was observed in two types of compounds, one made up of molecules with a straight rigid core and flexibles tails at the ends, while the second is made up of molecules with a bent core and flexible chains and in both types a unit cell consists of four left-handed columns and four right-handed chiral columns.

This project was concentrated on confirming the observations made from the experiments about the compounds with molecules having a straight core. It was also aimed at investigating whether other phases or configurations other than this one-to-one mix are possible. These molecules pack in space by trying to avoid clashes between tails. The best possible arrangement is one having them perpendicular to each other while the worst arrangement is one having them end to end. These interactions resemble those of 2D linear electric quadrupoles and hence were modelled as such. The model was then applied to a unit cell of the Fddd system as well as three other candidate configurations to determine whether the Fddd is indeed the ground state of this system.

Figure 1. g, h Two dimers of the straight core molecules on adjacent columns in g represented by quadrupoles in h. i, j Side and top views of co-rotating and counter-rotating columns made up to of quadrupoles, respectively. k Minimum-energy configurations on a 2D-hexagonal lattice; k1 system of two left- and two right-handed columns, Fddd, as observed experimentally; k2 system of three left- and one right-handed columns; k3 system of four right-handed columns; (k4) system of two left- and one right-handed columns. The red and pink columns are of the same handedness, while the blue columns are of the opposite handedness.

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Casimir force between real materials towards device applications

Professor GEORGIOS PALASANTZAS

When quantum vacuum fluctuations are confined within boundaries, then they manifest themselves by the generation of Casimir forces. However, boundaries between interacting bodies possess in many cases nanoscale surface roughness, which is both difficult to avoid and control. At short separations of less than 200 nm, nanoscale roughness starts to play an important role on the Casimir interaction between the bodies and their adhesion upon contact. Indeed, control of this short-distance interaction is crucial for MEMS/NEMS, and adhesion technologies. Although the Casimir forces for flat bodies can be described partly by Lifshitz theory that takes into account the actual measured optical properties of the interacting materials, for rough surfaces the problem is complicated by the nonadditivity of the dispersion forces. In my talk, I will discuss first the current state of the problem in Casimir force measurements between real materials with attention to metals (e.g. Au in ambient and liquids), poor conductors (SiC, phase change materials), and topological insulators offering the possibility for repulsive Casimir forces. Secondly, results will be shown with respect to actuation dynamics of devices towards chaotic behavior in terms of Melnikov and Poincare portrait analysis. The consequences of the Drude-Plasma model uncertainty on the actuation problems will also be addressed.

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New opportunities for liquid neutron spectroscopy at ISIS

Ross Stewart, David Voneshen, Russell Ewings

MC7: Exploring Liquid Properties in Confined Geometry (Up To Mesoscopic Scales) VII, August 24, 2022, 2:00 PM - 3:30 PM

Quasi-elastic neutron spectroscopy of liquids is in common usage at the ISIS Neutron and Muon Source, UK, to examine incoherent (non-propagating) dynamical properties, such as diffusion constants and local internal molecular modes. However, it is much more difficult to measure coherent excitations in liquids with neutrons due to their kinematical constraints - namely the rather limited range of excitation energies at low momentum transfers, where the coherent liquid modes must be measured. As a result, coherent liquid spectroscopy is most commonly attempted using inelastic X-ray scattering.

In principle, however, neutron spectroscopy should be able to provide much better data than IXS, since the energy resolution is generally much better, and the line-shape is a well-behaved Gaussian function rather than a Lorentzian.

We will present recent data taken on the LET and MERLIN direct geometry neutron time-of-flight spectrometers on propagating excitation modes in liquids, including measurements under pressure. We will also present an instrument concept called BRILL, which is a recently-proposed direct geometry neutron time-of-flight spectrometer at ISIS, dedicated to the measurement of low-momentum transfer propagating excitations.

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Non-ideality in lipid mixtures, a molecular dynamics study

Lisa Berezovska, Fabrice Thalmann

Biological membranes are complex environments characterized by multicomponent lipid mixtures[1]. We investigate in this work binary lipid bilayers using the SPICA coarse-grained molecular dynamics model. Adapting the Kirkwood-Buff theory of liquid mixtures [2] to finite wavelength density fluctuations statistics, we compare various practical approaches for determining the interaction parameters in theory of regular solution description of these numerical lipid mixtures.

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Jenny Griffiths

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Ultrafast optical generation and control of magnetic skyrmions

Stefan Eisebitt

MC47: X-ray FreeElectron Lasers for Condensed Matter & Materials Physics (XFELs for CMMP) I, August 22, 2022, 11:30 AM - 12:30 PM

Magnetic Skyrmions are spin textures which behave as quasi-particles and are characterized by a specific topology. Some types of skyrmions do exist in suitable thin magnetic multilayer film systems at room temperature, and they can be generated and efficiently moved laterally by spin- polarized current pulses. I will discuss how magnetic skyrmions can be generated via laser pulses instead of current pulses at unprecedented speed, with the topology change completed after 300 ps. Insight into the ultrafast laser-induced formation mechanism comes from time- resolved scattering experiments at X-ray lasers in comparison with atomistic spin simulations. Local topology fluctuations in a transient high temperature phase are identified as the key element for this topological phase transition [1] - a mechanism that may be applicable to phase transitions with a net change of topology in completely different material systems as well. Beyond the fundamental mechanism of skyrmion formation in thin magnetic films, recent results on control [2] and localization [3] of the optical creation and annihilation are briefly discussed, which will enable the study of nucleation dynamics via pump-probe experiments at high repetition rates in the future.

Fig. 1. Scheme of optical formation of magnetic skyrmions via a femtosecond laser pulse in the presence of an external magnetic field, starting from a previously uniform magnetization. The image in the circular field of view with 1 µm diameter shows an out-of-plane magnetization map obtained by x-ray holography after the optical pulse has been absorbed and skyrmions have formed. The skyrmions density can be controlled via the magnetic field.

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Sub-diffusion in random regular graphs

Luis Colmenarez

MC42: Broken Ergodicity and Localisation in Quantum Many-Body Systems IX, August 25, 2022, 11:30 AM - 12:30 PM

The scaling of the Thouless time with system size is of fundamental importance to characterize dynamical properties in quantum systems. In this work, we study the scaling of the Thouless time in the Anderson model on random regular graphs with on-site disorder. We determine the Thouless time from two main quantities: the spectral form factor and the power spectrum. Both quantities probe the long-range spectral correlations in the system and allow us to determine the Thouless time as the time scale after which the system is well described by random matrix theory. We find that the scaling of the Thouless time is consistent with the existence of a sub-diffusive regime anticipating the localized phase. Furthermore, to reduce finite-size effects, we break energy conservation by introducing a Floquet version of the model and show that it hosts a similar sub-diffusive regime.

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Neuromorphic computing with magnons

Katrin Schultheiss

MC44: New Perspectives in Magnonics, from 2D to 3D Systems II, August 22, 2022, 2:00 PM - 3:30 PM

Within the last decade, spintronics and magnonics have demonstrated an impressive development in the experimental realization of Boolean logic gates. However, the exponential growth of data and the rise of the internet of things are pushing the deterministic Boolean computing of von-Neumann architectures to their limits or are simply to energy consuming. Moreover, it is accepted commonly that conventional Boolean computer architectures are likely to remain inefficient for certain cognitive tasks in which the human brain excels, such as pattern recognition, particularly when incomplete or noisy data are involved.
One of the most generic and abstract implementations of brain-inspired computing schemes is reservoir computing, where the nonlinear response of a physical system is used to separate patterns hidden in a temporal data stream into distinct manifolds of a higher dimensional output space. In this presentation, I will demonstrate the experimental realization of pattern recognition based on reservoir computing using magnons.
Recently, we reported on the nonlinear scattering of magnons in vortices in micron-sized Permalloy discs [1] which we also learned to control and stimulate by means of other magnons [2]. Now, we utilize these phenomena to employ magnons for pattern recognition without actually relying on magnon transport in real space. I will present a comprehensive overview of experimental results and numerical simulations demonstrating the capabilities and advantages of magnon reservoir computing in reciprocal space.

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Gold nanoparticule supracrystals : structure and stiffness

Brigitte PANSU, Helen IBRAHIM, Marianne IMPEROR-CLERC, JF SADOC, Victor BALEDENT

MC8 : Complex Phases in Soft Matter VII, August 24, 2022, 2:00 PM - 3:30 PM

Spherical gold nanoparticules (NPs) grafted with hydrophobic ligands built 3D supracrystals with many different structures (FCC, BCC, Frank and Kasper C14 phase) depending on both the gold core diameter and on the ligand length (1). The main interactions between the NPS are the large van der Waals attraction between the gold cores and the complex interaction between the soft shells combining attraction and repulsion (2). The mechanical collective behavior of the soft matrix surrounding the gold cores inside the 3D crystals is a key parameter to analyze the balance between the different interactions.

The stiffness of the gold nanoparticule supracrystals has been investigated using High Pressure Small Angle X-ray Scattering (HP-SAXS). Under a hydrostatic pressure up to 8 GPa, the supracrystals show a high structural stability and the bulk elastic modulus of the supracrystal and of the soft matrix can be derived from the variations of the cell parameter (3). At higher pressure, the structure is highly affected and this transformation is irreversible. The role of the structure on the mechanical behavior of the supracrystals will be discussed.

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Density induced BCS-Bose evolution in gated two-dimensional superconductors: The role of the interaction range in the Berezinskii-Kosterlitz-Thouless transition

Carlos Sa De Melo

MC35: Collective Effects and Non-Equilibrium Phenomena in Quantum Gases and Superconductors VII, August 24, 2022, 2:00 PM - 3:30 PM

The evolution from Bardeen-Cooper-Schrieffer (BCS) to Bose superconductivity versus carrier density (n) in two-dimensional (2D) gated superconductors is discussed and the fundamental role that the interaction range plays in the Berezinskii-Kosterlitz-Thouless transition is addressed. [1] The density dependence of the critical temperature (Tc), superfluid density, order parameter, chemical potential and pair size are investigated. The most important finding is that it is essential to include classical and quantum phase fluctuations, as well as finite-ranged interactions to explain the non-monotonic behavior of Tc versus n and to guarantee that the upper bound on Tc is not exceeded in 2D superconductors, as experimentally observed in LixZrNCl [Science 372, 190 (2021)], a lithium intercalated layered nitride, and in magic-angle twisted trilayer graphene [Nature 590, 249 (2021)]. Furthermore, it is shown that from measurements of Tc and the order parameter, the effective mass of charge carriers and their interaction strength and range can be extracted.

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Moiré interlayer excitons in space and time: time-resolved momentum microscopy on twisted WSe2/MoS2

Marcel Reutzel, David Schmitt, Jan Phillip Bange, Wiebke Bennecke, AbdulAziz AlMutairi, Giuseppe Meneghini, Kenji Watanabe, Takashi Taniguchi, Daniel Steil, D. Russell Luke, R. Thomas Weitz, Sabine Steil, G. S. Matthijs Jansen, Samuel Brem, Ermin Malic, Stephan Hofmann, Stefan Mathias

MC16: Spin Control in Twisted Van Der Waals Heterostructures V, August 23, 2022, 2:00 PM - 3:30 PM

Transition metal dichalcogenides (TMDs) are an exciting model system to study ultrafast energy dissipation pathways, and to create and tailor new emergent quantum phases [1,2]. The versatility of TMDs results from the confinement of optical excitations in two-dimensions and the concomitant strong Coulomb interaction that leads to excitonic quasiparticles with binding energies in the range of several 100 meV. In TMD stacks consisting of at least two layers, the interlayer interaction can be precisely controlled by manipulating the twist angle: The misalignment of the crystallographic directions leads to a momentum mismatch between the high symmetry points of the hexagonal Brillouin zones. This strongly impacts the interlayer wavefunction hybridization, and, moreover, adds an additional moiré potential. Crucially, in this emergent energy landscape, dark intra- and interlayer excitons dominate the energy dissipation pathways. While these dark excitonic features are hard to access in all-optical experiments, time-resolved momentum microscopy [3] can provide unprecedented insight on these quasiparticles [4].

In my talk, I will present our recent results on the ultrafast formation dynamics of interlayer excitons in twisted WSe2/MoS2 heterostructures. First, I will report on the identification of a hallmark signature of the moiré superlattice that is imprinted onto the momentum-resolved interlayer exciton photoemission signal. With this data, we reconstruct the electronic part of the exciton wavefunction, and relate its extension to the moiré wavelength of the heterostructure. Second, I will show that interlayer excitons are effectively formed via exciton-phonon scattering, and subsequent interlayer tunneling at the interlayer hybridized Σ valleys on the sub-50 fs timescale. Finally, I will discuss our recent efforts to monitor the interlayer exciton formation dynamics with spatiotemporal resolution using femtosecond photoelectron dark-field microscopy.

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Probing tunneling processes into YSR states with microwaves

Janis Siebrecht, Haonan Huang, Piotr Kot, Sujoy Karan, Ciprian Padurariu, Björn Kubala, Joachim Ankerhold, Alfredo Levy Yeyati, Juan Carlos Cuevas, Christian R. Ast

MC21: Bound States in Hybrid Superconductor Nanostructures V, August 23, 2022, 2:00 PM - 3:30 PM

Microwaves are an important tool in the manipulation of multi-level systems such as single spins on a surface, nitrogen vacancies in diamond or double quantum dots. Here we use a scanning tunneling microscope (STM) at a base temperature of 0.56K to probe the intrinsic YSR states in a Vanadium tip in contact with a V(100) surface. The addition of an E-Band (60-90GHz) microwave antenna at the junction opens the possibility to study the behavior of YSR states with AC driving- a scenario which has been subject to many theoretical but very few experimental studies. Using microwave-assisted tunneling, we gain insight into how the excited state participates in the tunneling process and how this is related to Andreev processes and parity conservation. Our results point at a new path, namely microwave manipulation of YSR states, which could be an important step towards using YSR states as qubits.

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Perturbational Imaging of Molecules with the Scanning Tunneling Microscope

Mr Haoxuan Ding

MC18: Developments at the Frontiers of High-resolution Scanning Probe Microscopy II, August 22, 2022, 2:00 PM - 3:30 PM

Microscopic imaging of molecules is important for determination of molecular structures by providing real space snapshots. The scanning tunneling microscope (STM) is able to offer local perturbations to a molecule such that the molecule is locked in a transient state. This perturbation is tunable to certain extent, giving rise to the possibility to “pose” the molecule before a shot is taken. Here, we report the pose-and-shoot method applied to Au-adatom-diethylthiolate (CH3 CH2 S−Au−SCH2 CH3). This type of perturbational imaging significantly enhances the capability of the STM in providing a dynamic view of the molecule.

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Complex Supramolecular Tessellations with On-surface Self-Synthesized C60 Tiles through van der Waals Interaction

Mr Haoxuan Ding

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Supramolecular tessellation with self-synthesized (C60)7 tiles is achieved based on a cooperative interaction between co-adsorbed C60 and octanethiol (OT) molecules. Tile synthesis and tiling take place simultaneously on a gold substrate leading to a two-dimensional lattice of (C60)7 tiles with OT as the binder molecule filling the gaps between the tiles. This supramolecular tessellation is featured with simultaneous on-site synthesis of tiles and self-organized tiling. In the absence of specific functional groups, the key to ordered tiling for the C60/OT system is the collective van der Waals (vdW) interaction among a large number of molecules. This bicomponent system herein offers a way for the artificial synthesis of 2D complex vdW supramolecular tessellations.

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Anatomy of many-body localisation on the Fock space

Dr Sthitadhi Roy

MC42: Broken Ergodicity and Localisation in Quantum Many-body Systems V, August 23, 2022, 2:00 PM - 3:30 PM

A disordered, interacting quantum many-body system, in general, can be mapped onto a tight-binding problem on the complex, correlated Fock-space graph of the system. The problem of many-body localisation then maps onto an unconventional Anderson localisation problem on the high-dimensional Fock-space graph with strongly correlated disorder. In this talk, I will discuss several aspects of the anatomy of many-body localised eigenstates on this graph with a focus on the correlations between the eigenstate amplitudes. In particular, I will discuss how a lengthscale emerges on this graph in a many-body localised phase and how that leads to multifractality. I will also discuss the implications of these structures on local (in real-space) observables. Finally, I will present a scaling theory of the many-body localisation transition in terms of the statistics of these eigenstate amplitudes on the Fock-space graph.

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Modeling swift heavy ion track formation: how electrons heat the lattice

Dr. Nikita Medvedev

MC38: Controlled Irradiation Disorder in Model Systems, Organisation, Dynamics, and Transformations X, August 25, 2022, 2:00 PM - 3:30 PM

The effects of swift heavy ion (SHI) impact on the matter are a multiscale problem, posing challenges to theory and modeling. It starts from the energy deposition by the SHI to the electronic system of the target. Then, electrons exchange energy with the atoms. An atomic response may lead to transient disorder. After possible recrystallization, the remaining damage forms the observable nanometric track.
The crucial stage of the track formation is the energy exchange between excited electrons and the target lattice. The mechanisms of this atomic heating remained poorly understood for decades. There has been a puzzling discrepancy between slow electron-phonon coupling and the fast creation of swift heavy ion tracks. Track formation requires extremely fast energy transfer from the excited electrons to atoms [1]. In contrast, laser-irradiation experiments measured much too slow electron-phonon coupling, which is supported by various calculations [1]. This paradox led to the widespread use of electron-phonon coupling as a fitting parameter in calculations of SHI track creation.
We resolve this contradiction by noticing that electron-phonon coupling is not the sole mechanism of energy exchange between electrons and atoms in solids. The heating of electrons alters the potential energy surface of atoms. Appearing forces due to modification of the interatomic potential accelerate atoms increasing their kinetic energy (”nonthermal heating”) [1]. This non-thermal mechanism may be extremely fast – significantly faster than the electron-phonon coupling. At high deposited doses it may even lead to ultrafast nonthermal structure transformations.
Our results suggest that the nonthermal heating of atoms is a universal effect in nonmetallic crystalline materials under ultrafast energy deposition, and thus must be taken into account in appropriate models and interpretation of experiments [1].
Based on this knowledge, we propose a simple model to account for the nonthermal energy exchange between electrons and atoms in covalent materials via the conversion of the potential energy of electron-hole pairs into kinetic energy of atoms on-the-fly [2]. The model is free from fitting parameters. It is based on a combination of transport Monte Carlo (MC) simulations with classical molecular dynamics (MD). The advantage of such an approach is that it can readily be implemented into standard MC models, without complex ab-initio simulations of the effect. As it is the dominant channel of energy transfer from excited electrons to atoms in SHI tracks [1], the proposed simple model can significantly boost practical applications [2].

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Probing collective effects in a quantum critical Bose-Hubbard model using polarons.

Victor Colussi

MC35: Collective Effects and Non-Equilibrium Phenomena in Quantum Gases and Superconductors IX, August 25, 2022, 11:30 AM - 12:30 PM

We study the physics of a mobile impurity confined in a lattice, moving within a Bose-Hubbard bath at zero temperature. Within the Quantum Gutzwiller formalism, we develop a beyond-Fröhlich model of the bath-impurity interaction. Results for the properties of the polaronic quasiparticle formed from the dressing of the impurity by the quantum fluctuations of the bath are presented throughout the entire phase diagram, focusing on the quantum phase transition between superfluid and Mott Insulator. Here we find that the modification of impurity properties is highly sensitive to the different universality classes of the transition, providing an unambiguous probe of correlations and collective modes (Goldstone, Higgs, etc...) in a quantum critical many-body environment.

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Evidence of dual Shapiro steps in a Josephson junctions array

Nicolò Crescini, Samuel Cailleaux, Wiebke Guichard, Denis Basko, Kater Murch, Olivier Buisson, Nicolas Roch

MC23: Superconducting Circuits for Quantum Technologies V, August 23, 2022, 2:00 PM - 3:30 PM

The accuracy with which electromagnetic waves of specific frequencies can be both measured and produced have made frequency the basis for the definition of most physical units, including time, distance, and voltage. The modern primary voltage standard is based on the phenomena of Shapiro steps, where a tone applied to a Josephson junction yields a constant voltage determined by only the frequency of the light and fundamental constants. The duality of current and voltage has long suggested the possibility of dual Shapiro steps—that a Josephson junction device could produce current steps with heights determined only on the applied frequency. We embed an ultrasmall Josephson junction in a high impedance array of larger junctions to observe dual Shapiro steps resulting directly from microwave synchronised transport of Cooper pairs through the device. For multiple frequencies, we detect the presence of a RF mode in-phase with the tone at frequency f, and the corresponding emergence of flat steps in the IV curve with current 2ef , equal to the tunnelling of a Cooper pair with charge
2e per tone period. The observation of dual Shapiro steps opens a broad range of possibilities for future experiments, e. g. in the field of circuit quantum electrodynamics, many body quantum optics and quantum metrology.

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A Nano-Electromechanical Quantum Simulator

Stefan Forstner

Electron-phonon interactions lead to a plethora of phenomena in strongly correlated solid-state systems such as superconductivity and charge-density waves. However, the complex dynamics manifesting these phases can be beyond the reach of computational modelling, especially when taking into account electron-electron interaction. Therefore, one of the outstanding challenges in the field of correlated-electron physics is a widely tuneable model system that can mutually couple several electronic and phononic degrees of freedom. To date, no such system has been experimentally realized. While previous efforts have mostly focused on cold-atom configurations, nano-electromechanical systems are naturally suited to address this challenge. One of the most challenging requirements to engineering such a system is the achievement of ultrastrong electromechanical coupling, which has been recently demonstrated by our research group in a capacitively coupled carbon nanotube. Leveraging this capability, we work to engineer a model system in which electronic degrees of freedom are defined within four quantum dots and coupled to vibrational modes of a carbon nanotube. If successful, the project will enable the first experimental platform for quantum simulation of electron-phonon coupling.

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The best task performance in a superconducting hybrid machine

Full Professor Rosa Lopez, Associate Researcher Kun Woo Kim, Postdoctoral reseacher Jong Soo Lim

MC21: Bound States in Hybrid Superconductor Nanostructures VI, August 23, 2022, 4:30 PM - 6:00 PM

At the nanoscale, thermal engines are currently made by assembling a set of conductors attached to electronic and thermal reservoirs in which the action of electrical and thermal biases induces electron and heat flows with some specific purposes.
This research demonstrates that a better engine performance is achieved due to quantum effects, in particular, the coherence. The engine performance is characterized not only by the efficiency for doing some specific task but also by output stability represented by high suppression of fluctuations. Although the second law of thermodynamics dictates that entropy production must be zero or positive, imposing an upper bound for the efficiency, a more restrictive form for the entropy production is obtained through the so-called thermodynamic uncertainty relations (TUR). More specifically, in classical systems, entropy production constrains
the precision of the process under consideration. However, this restriction can be overcome when quantum coherence appears. With the aim of proving that quantum thermal engines benefit from coherence in optimizing the engine performance,
we investigate two interacting nanoscale conductors as a prototype. The setup consists of capacitively coupled double quantum dots. While one of the dots is connected to two normal leads, the other is connected to a normal lead and a superconducting lead which is the source of coherent states (Cooper pairs). When the system functions as a thermal machine, we explore the different operation modes and compute its efficiency when it performs a set of tasks and check the thermodynamic uncertainty relations considering the cross-responses for both charge and heat currents. We observe that it is possible to find a highly efficient quantum device operating with high precision. Definitely, our effort provides general guidelines for the design of quantum thermal
machines which can work in low dissipation, small fluctuation, and high efficiency regime.

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Electronic properties of marginally twisted 2D semiconductors

Astrid Weston, Dr Eli Castanon, Dr Volodya Enaldiev, Dr Fabio Ferreira, Dr Shubhadeep Bhattacharjee, Dr Nickolas Clark, Dr Alex Summerfield, Dr Teruo Hashimoto, Dr Andrey Kretinin, Prof Sarah Haigh, Prof Vladimir Fal'ko, Prof Roman Gorbachev

MC16: Spin Control in Twisted Van Der Waals Heterostructures I, August 22, 2022, 11:30 AM - 12:30 PM

Using the additional tool of rotational twisting of two-dimensional (2D) materials, there is almost unlimited scope for designing new metamaterials and engineer new and novel properties for the next generation of optoelectronic devices. In this work, we study low-twist-angle homobilayers of transitional metal dichalcogenides where the adjacent layers are stacked parallel ($\theta \sim 0^o$) or anti-parallel ($\theta \sim 180^o$) to study moiré superlattices resembling the 3R- or 2H- stacking polytype, respectively. Below a twist angle of $\theta \sim 2^o$, twisted bilayers of TMDs atomically reconstruct to form regions of energetically favourable domains of perfectly stack bilayers separated by boundaries of locally concentrated strain [1].

In this work, we reveal strikingly different domain formation due to lattice reconstruction leading to different electronic structures for each stacking polytype. Conductive atomic force microscopy (CAFM) revealed layer-polarised conduction band states caused by the lack of inversion and mirror symmetry of adjacent domains in the 3R-polytype configuration. Lattice reconstruction of 2H- polytypes revealed strong piezoelectric textures confined to the boundaries and intersections of the domain network.

Our most recent work reveals that for the 3R- stacking poly-type, lattice reconstruction enables ferroelectric domains with alternating out-of-plane polarisation arranged into a twist-controlled domain network [2]. Through the mechanism of domain wall sliding, polarised states can be ‘switched’ by applying out-of-plane electrical fields and has been visualized in-situ using back-scattered electron channelling contrast imaging (BSECCI) acquired using a scanning electron microscope. Prototype ferroelectric switches demonstrated pronounced hysteresis of the channel resistance in electrical transport measurements. This widens the scope for applications, for example, electronic/optoelectronic devices with built-in memory functions.

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Suspended nanowires as ultrasensitive force probes for the exploration proximity forces above surfaces and cavity nano-optomechanics

Philip Heringlake, Hugo Weltz, Francesco Fogliano, Benjamin Pigeau, Olivier Arcizet

MC17: Nanomechanical and Electromechanical Systems XI, August 25, 2022, 4:30 PM - 6:00 PM

We present the application of 2D force field imaging based on suspended SiC nanowires. In a first part we discuss the case of quasi realtime force sensing of electrostatic and proximity forces above a nano-structured surface that is approached to the nanowire's vibrating extremity. This technique uses an optical detection of the driven motion of a vertically oriented singly clamped nanowire.
The nanowire is free to oscillate in the horizontal plane with two perpendicular eigenmodes with similar frequencies. By tracking these changes of the modes' parameters we can reconstruct the force field gradient matrix and the force field itself. With a fast phase-locked loop based measurement a quasi realtime force gradient detection is possible with a sensitivity of fN/nm at 300K. At short distances the nanowire-surface interactions are dominated by electrostatic and proximity Casimir forces whose relative contributions can be tuned by adjusting bias voltages applied to the sample.
We mapped the nano-structures' topography by recording force fields quadratic in the bias voltage and imaged the impact of residual electrostatic fields produced by surface imperfections. Their contribution must be properly compensated to correctly measure the proximity forces in those novel geometries, which we achieve through a multi-electrode compensation scheme. In first measurements of the Casimir force above sub-micron trenches we find good qualitative agreement with numerical simulations.

In a second part, we present a cavity nano-optomechanical experiment where we inserted a sub-wavelength-sized nanowire in the optical mode of a fiber microcavity. The extreme sensitivity of the nanowires, their large optical scattering cross section enabled by internal Mie resonances, combined with the small mode volume of the micro-cavity provide a large optomechanical interaction sufficient to detect and map the optomechanical force exerted by less than a single mean intra-cavity photon.

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Suppressing heating by long-range interactions

Dr. DEVENDRA Bhakuni

MC42: Broken Ergodicity and Localisation in Quantum Many-Body Systems X, August 25, 2022, 2:00 PM - 3:30 PM

While periodically driven, many-body quantum systems typically reach an infinite temperature state, introducing strong disorder or sufficiently high driving frequency can yield a long, prethermal regime. In this talk, I will argue that long-range interactions can also efficiently suppress heating for specific initial conditions and low frequencies due to an effective fragmentation of the eigenenergies into bands.

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Kinetic constraints vs chaos in classical many-body dynamics

Dr Achilleas Lazarides, Dr Aydin Deger, Dr Roy Sthitadhi

MC42: Broken Ergodicity and Localisation in Quantum Many-body Systems V, August 23, 2022, 2:00 PM - 3:30 PM

I will present and discuss some recent results on ergodicity breaking in classical many-body spin systems. In particular, I will focus on a classical, clean (non-disordered) system of Heisenberg spins with kinetically constrained dynamics. The character of the dynamics depends on the strength of the constraint, with a transition between a chaotic regime and a localised regime in which the dynamics ceases.

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Inductive microwave response of Yu-Shiba-Rusinov states

Jens Paaske, Prof. Alfredo Levy Yeyati, Cecilie Hermansen

MC21: Bound States in Hybrid Superconductor Nanostructures IV, August 23, 2022, 11:30 AM - 12:30 PM

We calculate the frequency-dependent admittance of a phase-biased Josephson junction spanning a magnetic
impurity or a spinful Coulomb-blockaded quantum dot. The local magnetic moment gives rise to Yu-Shiba-Rusinov bound states, which govern the subgap absorption as well as the inductive response. We model the system by a superconducting spin-polarized exchange-cotunnel junction and calculate the linear current response to an ac bias voltage, including its dependence on phase bias as well as particle-hole and source-drain coupling asymmetry. The corresponding inductive admittance is analyzed and compared to results
of a zero bandwidth, as well as an infinite-gap approximation to the superconducting Anderson model. All three
approaches capture the interaction-induced 0–π transition, which is reflected as a discontinuity in the adiabatic
inductive response.

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SQUID-on-tip nanoscale magnetic and thermal imaging: Glimpse into dissipation in quantum systems down to atomic scale

Prof. Eli Zeldov

MC22: Nanoscale Fabrication of Superconducting Devices and their Applications XII, August 26, 2022, 9:00 AM - 10:00 AM

Energy dissipation is a fundamental process governing the dynamics of classical and quantum systems. Despite its vital importance, direct imaging and microscopy of dissipation in quantum systems are currently mostly inaccessible. We developed a scanning nanoSQUID that resides at the apex of a sharp pipette acting simultaneously as a nanomagnetometer with single spin sensitivity and as a nanothermometer providing cryogenic thermal imaging with four orders of magnitude improved thermal sensitivity of below 1 μK [1]. The non-contact non-invasive thermometry enables direct visualization and control of the minute heat generated by electrons scattering off a single atomic defect in graphene [2]. By further combining the scanning nanothermometry with simultaneous scanning gate microscopy we demonstrate independent imaging of work and dissipation, reveal the microscopic mechanisms that conceal the true topological protection in the quantum Hall state in graphene [3], and observe long-range dissipation and nontopological edge currents in charge-neutral graphene [4].

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Fermion Condensation in a Strongly Correlated 2D Electron System

Professor Sergey Kravchenko

I will review recent experimental results indicating that fermion condensation occurs in ultra-clean 2D electron systems in SiGe/Si/SiGe quantum wells. The effective electron mass at the Fermi level monotonically increases in the entire range of electron densities; in contrast, the energy-averaged mass saturates at low densities. The qualitatively different behavior of the two masses reveals a precursor to the interaction-induced single-particle spectrum flattening and suggests that fermions condense at the Fermi level in a range of momenta (unlike bosons).

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Non-local spectral signatures of many-body localization

Dr Abhishodh Prakash, Prof Manas Kulkarni, Prof Jedediah Pixley, Mr Mahaveer Prasad

I will describe non-local signatures of uncorrelated spectra that can be found in the spectral form factor of many-body-localized systems. This takes on a power-law scaling form with a specific exponent and is related to the underlying Poisson nature of the spectrum in the regime where it takes on the well-known linear `ramp' form for ergodic systems. While the latter arises from the intrinsic correlations and level repulsions and is robust to deformations and unfolding of the spectrum, this is unlikely true of the former. However, these signatures serve well to distinguish between the two phases and I will demonstrate its utility on a wide variety of models.

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Probing Mechanics of Plant Cells Using Atomic Force Microscopy

Dr Gleb Yakubov

MC2: Self-Organisation in Living Systems VIII, August 24, 2022, 4:30 PM - 6:00 PM

Atomic Force Microscopy is widely used to characterise the micromechanics of complex biological systems including cells. The attraction of using AFM for nanoindentation is its ability to measure very low forces and its operational versatility, as well as the potential to include in situ imaging. However, interpreting force indentation curves may present a significant challenge especially for biological materials and systems that are heterogeneous and comprise a number of morphological features, each having a unique set of micromechanical properties.
Here, I present a Multi Regime Analysis (MRA) algorithm that tackles these challenges enabling deconvolution of highly complex force indentation profiles. The MRA approach combines both well established and semi-empirical theories of contact mechanics within a single framework. I will illustrate the applicability of MRA for characterising the micromechanics of plant cells and isolated cell walls. In particular, I will show the unique capability of MRA to map micromechanical properties of individual suspension-cultured cells (SCCs), derived from Italian ryegrass (Lolium multiflorum) starchy endosperm, which show a distinct pattern of spatial distribution of elastic moduli across the surface in a form of ‘soft’ and ‘hard’ domains. These domains are found across length scales between 0.1 µm and 3 µm. The generality and wider applicability of this mechanical heterogeneity is verified through in planta characterization on leaf epidermal cells of Arabidopsis thaliana and L. multiflorum. The outcomes of this research provide a basis for uncovering and quantifying the relationships between local wall composition, architecture, cell growth, and/or morphogenesis.

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Mechanisms of interactions of swift heavy ions with embedded metal nanoparticles

Prof. Flyura Djurabekova, Dr. Aleksi A. Leino, Ville Jantunen, Prof. Kai Nordlund, Spyridon Korkos, Prof. Timo Sajavaara

MC38: Controlled Irradiation Disorder in Model Systems, Organisation, Dynamics, and Transformations X, August 25, 2022, 2:00 PM - 3:30 PM

Since the discovery in 2002 of metal nanoparticle elongation under swift heavy ions, numerous studies were devoted to understanding of physical mechanisms governing this process. In our previous studies, we used the two-temperature model to explain fairly well the elongation of nanoparticles along the ion track via material flow driven by thermal expansion. However, many assumptions in this early model remained to be clarified. In particular, the atomic interactions in energy barriers in the interface as well as a necessary recrystallization step prior the subsequent ion impact were simplified. In this talk, I will present our latest developments of the model that addresses the effect of energy barrier in the interface on the heat flow as well as corrected interaction of Au atoms with the surrounding silica matrix [1]. Our simulations show importance of atomic dynamics before and after the silica matrix solidifies. We see that the nanoparticle continues growing even when no significant dynamics is observed for silicon and oxygen atoms. We also observe the active role of the matrix: the elongation does not proceed without additional stress imposed by nearby track developed in vicinity of nanoparticles [2]. Moreover, we demonstrated recently that energetic ions can be used not only for shape modification, but also for manipulation of nanorod orientation [3]. This observation was made by imaging exactly the same nanorods before and after swift heavy ion irradiation using transmission electron microscope. Our atomistic simulations were helpful to reveal a complex mechanism of nanorod re-orientation, which proceeded via incremental shape modification, however, eventually assuming the initial nanorod shape, but oriented along the ion track. The reorientation is found to be dependent of the nanorod size.

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Classical route to ergodicity and scarring phenomena in two-component Bose-Josephson junction

Mr. Debabrata Mondal, Mr. Sudip Sinha, Dr. Sayak Ray, Prof. Dr. Johann Kroha, Prof. Subhasis Sinha

MC42: Broken Ergodicity and Localisation in Quantum Many-body Systems V, August 23, 2022, 2:00 PM - 3:30 PM

We consider a Bose-Josephson junction (BJJ) formed by the binary mixture of ultracold atoms to investigate the manifestation of coherent collective dynamics on ergodicity and quantum scars, unfolding the connection between them. By tuning the inter and intra-species interaction, we demonstrate a rich variety of Josephson dynamics and transitions between them, which plays a crucial role in controlling the overall ergodic behaviour. The signature of underlying classicality is revealed from the entanglement spectrum, which also elucidates the formation of quantum scars of unstable steady states and of periodic orbits leading to athermal behaviour in a reduced Hilbert space. We show how the degree of ergodicity across the energy band and the scarring phenomena can be probed from the auto-correlation function as well from the phase fluctuation of the condensates, which has relevance in cold atom experiments. The model can also be realized in spin systems with application to information processing and lattice-gauge simulation.

Reference: Debabrata Mondal, Sudip Sinha, Sayak Ray, Johann Kroha and Subhasis Sinha, arXiv:2204.12422 (2022).

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Bespoke superconducting resonators as probes of materials and decoherence in quantum circuits

Sebastian de Graaf

MC22: Nanoscale Fabrication of Superconducting Devices and their Applications X1, August 25, 2022, 4:30 PM - 6:00 PM

Understanding and eliminating sources of decoherence is of paramount importance for a wide range of applications in quantum sensing and metrology and a key challenge for building a fault-tolerant superconducting quantum computer. Atomic scale material defects are a major factor limiting the coherence of quantum circuits, yet to date very little is known about the structural or chemical origin of such defects, which complicates mitigation strategies. The challenge lies in the very low density and low energy scales of the defects: existing materials science cannot access these defects and we must develop new techniques bridging in-situ defect detection with surface science capable of revealing useful chemical or structural information. Here we discuss the use of specially designed superconducting resonators for a range of applications in understanding the origins of decoherence in superconducting quantum circuits. This includes the use of resonators micromachined on scanning probe tips for individual defect imaging and single microwave photon imaging of quantum circuits, engineering magnetic field resilience for in-situ electron spin resonance detection of spurious surface spins, to advanced designs and fabrication processes enabling kinetic inductance fast-frequency tuning to track and study dynamics of individual defects in situ with devices. These routes allow to develop new techniques and experiments that can locate and probe previously inaccessible properties of both individual defects and ensembles thereof, allowing to link them to a physical, structural or chemical entity.

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Self-assembly of Co-C60 clusters on Au(111) surface

Mr HAOYU ZHAO

In the previous experiments of our group, we studied the structure of Au-C60 clusters and elucidated the self-assembly mechanism of Au-C60 clusters. Cobalt is a more reactive metal than gold. Based on the experiments, we found that the Co-C60 clusters showed a structure similar to that of gold at the correct deposition order and annealing temperature. Further, at different experimental steps and annealing temperatures, we observed the unique behavior of cobalt-C60 clusters on Au(111) surface and tried to reveal the physical mechanism behind this phenomenon.

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Quantum fluctuation based cooling mechanism at low temperatures

Bernd Braunecker

MC24: Quantum Electronics at Ultra-low Temperatures VII, August 24, 2022, 2:00 PM - 3:30 PM

Through adiabatic demagnetisation methods it is possible to cool systems of magnetic moments such as nuclear spins to ultra-low temperatures. If the magnetic moments are embedded in a metal it is then possible to used the magnetic moments as a coolant for the conduction electrons. Here, however, a bottleneck of the method is apparent. On the one hand, the ultra-low temperatures of the magnetic moments can be reached because at low enough temperatures the relaxation between the moments and the electrons slows down and an effective decoupling between the magnetic moment temperature and the electronic temperature is obtained. On the other hand, it is exactly this relaxation providing the heat flow between the two subsystems that make the magnetic moments act as a coolant. As the relaxation rate is proportional to the temperature (expressed through the Korringa relation) the cooling becomes ineffective where it would be of most interest.

In this talk, as formulated in our work [1], I will discuss a proposal to overcome this bottleneck based on repeatedly triggering relaxation caused by temperature insensitive quantum fluctuations. This is based on the observation that the free induction decay of a magnetic moment passes initially through a short time span in which quantum correlations build up with the conduction electron environment. This physics has been studied over the last years under the designation of non-Markovian dynamics, or phenomenologically as an initial slip, and it causes a rapid, temperature independent relaxation of the moment, although of a quite small amplitude.

In [1] we obtained a fully analytical description of the initial relaxation and its cross-over to the temperature dependent further conventional relaxation in a Fermi liquid. Based on this we proposed to employ the temperature insensitivity of the non-Markovian decay to transport heat out of the electron system and thus, by repeated re-initialisation of a cluster of magnetic moments, to cool the electrons at very low temperatures. Estimates can then be provided for the conditions on the cooling efficiency versus reheating by the re-initialisations and heat leaks. While this work so far takes into account the relaxation and cooling of a Fermi liquid, I will also address our more recent findings on the changes occurring in a strongly correlated metal [2].

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458

Ergodicity, entanglement, and many-body localization

Dmitry Abanin

MC42: Broken Ergodicity and Localisation in Quantum Many-body Systems IV, August 23, 2022, 11:30 AM - 12:30 PM

e are used to describing systems of many particles by statistical mechanics. However, the basic postulate of statistical mechanics – ergodicity -- breaks down in many-body localized systems, where disorder prevents particle transport and thermalization. In this talk, I will review recent developments in many-body localization (MBL), based on new insights from quantum entanglement. In contrast to ergodic systems, MBL eigenstates are not highly entangled, but rather obey so-called area law, typical of ground states in gapped systems. This property gives rise to an infinite number of emergent local conservation laws in MBL phases, in terms of which the Hamiltonian acquires a universal form. Turning to the experimental implications, I will show that MBL systems exhibit a universal response to quantum quenches: surprisingly, entanglement shows logarithmic in time growth, reminiscent of glasses, while local observables exhibit power-law approach to “equilibrium” values. I will close by discussing experimental advances and outstanding challenges in exploring ergodicty and its breakdown in quantum many-body systems, including many-body mobility edges and stability of MBL in two-dimensional systems.

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Van der Waals Heteroepitaxy: Intrinsic Epitaxial Alignment of Perfluoropentacene Films on Transition Metal Dichalcogenides

Maximilian Dreher, Darius Günder, Gregor Witte

MC52: Heterostructures, Combining Organic Molecules and 2D Materials IV, August 23, 2022, 11:30 AM - 12:30 PM

Van-der-Waals bound heterosystems and organic semiconductors (OSC) combine outstanding charge carrier transport properties with tunable optoelectronic properties and offer promising hybrid systems for future electronic devices. [1,2] In this work, we have studied the formation and azimuthal alignment of crystalline adlayers of the OSC perfluoropentacene (PFP) on the basal plane of various transition metal dichalcogenides (TMDC) as well as graphite and hBN single crystals. Such quite inert basal planes enable an unrestricted growth of OSCs without the requirement of relaxation in terms of commensurability at the interface, since molecules exhibit a stronger mutual interaction than with the substrate. Nevertheless, the crystalline PFP multilayers exhibit distinct azimuthal twist angles relative to the substrate surface, which we could rationalize by so called 'on-line coincidences' introduced by Forker et al. recently. [3] Here, the molecules do not favor a specific adsorption site at the interface as it is often described by commensurate superstructures. Instead the bulk crystal structure remains unperturbed down to the interface, but a specific twist angle is adopted, where molecules avoid unfavored adsorption sites. The extreme sensitivity of the resulting twist angles by small deviations in the crystal structure enabled us further to use the large thermal expansion of the OSC (compared to TMDCs) [4] to control the twist angles by varying the substrate temperature during deposition. [5]

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Detecting "Axion" Dark Matter with Novel Materials

Dr David Marsh

MC28: Condensed-matter Quantum Technology on the Hunt for Dark Matter I, August 22, 2022, 11:30 AM - 12:30 PM

Axions are a class of dark matter candidate, which, due to the very small particle mass, display macroscopic wavelike behaviour. The frequency of the waves is unknown, but for canonical models spans roughly from kHz to THz. Axions interact with ordinary matter very weakly, via parity violating couplings to electrons, nucleons, or directly to the electromagnetic field. One can detect axions these interactions resonantly excite ordinary matter (either materials, or the vacuum). I will briefly review the theory of axions, and describe various possible dark matter detection methods currently in use, including microwave cavities, ferromagnetic resonance, and NMR. I will then focus on a new proposal for detection via axion dark matter interaction with "axion quasiparticles", a hypothetical THz antiferromagnetic excitation of certain magnetic topological insulators. The detection principle I describe can also be applied to phonon-polaritons and plasmons. Successful axion detection in THz requires extremely low loss materials (Q>1000) and low dark count, high efficiency, THZ single photon detectors.

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Defects and superionic transition in UO2

Dr Paul Fossati, Miss Giulia Porto, Dr Laurent Van Brutzel, Dr Johann Bouchet, Dr Alain Chartier, Prof. Alexandre Boulle

MC38: Controlled irradiation Disorder in Model Systems: Organisation, Dynamics, and Transformations VII, August 24, 2022, 2:00 PM - 3:30 PM

Crystals with the fluorite structure at room temperature, such as UO2 and actinides mixed oxides (MOX) used as nuclear fuels, undergo a phase transition to a superionic conductor state on heating. The basic mechanisms responsible for this transition have been described and result from the mechanical instability of one of the two constitutive sublattices of the fluorite structure. For a long time, this was explained by the natural production of Frenkel pairs leading to the collapse of the oxygen sublattice. However, more recent calculations show that the softening of an oxygen vibration mode could explain the transition, for example in CeO2. Nevertheless, our current understanding of how structure affect the superionic transition is still quite limited. Under the defects hypothesis, we would expect pre-existing defects to destabilise of the structure, facilitating the superionic transition. Defects could also change the characteristics of the soft mode, which would also affect the transition.

We investigated this issue by simulation UO2 crystals with pre-existing defects such as Frenkel pairs, Schottky defects, grain boundaries, and dislocations. We used for this purpose molecular dynamics (MD) techniques with the Cooper-Rushton-Grimes (CRG) potential. We will present our results showing how radiation-induced defects change thermodynamical properties of UO2 at the onset of the superionic transition, particularly the heat capacity and ionic diffusion, as well as the characteristics of the superionic phase.

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Indium Selenide based van der Waals heterostructures for emerging technologies

Dr. Nilanthy Balakrishnan, Dr. Zakhar Kudrynskyi, Dr. David Buckley, Dr Eli Castanon, Mr. Shihong Xie, Mr. Anubhab Dey, Dr. Wenjing Yan, Dr Tom Vincent, Prof. Zakhar Kovalyuk, Dr. Oleg Kolosov, Prof. Alexander Tzalenchuk, Dr. Oleg Makarovsky, Prof. Kaiyou Wang, Prof. Amalia Patanè

MC52: Heterostructures, Combining Organic Molecules and 2D Materials VI, August 23, 2022, 4:30 PM - 6:00 PM

The pressing demand for miniaturize devices can be fulfilled by two-dimensional (2D) semiconducting materials. Among the 2D semiconducting materials, indium selenide (InSe) compounds are attracting great attention due to their desirable electronic and optical properties [1-2]. InSe compounds can exist with different stoichiometries (e.g. InSe, In_2Se_3 and In_4Se_4) and polytype phases (α, β, γ, etc.), providing band gaps tunable from the near infrared to the visible range (1.2 - 2 eV) of the electromagnetic spectrum [2], a high electron mobility at room temperature (> 0.1 m^2/Vs) [1], room temperature ferroelectricity [3] and strong carrier correlations in atomically thin layers due to an inverted “Mexican hat” valence band [4].

Here, we review our recent work on InSe compounds based van der Waals heterostructures of interest for optoelectronics, thermoelectrics and nanoelectronics (see Figure 1). Both InSe/GaSe and InSe/In_2O_3 heterojunctions exhibit room temperature electroluminescence (EL) and spectral response from the near-infrared to the visible and near-ultraviolet ranges. This demonstrates the technological potential of heterostructures based on direct-bandgap layered GaSe and InSe compounds with an optical response over an extended wavelength range [5-6]. On the other hand, the nanoscale thermal properties of InSe layers shows an anomalous low thermal conductivity, which is smaller than that of low-κ dielectrics, such as SiO_2 [7]. The thermal response of free-standing InSe layers and layers supported by a substrate, reveals the role of interfacial thermal resistance, phonon scattering, and strain. These thermal properties are critical for future emerging technologies, such as field-effect transistors that require efficient heat dissipation or thermoelectric energy conversion with low thermal conductivity, high electron mobility 2D materials, such as InSe. Furthermore, we report on the ferroelectric semiconductor α-In_2Se_3 embedded between two single-layer graphene electrodes. We show how the ferroelectric polarization of the In_2Se_3 layer can modulate the transmission of electrons across the graphene/In_2Se_3 interface, leading to memristive effects that are controlled by an applied voltages and/or by light [8].

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Dynamics in Fermi gases quenched to unitarity

Chris Vale

Semi-plenary: Professor Chris Vale, August 25, 2022, 10:00 AM - 11:00 AM

Ultracold atomic gases with tunable interactions provide a versatile setting to study quantum systems out of equilibrium. Here, we study Fermi gases following a rapid interaction quench to the unitarity limit. For quenches that cross the normal to superfluid phase transition, we observe both pair formation and pair condensation, along with the corresponding timescales to equilibrate. Smaller quenches in the superfluid phase excite the Higgs amplitude mode, which we observe using Bragg spectroscopy. The amplitude oscillations provide a direct measure of the pairing gap and decay according to a power law with a damping exponent approximately midway between the BCS and BEC limits.

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Signatures of interactions in the Andreev spectrum of nanowire Josephson junctions

Francisco Jesús Matute-cañadas, Cyril Metzger, Sunghun Park, Leandro Tosi, Peter Krogstrup, Jesper Nygård, Marcelo F. Goffman, Cristian Urbina, Hugues Pothier, Alfredo Levy Yeyati

MC21: Bound States in Hybrid Superconductor Nanostructures V, August 23, 2022, 2:00 PM - 3:30 PM

Hybrid semiconducting/superconducting nanostructures combined with circuit-QED techniques are allowing to explore superconducting proximity effects with an unprecedented degree of detail. For instance, these techniques have permitted to reveal the fine structure, due to spin-orbit coupling, of Andreev states in semiconducting nanowire Josephson junctions [1]. While some of the observed transition lines of the microwave spectrum could be explained in terms of non-interacting models with a few conducting channels [1-3], other expected transition lines from these models could not be clearly identified and some other experimental features remained unexplained.

In this work [4] we show that the inclusion of electron-electron interactions in the normal region of the junction is necessary to account for these unexplained features, which consist in the splitting of certain degeneracies expected in the non-interacting models. This allows to identify the corresponding transition lines in the experimental spectra.

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Non-Markovian transients in non-equilibrium transport between chiral quantum wires coupled through a point-contact

Mr. Nikhil Danny Babu, Prof. Girish Setlur

The exact dynamical non-equilibrium Green functions (NEGF) are obtained analytically for a system of two quantum wires with non-interacting fermions of opposite chirality coupled through a point contact tunnel junction driven out of equilibrium by the application of a generic time-dependent bias [1]. The NEGF is written down in a closed form in terms of simple functions of position and time. This allows us to obtain the tunneling I-V characteristics in the presence of an arbitrary time-dependent bias. In addition to this, our method is able to account for transient behaviour in the Green functions as well as approach to steady state. In the present work we also consider the case of a finite momentum bandwidth in the point-contact and show that the non-equilibrium transport properties exhibit non-Markovian behaviour. Upon sudden switch on of a subsequently constant bias, the tunneling current shows a transient buildup before attaining its steady state value. This is in contrast to the infinite bandwidth case where no transients are present in the I-V characteristics. The expression for the tunneling current involves an integral over the past history of the system and hence it is of a non-Markovian nature. Previous numerical simulations of lattice systems using time-dependent DMRG (tDMRG) [2] that predict this transient property suggests that this transient buildup arises merely due to the presence of a short-distance cutoff in the problem description.

From the exact expressions for the non-equilibrium two-point functions we also obtain the four-point functions using Wick's theorem. These correlations can be used in conjunction with powerful novel bosonization techniques [3,4,5] to study non-equilibrium transport between chiral fermionic edges with mutually interacting particles like in the case of fractional quantum Hall edge states. As a starting step towards this we formulate an unconventional bosonization ansatz and use it to obtain the NEGF for the noninteracting problem [6].

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MICROWAVE RESPONSE OF A BOUND STATE IN A HYBRID SUPERCONDUCTOR NANOSTRUCTURE

Leonid Glazman, Vladislav Kurilovich, Valla Fatemi, Pavel Kurilovich, Bernard van Heck, Chaitanya Murthy, Chetan Nayak, Michel Devoret

MC21: Bound States in Hybrid Superconductor Nanostructures IV, August 23, 2022, 11:30 AM - 12:30 PM

We evaluate the admittance of a weak link between two superconductors connected by a semiconductor quantum wire. Our theory predicts the dependence of the microwave response on the link's parameters, including its length, transparency for electrons propagating across it, and the applied phase bias. The focus of our study is on the response in the absence of an external magnetic field, and on the response near the field-driven topological transition. Most of the current microwave measurements are performed in the absence of a magnetic field; we apply our theory to analyze the latest measurements data. Understanding of the response near the topological transition is conceptually important. The dependence of the admittance on frequency and temperature at the critical point is universal and determined by the symmetries of the system. Despite the absence of a spectral gap at the transition, the dissipative response may remain weak at low energies, in a striking difference from the electromagnetic response of a normal metal.

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Nanomechanical and electromechanical systems

Dr. Jana Ochs, Gianluca Rastelli, Dr. Maximilian Seitner, Prof. Mark Dykman, Prof. Eva Weig

We study the response of a weakly damped vibrational mode of a nanostring resonator to a moderately strong resonant driving force. Because of the geometry of the experiment, the studied flexural vibrations lack inversion symmetry. As we show, this leads to a nontrivial dependence of the vibration amplitude on the force parameters. For a comparatively weak force, the response has the familiar Duffing form, but for a somewhat stronger force, it becomes significantly different. Concurrently there emerge vibrations at twice the drive frequency, a signature of the broken symmetry. Their amplitude and phase allow us to establish the cubic nonlinearity of the potential of the mode as the mechanism responsible for both observations. The developed theory goes beyond the standard rotating-wave approximation. It quantitatively describes the experiment and allows us to determine the nonlinearity parameters.

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Disorder-robust phase crystal in high-temperature cuprate superconductors from topology and strong correlations

Annica Black-Schaffer, Debmalya Chakraborty, Tomas Löfwander, Mikael Fogelström

MC41: Real Space Simulations of Topological Matter and Disordered Materials III, August 22, 2022, 4:30 PM - 6:00 PM

The simultaneous interplay of strong electron-electron correlations, topological zero-energy states, and disorder is still a largely unexplored territory despite their inevitable presence in many materials. Copper oxide high-temperature superconductors (cuprates) with pair breaking edges host a flat band of topological zero-energy states, making them an ideal playground where strong correlations, topology, and disorder are strongly intertwined. Here we perform fully self-consistent calculations of the superconducting state in cuprate superconductors and find that strong correlations stabilize a fully gapped phase crystal state along the pair breaking [110] edge. The phase crystal breaks both translational and time reversal invariance and is characterized by a nanoscale modulation of the phase of the d-wave order parameter. In particular, we first show how strong correlations increase the number of zero-energy states for any uniform superconducting phase, contradicting simple topological arguments. Then, when allowing for a non-uniform solution, we find a cascade of phase transitions occurring at different temperatures: d-wave superconductivity occurs below a transition temperature Tc, the phase crystal appears further below at temperature T* ~ 0.2Tc, and, finally, an additional extended s-wave order, with the same spatial modulations as the phase crystal, is generated below Ts, producing a full energy gap. Taken together, these phase transitions explain a set of so far seemingly contradictory experimental results. Furthermore, we find that the phase crystal state is unexpectedly very robust to disorder, but notably only in the presence of strong correlations. Our results show that the combined effects of strong correlations and topology lead to the emergence of novel phases of matter that survives strong disorder in a highly non-intuitive manner.

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Modeling of dynamics of nonlinear wave propagation in phononic crystals

Jun Takayanagi

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter XIII, August 26, 2022, 10:00 AM - 11:00 AM

Metamaterials are getting greater attention for their property which can be used for wide applications. Among them, one of the most attracting characteristics of metamaterials is existence of band gap. For example, phononic band gap (PnBG) appears in phononic crystals (PnCs), which is a type of artificial structure in which a scatterer made of a hard material is embedded in the base of a soft material. Moreover, new properties have been realized by applying nonlinear dynamics in metamaterials. For example, it has been reported that the PnC can realize switching behavior by combining the PnBG and nonlinear wave propagation. This structure is called switching structure (SS). The SS has a structure in which the PnC scatterers are partially replaced with structures with different property. The switching behavior at which wave does not propagate when the amplitude of the wave is increased at certain frequency, is expected to be applied to logic gates. However, in order to put the SS to practical use, it is necessary to understand the mechanism of this nonlinear behavior. In this study, we construct a dynamics model of PnCs and the SS to understand this nonlinear behavior.

The model consists of mass points and linear springs. To represent the difference in material properties between the background and the scatters, mass of the scatter mass points is multiplied by 10 times and similarly spring constant of the adjacent springs is by 1000 times compared to them of the background. Moreover, nonlinearity is added to the model by changing the mass of each mass point in response to the displacement of the mass point.

We perform frequency response simulations in the model. In this simulation, a forced vibration is applied to the one end of the model to investigate how the wave propagation behavior changes in response to the frequency of forced vibration. The numerical results shows that the vibration propagated only near the natural frequencies of the model. It is also confirmed that a band gap is realized in the model in the frequency range where no natural frequency exists (f = 0.26-0.32 [Hz]). Moreover, Fourier analysis of these results show that the frequency distribution disperses in proportion to the distance from the one end of the model, but that only the frequency components near the natural frequency propagate. And, dispersion curve of this model indicates existence of band gap near this frequency band (f = 0.26-0.32 [Hz]), which shows validity of the model.

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Hunting Majorana Bound States in Topological Systems:

Dr Oindrila Deb

MC21: Bound states in hybrid superconductor nanostructures VIII, August 24, 2022, 4:15 PM - 6:00 PM

Topological materials have fundamentally enriched our understanding of quantum phases of matter and have the hallmark of hosting quantum states at their boundaries which are protected from disorder. In this colloquium, I will talk about a particular kind of topological material known as topological superconductors (TSCs) which hosts exotic zero-energy modes at the boundary. These boundary modes called Majorana bound states (MBSs), named after Ettore Majorana who postulated their existence in 1937, are their own antiparticles and one of the most important candidates to build a topological qubit for quantum computation. In this talk, I will first introduce a one-dimensional toy model of TSC to demonstrate the emergence of an MBS at the system boundary. Experiments to detect MBS, even while extremely difficult and novel, are often inconclusive about a Majorana detection potentially due to other effects in the system. While providing some examples of such experimental efforts, I will discuss our recent work where we find that even two spin impurities in a two-dimensional TSC can lead to experimental signatures that can mimic those of MBS. I will conclude by providing the future directions towards hunting MBS in various quantum condensed matter systems.

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Dark matter: motivation, candidates and experimental prospects

Edward Hardy

MC28: Condensed-matter Quantum Technology on the Hunt for Dark Matter I, August 22, 2022, 11:30 AM - 12:30 PM

I will discuss the evidence for dark matter and some of the different (as yet undiscovered) particles that could account for it. After reviewing candidates such as WIMPs and asymmetric dark matter, I will focus on the alternative possibility that dark matter is a particle with small (less than eV) mass, in which case it has wave-like properties in the present day Universe. One of the foremost such dark matter candidates is the QCD axion, and I will describe what is known theoretically and the remaining uncertainties in this case. I will also discuss current experimental detection approaches and possible future directions.

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From quantum tunneling in a topology-changing fermionic bath to topological quantum superpositions

Elis Roberts, Jan Behrends, Benjamin Béri

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Coupling a quantum particle to a fermionic bath suppresses the particle's amplitude to tunnel, even at zero temperature. While this effect can generally be neglected for gapped baths -- a key feature for superconducting qubits -- , it is possible for the bath to be gapped near the potential minima between which the particle tunnels, but different minima to correspond to different bath topologies. This enforces the bath to undergo gap closing along the tunneling path. In this work, we investigate quantum tunneling in the presence of such a topology-changing fermionic bath. We develop a field theory for this problem, linking the instantons describing tunneling in a bath of d space dimensions to topological boundary modes of systems in d+1 dimensions, thus stepping a level higher in a dimensional hierarchy. We study in detail a d=1 example, inspired by planar Josephson junctions where the particle coordinate is the superconducting phase whose value sets the electronic topology. We find that the topology change suppresses tunneling by a factor scaling exponentially with the system size. This translates to a correspondingly enhanced suppression of the energy splitting for the lowest-lying states, despite these being linear combinations of states near potential minima where the bath is gapped. Our results help to estimate the influence of charging energy on topological phases arising due to the Josephson effect and, conversely, to assess the potential utility of such topological systems as superconducting qubits. For moderate-sized baths, the incomplete suppression of tunneling opens the prospects of quantum-mechanical superpositions of many-body states of different topology, including superpositions of states with and without Majorana fermions.

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On the reliability and reduction of error of resonance circle fits

Dr Paul Baity, Connor Maclean, Valentino Seferai, Tania Hemakumara, Yi Shu, Harm Knoops, Russ Renzas, Prof Martin Weides

MC23: Superconducting Circuits for Quantum Technologies III, August 22, 2022, 4:30 PM - 6:00 PM

The control of material losses is playing an increasingly more important role for improving coherence times of superconducting quantum devices [1,2]. Such material losses can be characterized through the measurement of planar superconducting resonators, which reflect losses through the resonance's quality factor Ql. This resonance quality factor reflects both internal losses (i.e. material losses) as well as external losses when resonance photons escape into the measurement circuit. The combined losses then contribute as 1/Ql = 1/Qc + 1/Qi, where Qc and Qi are the external and internal quality factors of the resonator, respectively. The resonance response projects onto the complex plane as circle, which can be fit by geometric or algebraic means [3,4] to extract the resonator's quality factors. Diameter-correcting circle fits, such as those used by Probst et al. [5], use algebraic means to distinguish the internal and external quality factor contributions. However, for low-loss materials with Qi>>Qc, external losses dominate the resonator response, making a reliable determination of the internal quality factor more difficult. While in principle, this can be resolved by resonator design changes, for materials and process exploration purposes, it may not be possible to accurately predict internal losses prior to fabrication of the design. Therefore, a robust fitting algorithm is required that can accurately fit for quality factors over a wide range of design parameters. To address this issue, we have used a combination of simulations and experiments to determine the reliability of the fitting algorithm of Ref. [5] across a wide range of quality factor values from Qi>>Qc to Qc>>Qi. We perform an analysis of the fit error contributions and conclude that while fit errors depend on the ratio Qi/Qc, Qi determination can still be reliable when noise levels are sufficiently low and the number of data points remains large. In addition, we have also explored alternative measurement protocols to minimize the errors on resonance circle fit parameters.

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Sachdev-Ye-Kitaev circuits for braiding and charging Majorana zero modes

Jan Behrends, Benjamin Béri

MC21: Bound States in Hybrid Superconductor Nanostructures V, August 23, 2022, 2:00 PM - 3:30 PM

The Sachdev-Ye-Kitaev (SYK) model is an all-to-all interacting Majorana fermion model for many-body quantum chaos and the holographic correspondence. Here we construct fermionic all-to-all Floquet quantum circuits of random four-body gates designed to capture key features of SYK dynamics. Our circuits can be built using local ingredients in Majorana devices, namely charging-mediated interactions and braiding Majorana zero modes. This offers an analog-digital route to SYK quantum simulations that reconciles all-to-all interactions with the topological protection of Majorana zero modes, a key feature missing in existing proposals for analog SYK simulation. We also describe how dynamical, including out-of-time-ordered, correlation functions can be measured in such analog-digital implementations by employing foreseen capabilities in Majorana devices.

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Weak ferroelectricity in few-layer graphenes

Dr. Aitor Garcia-ruiz, Dr. Vladimir Enaldiev, Dr Vladimir I. Fal'ko

MC12: Physics in 2D Nanoarchitectonics IV, August 23, 2022, 11:30 AM - 12:30 PM

Ferroelectric van der Waals heterostructures have attracted a lot of research attention, as they could be used on a wide range of device applications, such as non-volatile memory devices or pyroelectric sensors [1]. Experimentalists have constructed such structures using hexagonal boron nitride [2] or transition-metal dichalcogenides [3]. However, there has been no theoretical or experimental reports on single-element ferroelectric materials yet.
In this presentation, I will discuss a family of carbon-based structures that host a weak ferroelectric effect, with special focus on marginally twisted double bilayer graphene (AB/BA). In this material, each domain of the moiré unit cell breaks inversion symmetry, as the top three layers have a different stacking from the bottom three layers (see Fig. 1). Following previous works [4], we find that the charge distribution across the layers inherits this feature from the crystal symmetry and develop a method to compute the ferroelectric polarisation map across the moiré unit cell, including the effects of lattice relaxation. We find that the ferroelectric polarisation has a definite orientation in each domain and propose an experimental setup that enable us to observe ferroelectricity.

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Controlling the Shape of finite 2D Systems by Surfactants

Mr Birkan Emrem, Mr Jan-Ole Joswig, Mr Thomas Heine

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

In the field of the nanotechnology, controlled synthesis of two−dimensional (2D) nanoplatelets is one of the biggest challenges faced since the beginning of the era of 2D materials. In this study, we investigate if surface-active agents (surfactants) can be used to manipulate the growth direction of selected 2D materials.

Finite transition metal dichalcogenide (TMDC) 2D nanoplatelets offer several attack positions for surfactants, for instance, edges, vertices, or the basal plane. By their natures, these sites have different activity levels, and, consequently, these lead to non-similar surfactant binding affinities. Using different activity levels, surfactant-assisted colloidal synthesis can be used to grow different shapes of TMDC nanoparticles. Triangular shaped nanoparticles in 2H phase, hexagonal and star−shaped nanoparticles in 1T phase can be given as examples. Promoted growth of star-shaped systems is particularly interesting, as it allows maximizing catalytic activity at the edges.

We have used dispersion-corrected density-functional theory (DFT) for finite triangular MoS2 systems with the surfactants methylamine, methyl alcohol, and formic acid. As for now, the initial results show lower surfactant binding energies at the edges rather than at a vertex or the basal plane of the particles. From a thermodynamic point of view, a faster growth at the edge centers can be expected in comparison to the vertices due to the lower binding energies at this place and a corresponding faster exchange of molecular species.

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Laser heating for analyzing the energy dissipation due to Casimir-like interactions in colloidal systems within critical baths.

Ignacio A. Martinez

MC19: Advances in the Casimir Force and Heat Transfer Phenomena V, August 23, 2022, 2:00 PM - 3:30 PM

Critical Casimir interactions represent a perfect example of bath-induced forces in the mesoscale that may have a relevant role in the living systems as well as a role in the design of nanomachines fueled by environmental fluctuations. Since the thermal fluctuations are enhanced in the vicinity of a demixing point of a second-order phase transition, we can modulate the magnitude and range of these Casimir-like forces by slight changes in the temperature. Here, we control them by warming the mixture using laser-induced heating, whose local application ensures a high reproducibility. Once the optically trapped two-particle system is warmed, we use the critical interactions as the system's self-thermometer using different observables. Finally, we use our experimental scheme for analyzing the energetics of a critical colloidal system under a non-equilibrium-driven protocol. We quantify how the injected work can be dissipated to the environment as heat or stored as free energy. Indeed, our system allows us to use the fluctuation theorems framework for analyzing the performance of this critically-driven toy model. Our work paves the way for future experimental studies on the non-equilibrium features of the bath-induced forces and the design of critically driven nanosystems.

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Re-entrant percolation in active Brownian colloids

Dr Mark Miller, Mr David Evans, Mr José Martin-Roca, Dr Chantal Valeriani

MC6: Emergent Phenomena in Driven Soft, Active and Biological Matter VI, August 23, 2022, 4:30 PM - 5:30 PM

Percolation is the sudden emergence of a macroscopic, system-spanning cluster at a critical set of conditions. In colloidal matter, percolation is typically triggered at a threshold in the packing fraction and/or interaction strength between particles. For passive matter at equilibrium, percolation can often be understood using a range of heuristic observations, numerical calculations, and analytical theories.

In this contribution, I will describe ongoing computational work into percolation in a non-equilibrium colloidal model, namely two-dimensional active Brownian hard disks. This system is known to undergo motility-induced phase separation (MIPS) at sufficiently high Peclet number and density. However, very weak activity (far below the MIPS transition) leads to enhancement of percolation, lowering the packing fraction at which system-spanning clusters are seen. For stronger activity, but still below the MIPS transition, the percolation threshold passes through a minimum before rising, leading to re-entrant percolation as a function of activity over a window of densities.

The weakly active case can be understood as a perturbed passive system with an effective attraction, which we quantify. Scaling laws for the percolation probability function continue to work up to moderate levels of activity, allowing the percolation threshold to be well defined. However, empirical rules of thumb such as a critical coordination number become steadily less reliable with increasing activity. Our study provides insight into the evolution of active Brownian particles both far from the onset of MIPS and into the phase-separated regime.

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Microwave spectroscopy of Andreev states in a InAs nanowire Josephson weak link close to pinch-off

Manas Ranjan Sahu, Maria Benito, Cyril Metzer, FJ Cañadas, Sunghun Park, L Tosi, P Krogstrup, J Nygård, A Levy Yeyati, MF Goffman, C Urbina, H Pothier

MC21: Bound States in Hybrid Superconductor Nanostructures V, August 23, 2022, 2:00 PM - 3:30 PM

We performed the microwave spectroscopy of an InAs Josephson weak link close to pinchoff, revealing the interplay of strong coulomb interactions and superconducting proximity effect. In the regime where the semiconducting nanowire behaves as a quantum dot (QD), it is predicted that the ground state can change from singlet to doublet, depending on different competing energy scales, namely, charging energy, superconducting pairing energy and coupling strengths to the superconducting leads. We observed signatures of transitions from singlet to doublet ground state and explored the underlying phase diagram as a function of gate voltage and the phase difference across the weak link. Two-tone microwave spectra display anomalous parity switching transitions, which we tentatively interpret as signatures of the presence of more than one QDs in the weak link.

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Probing Josephson Weak Links near pinch–off using microwave spectroscopy

Maria Benito, Manas Ranjan Sahu, Hugues Pothier, Marcelo Goffman, Cyril Metzger, Francisco Jose Matute Cañadas, Alfredo Levy Yeyati, Sunghun Park, Cristian Urbina

We use Circuit Quantum Electrodynamics (cQED) techniques to probe the spectrum of Andreev Bound States in a Josephson Weak Link consisting of an InAs nanowire contacted by two superconducting Al electrodes, and placed in a superconducting loop. Readout of the quantum state is accomplished by coupling it to a coplanar-stripline (CPS) λ/4 resonator.

Single-tone measurements performed near the region where the nanowire is completely depleted from electrons ("pinch-off" regime), show abrupt changes in the resonance frequency. We interpret these sharp jumps as parity changes from singlet to doublet state, considering the formation of a quantum dot given this low bias configuration. Theoretically, such a transition is predicted to depend on the charging energy of the quantum dot, the superconducting-pairing energy, the coupling strength to the superconducting leads and the phase difference between them. Experimentally, we explore the effect of those parameters: a gate voltage tunes both the Fermi energy in the nanowire and the coupling strength to the leads; a magnetic field applied perpendicular to the sample controls the magnetic flux through the superconducting loop, which enables us to control the phase difference across the nanowire. The population and rates between the singlet and doublet ground states are extracted as a function of both gate and flux.

Two-tone microwave spectroscopy will also be discussed. I will present the model developed by our theoretical collaborators , which accounts for the data by introducing a second quantum dot weakly coupled to the main one.

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Universal principles of moiré band structures

Simon Trebst

MC41: Real Space Simulations of Topological Matter and Disordered Materials II, August 22, 2022, 2:00 PM - 3:30 PM

Moiré materials provide a highly tunable environment for the realization of band structures with engineered physical properties. Specifically, moiré structures with Fermi surface flat bands — a synthetic environment for the realization of correlated phases — have moiré unit cells containing thousands of atoms and tantalizingly complex bands structures. In this talk, I will show that statistical principles go a long way in explaining universal physical properties of these systems. Our approach builds on three conceptual elements: the presence of quantum chaos caused by the effective irregularity of the atomic configurations on short length scales, Anderson localization in momentum space, and the presence of approximate crystalline symmetries. Which of these principles dominates depends on material parameters such as the extension of the Fermi surface or the strength of the moiré lattice potential. The phenomenological consequences of this competition are predictions for the characteristic group velocity of moiré bands, a primary indicator for their average flatness. In addition to these generic features, we identify structures outside the statistical context, notably almost flat bands close to the extrema of the unperturbed spectra, and the celebrated zero energy ‘magic angle’ flat bands, where the latter require exceptionally fine tuned material parameters.

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Spontaneous trail formation in populations of signalling active walkers

Zahra Mokhtari, Robert I. A. Patterson, Felix Höfling

MC6: Emergent Phenomena in Driven Soft, Active and Biological Matter VI, August 23, 2022, 4:30 PM - 5:30 PM

How do ants form long stable trails? Despite abundant evidence that trail formation in colonies of insects or bacteria originates in their sensing of and responding to the deposits of chemicals that they produce, there is no consensus on the minimum required ingredients for this phenomenon. To address this issue, here, we develop an agent-based model in terms of active random walkers communicating by means of pheromones, which can generate trails of agents from an initially homogeneous distribution.

Based on extensive off-lattice computer simulations we obtain qualitatively the non-equilibrium state diagram of the model, spanned by the strength of the agent-chemical interaction and the number density of the population. In particular, we demonstrate the spontaneous formation of persistent, macroscopic trails, and highlight some behaviour that is consistent with a dynamic phase transition. This includes a characterisation of the mass of system-spanning trails as a potential order parameter. We also propose a dynamic model for few macroscopic observables, including the sub-population size of trail-following agents, which captures the early phase of trail formation.

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Engineering the Electronic properties of 2D Quantum Materials with Tunable Superlattices

Kevin Garcia Diez, Guillaume Vasseur, Ignacio Piquero-Zulaica, Frederik Schiller, Julien Raoult, Miguel Angel Valbuena, Stefano Schirone, Sonia Matencio, Jose Enrique Ortega, Jorge Lobo-Checa, Massimo Tallarida, Aitor Mugarza

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Materials exhibiting spin-orbit coupling (SOC) have triggered an immense research activity that led to the opening of a new field in spintronics, the so-called spin-orbitronics [1]. As for any other material, their successful technological application depends on two factors: a fundamental understanding of the emerging phenomena, and the capability to engineer and tune their key properties. Exposing electrons to superlattice potentials is a very attractive approach to simultaneously realize these two conditions [2,3].

Here we present the first realization of periodic resonator arrays on the BiAg2 atom-thick surface alloy with atomic precision, and demonstrate their potential ability for tailoring the giant-split helical Rashba states [4]. By using curved crystals to select local vicinal planes we achieve arrays of BiAg2 monoatomic steps with distinct step structure and spacing, as experimentally determined from scanning tunneling microscopy and low energy electron diffraction. Scanning the photon beam across the BiAg2 curved surface in angle-resolved photoemission experiments, and comparing results with Density Functional Theory, allow us to assess the interaction of the Rashba helical states with the step arrays. We find that coherent scattering induces a strong anisotropy in the dispersion and orbital, and hence spin texture of Rashba bands. Finally, we present our latest efforts on extending the method to study Bismuthene superlattices.

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Numerical renormalization group study of the Loschmidt echo in quenched quantum impurity systems

Kacper Wrześniewski, Tomasz Ślusarski, Ireneusz Weymann, Nicholas Sedlmayr, Tadeusz Domański

MC21: Bound States in Hybrid Superconductor Nanostructures VI, August 23, 2022, 4:30 PM - 6:00 PM

We analyze the time evolution of the Loschmidt echo following a quench in Hamiltonian variables applied for two different models. Firstly, we study the one-channel Kondo model, where universal behavior of the Loschmidt echo is revealed with the time scale given by the inverse of the Kondo temperature. For the two-channel Kondo model, we focus on the quench leading to the formation of the non-Fermi liquid state and discuss relevant dynamics. Finally, we study the case when the system initially prepared in Fermi liquid phase is suddenly coupled to the second screening channel. Here, a new time scale emerges, which is associated with the channel anisotropy.

Furthermore, we consider the Loschmidt echo in the case of a quantum dot embedded between normal and superconducting electrodes. We focus on the singlet-doublet dynamical phase transition upon traversing the phase boundaries between the ground states. The analysis of the Loschmidt echo and non-analytic cusps in the return rate reveal signatures of dynamical quantum phase transitions periodically occurring at critical times.

483

Two Dimensional Soft Molecular Architectures on Hard Surfaces

Rasmita Raval

Molecules represent the most versatile, functional entities available in Nature and are central components in the machinery of life. This has inspired scientists to translate molecular systems to 2D surfaces in order to engineer 21st century nanotechnology. A critical transition from a simple isolated molecule to a complex 2D molecular collective is required in order to deliver a functional interface. This talk will outline the pivotal role of scanning probe microscopy, surface spectroscopies and periodic density functional theory in demonstrating how organic and biological molecules come together at surfaces and how their extended 2D organisations and macroscale attributes are determined by single bond and single molecule orientations at the interface. In addition, the surface provides a reactive environment in which molecules can couple covalently to create complex organic matter, with the direct emergence of structural and topological complexity, often giving rise to new types of molecular materials. Such 2D supramolecular and covalent assemblies give rise to complex physical and chemical functions at surfaces like chiral recognition and separation, stimuli-responsive behaviour and provide a platform for simple molecular machines.

495

Effect of the electric field in High Chern number magnetic Topological insulators

Yuriko Baba, Francisco Domínguez-Adame, Rafael A. Molina

MC14: Beyond Charge Transport in Nanostructures and 2D Materials via Geometric Design IX, August 25, 2022, 11:30 AM - 12:45 PM

The Quantum Anomalous Hall state can be realized in a high Chen number configuration in magnetically doped topological insulators such as Cr-doped Bi2(Se,Te)3 . In three-dimensional structures of magnetically doped and undoped layers, the number of chiral edge channels can be controlled by the width and number of layers generating an effective 2D Quantum Anomalous Hall state, measured in transport experiments showing this feature up to C = 5 [1].

In this work, we explore the possibilities of tuning the chiral channels of the aforementioned materials in the presence of electric fields in multilayered structures. Due to the external field, the Chern number is modified dynamically, with a remarkable impact on the transport properties of pristine and disordered samples.

[1] Zhao, Y. F. et al., Nature, 588 (2020) 419

484

Imaging quantum materials with scanning SQUID microscopy

Prof. Beena Kalisky

MC22: Nanoscale Fabrication of Superconducting Devices and Their Applications X, August 25, 2022, 2:00 PM - 3:30 PM

Competition or cooperation between different electronic orders with similar energy scales often gives rise to new or unexpected behaviors. Detecting traces of such orders requires versatile probes, which can probe different aspects of the system, such as conductivity, superconductivity and magnetism. In my talk, I will describe two systems where our local view uncovered surprising mesoscopic effects. In the oxide interface LaAlO3/SrTiO3, we imaged the current flow close to a metal-insulator transition. We found that the critical behavior is controlled by structural domain patterns in the substrate, rather than by universal scaling laws. In the transition metal dichalcogenide 4Hb-TaS2 we show that the superconducting state hosts a spontaneous vortex phase, where vortices appear in the absence of an external field. I will show evidence that this spontaneous vortex phase is caused by unconventional magnetism in the normal state.

492

All-optical switching in Co/Pt multilayers

Mr Wenjia Li, Mr Kaiyu Tong, Miss Zhuoyi Li, Dr Xianyang Lu, Dr Jing Wu, Prof Yongbing Xu

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

The demands for the ever-increasing speed of magnetic storage of information in magnetic media and the intrinsic limitations imposed by magnetic-field-driven writing techniques in magnetic recording have triggered intense searches for ways to control magnetisation by means other than magnetic fields. The discovery of ultrafast magnetisation dynamics induced by femtosecond laser pulses potentially provides such a means and at the same time spin dynamics becomes one of the most challenging and outstanding questions in today's condensed matter physics. The heating and helicity effects induced by circularly polarized laser excitation are entangled in the helicity-dependent all-optical switching (HD-AOS), which hinders the understanding of magnetization dynamics involved. Here, HD-AOS in Co/Pt multilayer has been investigated by applying a dual-pump laser excitation, first with a linearly polarized (LP) laser pulse followed by a circularly polarized (CP) laser pulse. The contribution from heating and helicity effects in HD-AOS in Co/Pt multilayers are identified. When the sample is preheated by the LP laser pulses to a nearly fully demagnetized state, CP laser pulses with a much-reduced power switches the sample's magnetization. By varying the time delay between the two pulses, heating and helicity effects can be tuned with the unique dual-pump laser excitation, which will enable HD-AOS in a wide range of magnetic material systems.

488

Proximity-induced superconductivity generated by thin superconducting films: the role of disorder

Tudor Stanescu

MC21: Bound States in Hybrid Superconductor Nanostructures I, August 22, 2022, 11:30 AM - 12:30 PM

We examine the role of surface disorder characterizing a thin superconducting film in determining the strength of the proximity effect induced by the superconductor across an interface with a semiconductor. Using a three-dimensional model, we examine both the positive and the negative effects of the surface disorder, including the possibility of inducing effective disorder inside the semiconductor subsystem. Possible implications regarding proximity-induced topological superconductivity and Majorana-type bound states are discussed.

517

Oscillations in cell cycle times in Drosophila abdomen modelled as cell phase synchronization

Riya Nandi, Andrea Cairoli, John J. Williamson, Ana Ferreira, Anna P. Ainslie, John Robert Davis, Nicolas Tapon, Guillaume Salbreux

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Analysis of tissue growth in Drosophila abdomen has revealed that the cell cycle times are correlated in space and time. One manifestation of such correlations is through the average rate of cell division in the Histoblast nests which has been observed to oscillate with a period of roughly four hours, before decaying after 28 hAPF. As a simple explanation for such oscillations, we propose that neighbouring cells have synchronous cycles. We develop a model of the cell cycle where each cell is a phase oscillator evolving from a phase of 0 to 2π between birth and division. We then study phase synchronization for a growing and dividing population of cells using a variant of the standard Kuramoto model with nearest neighbour coupling and a Gaussian noise term. Such a model reproduces oscillations in the cell-division rate, and limit-cycle trajectories of the global phase of the system, as observed experimentally. This model exhibits a continuous phase transition with a psuodo-synchronous phase for high values of the coupling constant. We further discuss the critical behaviour and extract the various exponents for this model.

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High Temperature Superconductor Materials Modification with Focused Helium Ions for Nano Josephson Devices

Professor Shane Cybart

MC22: Nanoscale Fabrication of Superconducting Devices and their Applications X1, August 25, 2022, 4:30 PM - 6:00 PM

In Feynman’s infamous 1959 lecture entitled, "There's Plenty of Room at the Bottom " he inspired and foreshadowed the emergence of nanoengineering. He suggested that finely focused electron, and ion beams would aid our eyes and hands to precisely engineer structures at the atomic level. Currently, electron beam lithography systems and gallium focused ion beams are ubiquitous in nanotechnology and can routinely be used to create structures of the order of tens of nanometers. However, the ability to scale to the sub-10 nm has been a technological challenge until the development of gas field ion sources (GFIS) over the past decade. The GFIS source, utilizes a single crystal tungsten wire sharpened to just 3 atoms. Helium gas is field ionized by one of these atoms, creating a helium ion beam with diameter of only 0.25nm! This instrument is emerging as an important tool for sub-10nm structuring of superconducting materials. Helium ion beams have significant advantages. Helium is small and chemically inert which allows it to be used for direct modification of materials properties without etching away material or employing resists.
My research group has been utilizing GFIS for direct patterning of ceramic high-temperature superconducting materials for quantum electronics. The helium ion beam induces nanoscale disorder from irradiation into the crystalline structure which converts the electrical properties of the material from superconductor to insulator. Insulating feature sizes of less than 2nm have been successfully demonstrated and many unique novel devices have been realized. Much of this success is due to the irradiation sensitivity of electrical transport in high temperature superconductors. This sensitivity results from loosely bound oxygen atoms (~1-8ev) in the crystal lattice that are easily displaced into interstitial or anti-site defects. I will describe details of the GFIS materials modification process and highlight applications in nanoelectronics.

491

Quantum Sensors for the Hidden Sector (QSHS)

Dr Paul J Smith

MC28: Condensed-matter Quantum Technology on the Hunt for Dark Matter II, August 22, 2022, 2:00 PM - 3:30 PM

Great progress has been made in device physics towards new classes of detectors and coherent quantum amplifiers that can detect individual quanta, and in particular individual photons or other more exotic electrodynamic states. Such detectors in the right instrument may be able to reveal new unexplored structures close to the ground state, the vacuum, of physics. Such phenomena may turn out to be the solution of the dark matter problem, and even provide information about the very early phase of evolution of the Universe. Probing these hidden sector phenomena is the aim of the QSHS (Quantum Sensors for the Hidden Sector) collaboration, a UK based collaboration funded by STFC. We will describe the proposed QSHS facility and give an outline of its major physics goals.

514

Floquet-Andreev resonances in a voltage-biased Andreev molecule

Andriani Keliri, Benoît Douçot

MC21: Bound States in Hybrid Superconductor Nanostructures III, August 22, 2022, 4:30 PM - 6:00 PM

We study the three terminal S-QD-S-QD-S Josephson junction biased with commensurate voltages. In the absence of an applied voltage bias, the Andreev bound states on each quantum dot hybridize forming an artificial molecule, termed the 'Andreev molecule'. However, understanding of this system in a non-equilibrium setup is lacking.

Applying a dc voltage on the bijunction makes the system time-periodic, and the equilibrium Andreev bound states evolve into a ladder of resonances with a finite lifetime due to multiple Andreev reflections (MAR). Starting from the time-periodic Bogoliubov-de Gennes equations we use Floquet theory to obtain an infinite tight-binding chain. We calculate the spectrum of the Andreev resonances which could be experimentally probed by performing local tunneling spectroscopy on one of the dots. A second observable we consider is the subgap current, which is known to exhibit steps at odd subdivisions of the superconducting gap. We show how the Floquet resonances leave a trace in the current, determining the position of the MAR steps. Proximity of the two dots changes drastically the subgap structure compared to the single S-QD-S case.

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Emergent Hyper-Magic Manifold in Twisted Kitaev Bilayers

Samuel Haskell, Alessandro Principi

MC14: Beyond Charge Transport in Nanostructures and 2D Materials via Geometric Design VIII, August 24, 2022, 4:30 PM - 6:00 PM

Kitaev quantum spin liquids have been the focus of intense research effort thanks to the discovery of various materials (e.g., RuCl3) that approximate their intriguing physics. In this paper we construct a mean-field approximation for a moire superlattice emerging in twisted Kitaev bilayers in terms of solutions of commensurate bilayers. We show that the band structure of deconfined spinons, defined on the mini-Brillouin zone of the superlattice, is greatly modified. The system exhibits a hyper-magic manifold: a series of nearly perfectly-flat bands appear at energies above the lowest gap. When accounting for intralayer modulation, such bands become isolated from other dispersive ones. Intriguingly, flat-band eigenstates exhibit a localization akin to wavefunctions of Kagome lattices

494

Anderson Localization in the Fractional Quantum Hall Effect

Songyang Pu, G J Sreejith, J K Jain

MC42: Broken Ergodicity and Localisation in Quantum Many-body Systems VII, August 24, 2022, 2:00 PM - 3:30 PM

The interplay between interaction and disorder-induced localization is of fundamental interest. This article addresses localization physics in the fractional quantum Hall state, where both interaction and disorder have nonperturbative consequences. We provide compelling theoretical evidence that the localization of a single quasiparticle of the fractional quantum Hall state at filling factor $\nu=n/(2n+1)$ has a striking {\it quantitative} correspondence to the localization of a single electron in the $(n+1)$th Landau level. By analogy to the dramatic experimental manifestations of Anderson localization in integer quantum Hall effect, this leads to predictions in the fractional quantum Hall regime regarding the existence of extended states at a critical energy, and the nature of the divergence of the localization length as this energy is approached. Within a mean field approximation these results can be extended to situations where a finite density of quasiparticles is present.

523

Scattering of a diffracted electron wave from nanoscale potential barriers on graphene

Dylan Jones, Adelina Ilie, Marcin Mucha-Kruczynski

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Following its discovery, it was found that graphene's electrons exhibit the Klein tunneling effect. This prompted research into the tunneling/scattering of graphene electrons from electrostatic potentials of various geometries and the associated potential applications. This included the use of on-sheet scattering from nanoscale circular potential barriers, or, circular quantum dots (CQDs) in graphene-based circuitry applications [1, 2]. The main results of these theoretical works were the predictions of anisotropic electron flow in the far-field scattered probability current density from the CQD due to scattering of a plane wave. However, these predicted scattering effects would not be measurable in a realistic device setting since a plane wave corresponds to current injection from a large electrode whose lateral size is much greater than the CQD; local perturbations to the total current density would be dominated by the incident current field.

Within the framework of the low-energy, single-valley continuum approach we model the scattering of a diffracted electron plane wave from a CQD on the surface of graphene. The diffracted wave is modelled by solving the spinor Helmholtz equation [3] through calculation of the derived graphene Green's matrices. Then, the scattering problem at the CQD boundary is solved through partial wave analysis as in [1, 2]. Calculation of the resulting total probability current densities show that tunable anisotropic scattering in the far-field can be achieved following the scattering of a diffracted graphene electron wave, unlike the case of simple plane wave scattering.

Our findings open the door for the design and realisation of a multi-terminal device based on the anisotropic distribution of current scattered from a CQD on graphene. In such a device, the Fermi wavelength, and hence the scattering behaviour of the CQD, could be controlled by the switching of a gate voltage. This work also permits the detailed device behaviour, i.e., conductances through the multiple terminals, to be modelled using tight-binding simulations.

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[2] Schulz, C., Heinisch, R.L. and Fehske H., 2014. Electron flow in circular graphene quantum dots. arXiv preprint arXiv:1412.2539
[3] Hillion, P., 1978. The spinor Helmholtz equation. Journal of Mathematical Physics, 19(1), pp.264-269

497

Organic molecules meet transition metal dichalcogenides for solar energy conversion

Dr Juliana Morbec

MC52: Heterostructures, Combining Organic Molecules and 2D Materials IV, August 23, 2022, 11:30 AM - 12:30 PM

Combining two-dimensional (2D) materials with organic materials can be very attractive for applications that require flexibility and where size and weight are important parameters to be considered, such as in wearable, portable and mobile applications. Organic materials usually exhibit excellent optical absorption efficiency and photo- and temperature-induced conformational changes, while 2D materials often show relatively high carrier mobility, superior mechanical flexibility, and tunable electronic and optical properties. Combining both systems can stabilize the organic materials and lead to heterostructures with both high carrier mobility and high optical absorption efficiency, which is promising for solar energy conversion. In this work we investigate, by means of density-functional-theory calculations, heterostructures composed of organic molecules (for example, pentacene and azulene) and transition metal dichalcogenides (TMD) for application in photovoltaic devices. We examine the interaction between the molecules and monolayer TMDs as well as the band alignment of the heterostructures, considering effects of the molecular coverage and dielectric screening.

Acknowledgements: This work has been partially funded by the German Research Foundation (Deutsche Forschungsgemeinschaft, DFG) – 406901005. This work used the Cirrus UK National Tier-2 HPC Service at EPCC funded by the University of Edinburgh and EPSRC (EP/P020267/1).

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Microkelvin electronics on a pulse-tube cryostat with a gate Coulomb blockade thermometer

Dr. Christian Philipp Scheller, Dr. Mohammad Samani, Dr. Nikolai Yurttagül, Dr. Kestutis Grigoras, Dr. David Gunnarsson, Omid Sharifi Sedeh, Dr. Alexander T. Jones, Dr. Jonathan R. Prance, Prof. Richard P. Haley, Prof. Mika Prunnila, Prof. Dominik M. Zumbühl

MC24: Quantum Electronics at Ultra-low Temperatures XII, August 26, 2022, 9:00 AM - 10:00 AM

Cryogen-free dilution refrigerators are the future of low temperature experiments. They offer plenty of experimental space in addition to independence of liquid helium. Those benefits, however, come at the cost of mechanical vibrations induced by the pulse tube which, if not addressed properly, render microkelvin experiments impossible.
In this work we develop a low heat-release microkelvin sample enclosure equipped with rigid sample wiring to effectively suppress the effect of pulse tube vibrations. In addition, a new type of Coulomb blockade thermometer (CBT) is introduced – the gate CBT – where the island capacitance to ground dominates over the junction capacitance thus effectively rendering individual islands independent. This leads to more narrow conductance distribution as a function of offset charge configurations and allows us to significantly extend the validity range of the thermometer down to about 20% of the charging energy.
With those improvements we demonstrate on-chip electron temperatures down to 224 µK with a hold-time exceeding 1 day below 300 µK. Despite the CBT array structure, the low temperature results are currently limited by voltage noise rather than actual sample cooling. Finally, we give an outlook for cooling below 50 µK in a new generation of experiments.

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Force volume data processing for advanced electrical SPM experiments

Petr Klapetek, David Nečas

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Scanning Probe Microscopy methods related to conductive Atomic Force Microscopy are extremely valuable when studying various functional thin films. During last years, novel scanning regimes were introduced for nano-electrical measurements, providing data sets of higher dimensionality than images. In the regimes like PeakForceTUNA by Bruker one can quickly obtain volume dependencies of electrical current flowing through the probe-sample area at different contact forces. Such regimes also allow combining multiple channels, like mechanical and electric response. Force volume based approach has a potential to both overcome the limitations related to unknown aspects of the probe-sample contact formation and to explore unique material properties that were inaccessible to Scanning Probe Microscopes earlier. In this contribution we will present some of the tools that were recently developed for processing data of higher dimensionality coming from this type of experiments in the open source software Gwyddion. This includes discussion of different data types and their most efficient representation, description of tools for data pre-processing and tools for the quantitative analysis. Finally, we will also discuss various ways how to link the measured data to numerical tools when an analysis of measurement uncertainties is performed and when the data interpretation is not straightforward and model based approach needs to be used.

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Hybrid carbon nanotube resonators for ultrasensitive scanning probe experiments

Gernot Gruber, Christoffer Moller, Johann Osmond, Pierre Verlot, Adrian Bachtold

MC17: Nanomechanical and Electromechanical Systems XI, August 25, 2022, 4:30 PM - 6:00 PM

Nanomechanical resonators are excellent sensors for the detection of minuscule forces at the nanoscale.[1-3] Due to their small size and mass, carbon nanotubes are a class of resonators holding great potential for the force detection of individual nuclear spins. Recently, our group reported on a hybrid carbon nanotube cantilever, with an impressive force sensitivity of 767 zN/√Hz at room temperature.[4] The resonator is composed of a singly clamped nanotube grown by chemical vapour deposition. Subsequently, a platinum nanoparticle is deposited at the free end of the nanotube via an electron microscope with a gas injection system. The nanoparticle efficiently scatters light, enabling the optical detection of the thermal vibrations of the nanotube with high signal to noise ratio. We recently introduced a mass sensing method to control the amount of deposited material during growth with a mass resolution in the zeptogram range.[5] This technique relies on monitoring the resonance frequency of the resonator during the deposition process via e-beam electro-mechanical coupling. The device design can be modified such that the Pt particle is grown with an offset from the apex. This allows the device to approach a surface and to serve as a scanning probe. In addition, a second particle of a different material can be deposited at the apex to functionalize the nanotube tip.
Here, we show further advancements in the fabrication of hybrid nanotube cantilevers and their application as ultra-sensitive vectorial scanning probes. We present opto-mechanically acquired 2D maps of nano-patterned Au wires and investigate effects on the mechanical resonance due to interactions of the cantilever tip with the Au surface. Furthermore, we give a perspective on our recent progress towards magnetic resonance force microscopy[3] employing nanotube cantilevers.

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[5] G. Gruber, et al., Nano Lett. 19, 6987 (2019).

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Coulomb blockade thermometry: a master equation, and Monte Carlo approach

Omid Sharifi Sedeh, Dr Christian Philipp Scheller, Prof. Dr. Dominik Zumbühl

MC24: Quantum Electronics at Ultra-low Temperatures VII, August 24, 2022, 2:00 PM - 3:30 PM

Accessing microkelvin temperatures would pave the way for the discovery of new phenomena. This is accompanied by a demand for accurate thermometry in this regime. Microkelvin electronics, however, has demonstrated temperatures, as low as 224 μK, using Coulomb blockade thermometers (CBTs). To perform the thermometry, a translation of the measured conductance into temperature takes place. This has been done using the master equation approximation, and/or Monte Carlo simulation. Here, however, we solve the master equation numerically, in steady-state, for few-junction CBTs utilizing the damped simple iteration method, and compare the results with the aforementioned approaches. Additionally, we develop a Monte Carlo simulation that allows studying the accuracy of the junction, and gate CBTs in the presence of temperature non-uniformity over the islands and source-drain reservoirs. Plus, using the generalized Monte Carlo algorithm, we investigate the possibility of employing the top-gate in the recently established gate CBTs [arXiv:2110.06293].

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Fate of Stark Many-Body Localization in a purely linear potential

Benedikt Kloss, Jad Halimeh, Achilleas Lazarides, Yevgeny Bar Lev

MC42: Broken Ergodicity and Localisation in Quantum Many-Body Systems X, August 25, 2022, 2:00 PM - 3:30 PM

Whether many-body localization (MBL) can exist in one-dimensional systems with local interactions in the absence of quenched disorder is an open question. Recently, interacting systems in a tilted field have emerged as a candidate to exhibit MBL-like behaviour. In this talk we will provide a thorough numerical analysis of this proposition. In particular, the role of an additional discrete symmetry in the case of a purely linear field and its implications for localization are discussed.

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Simulating active agents under confinement with Dissipative Particles (hydro)Dynamics

José Martín-roca, C. Miguel Barriuso Gutierrez, Valentino Bianco, Ignacio Pagonabarraga, Chantal Valeriani

MC6: Emergent Phenomena in Driven Soft, Active and Biological Matter IV, August 23, 2022, 11:30 AM - 12:30 PM

In this ongoing work we are developing a framework to simulate active agents taking into account both hydrodynamics and thermal fluctuations. Currently we are limiting our study to colloids and polymers although the framework will be applicable to agents with a wide range of structures. To achieve this we propose an extension of the widely known simulation software LAMMPS [1] that allows the implementation of hydrodynamic self-propulsion via force redistribution among solvent particles, this extension, in combination with the Dissipative Particle Dynamics (DPD) package [2], enables these kind of simulations. Similar approaches using lattice Boltzmann (LB) methods [3] and Multi-Particle Collision dynamics (MPC) [4] have been already well studied. With DPD and MPC dynamics we can easily simulate agents with more complex shapes taking into account thermal fluctuations, both of which are harder to implement using LB methods. Our approach takes advantage of the versatility of the LAMMPS code, being MPI-parallelizable and allowing the combination of our implementation with the wide range of features LAMMPS offers. We are interested in the subsets of active matter systems known as active colloids and active polymers, which have very useful and broad applications. Their collective behaviour is rich and complex, and in many cases cannot be ascribed solely to the agents motion: hydrodynamic interactions need to be taken into account . This is the case, for example, of many self-propelled microorganisms, or microswimmers, whose movement is an essential aspect of life. A successful model for this systems is the so-called squirmer, in their simplest form these are hard spheres that take into account the propulsion induced by the beating cilia and flagella as a prescribed steady velocity of the solvent particles tangential to the surface of the sphere. This model serves as inspiration for our project.

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516

Confinement of sulfur in porous carbon matrices

Dr. Vanessa Coulet, Loic Gourmellen, Dr. Renaud Denoyel

MC7: Exploring Liquid Properties in Confined Geometry (up to mesoscopic scales) IX, August 25, 2022, 11:30 AM - 12:30 PM

Sulfur is the most puzzling element in the chalcogen family, in the liquid as well in the solid state. It is the element of the periodic table with the highest number of allotropes in the solid state [1]. At the melting point (Tm= 115°C), the liquid is essentially composed of S8 rings and has a low viscosity. Around 159°C, a reversible polymerization transition is observed and the chain formation leads to an increase in the viscosity of almost four orders of magnitude. At 445°C, the sulfur sublimes into vapor consisting of Sn molecules (n = 2 - 10) in proportions depending on temperature and pressure.

A few works on the confinement of sulfur in porous matrices were published in the late nineties. At that time, the aim was to identify, essentially by spectroscopic methods, the allotropes (rings or chains) that can be stabilized in the pores [2]. Within the last decade, sulfur confinement has attracted much attention since it is considered as a promising component of electrode material for the next generation of Li-ion batteries [3]. For such application, sulfur is confined into porous carbon materials: the carbon ensures the conductivity and the pores are supposed to retain the polysulfides that are formed during the electrochemical cycles [4]. Various hosts are considered such as mesoporous carbon, microporous carbon or carbon nanotubes. However, one can regret that the confinement itself of sulfur is never at the center of the published works. Our studies aim to open a path to the rationale of the impregnation of porous carbon by sulfur. Our objectives are to understand the interaction between liquid sulfur and porous carbon and the influence of confinement on sulfur thermodynamic properties

In this contribution, immersion calorimetry studies will be first presented. To the best of our knowledge, it is the first time that this method is used at high temperature and with liquid sulfur. It allows the evaluation of the energy of interaction of liquid sulfur with the porous material and to follow the kinetics of wetting. It will be demonstrated that, below the polymerization transition, the kinetics of wetting is rather fast and that S8 rings are able to enter the micropores. The second part concerns the physicochemical characterization of various carbon-sulfur composites synthetized at different impregnation temperatures in the liquid (before and after polymerization) and in the vapor states. It will be shown that the sulfur loading in the porous carbon hosts is related to the impregnation temperature and that the sulfur stability is linked to the pore network.

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Heating effects in hybrid superconductor-semiconductor nanowire deivces

Eduardo Lee, Angel Ibabe, Mario Gomez, Gorm Steffensen, Jesper Nygard, Alfredo Levy Yeyati

MC21: Bound States in Hybrid Superconductor Nanostructures VI, August 23, 2022, 4:30 PM - 6:00 PM

Hybrid superconductor-semiconductor nanowires have been widely studied in the past decade, largely motivated by prospects of applications in quantum technologies both in the trivial and in the topological regimes. A key element for the above developments relies on the quality of materials and in their reproducible properties. Despite the impressive improvements related to nanowire growth in the past years, it can be arguably said that there still exists a great deal of variability in the behavior of fabricated devices. As such, there is a need for techniques and protocols that allow for a thorough characterization of hybrid devices. Here, we show that Joule heating effects can be used as a characterization tool, providing rich information regarding the properties of hybrid superconductor-semiconductor devices that is complementary to that obtained by transport measurements. We have studied devices with a Josephson junction geometry, as well as mesoscopic superconducting islands. We show that heating effects can drive a superconductor-to-normal metal transition of the epitaxial shell, which can be used to obtain information regarding heat dissipation, as well as of the superconductivity in different parts of our devices.

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Non-equilibrium generation of spin-wave solitons in magnetic nanostructures

Hermann Durr

MC47: X-ray Free Electron Lasers for Condensed Matter & Materials Physics (XFELs for CMMP) II, August 22, 2022, 2:00 PM - 4:00 PM

Spin waves are the fundamental excitations in magnetic systems. At low densities, they behave as independent quasiparticles that can be used to transport information in technology. At sufficiently high densities, spin waves can condense into solitons that derive their stability from non-linear spin precession. Generation of spin-wave solitons requires a conservative environment, where dissipation is matched by excitation, realized within spin-torque nano-contacts. Here we show that non-equilibrium conditions via demagnetization with a femtosecond laser pulse provides an alternative generation mechanism for spin-wave solitons. Tailoring materials properties such as the magneto-crystalline anisotropy enables the generation of spin textures close to their fundamental limit given by the magnetic exchange length.

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Tuneable Correlated Disorder and Disorder-Phonon Coupling in the Pseudo-bcc Uranium Molybdenum System γ-(U1-xMox)

Dr Daniel Chaney, Dr Aloïs Castellano, Dr Alexeï Bosak, Dr Johann Bouchet, Dr François Bottin, Dr Boris Dorado, Dr Luigi Paolasini, Dr Sophie Rennie, Dr Christopher Bell, Dr Ross Springell, Prof Gerard Lander

MC38: Controlled Irradiation Disorder in Model Systems: Organisation, Dynamics, and Transformations XI, August 25, 2022, 4:30 PM - 6:00 PM

Understanding the role of disorder, and the correlations that exist within it, is one of the defining challenges in contemporary materials science. However, there are few material systems, devoid of other complex interactions, that can be used to systematically study the effects of correlated disorder arising from crystallographic conflict. The pseudo-bcc uranium molybdenum system is however an exemplar case study and as such we fabricated thin (~300 nm) epitaxial films of γ-(U1-xMox) alloys in the range $0.16 < x < 0.31$ to be studied that the ID28 beamline (ESRF, France).

We established, via extensive diffuse x-ray scattering studies [1], that the intrinsic symmetry conflict; where uranium, which prefers a locally anisotropic environment, is forced into an isotropic bcc global symmetry, produces a new form of correlated disorder where every atom is displaced to form a short-range superstructure with correlations existing over nanometre sized regions. Furthermore, we show that the strength of this unusual form of disorder displays both intrinsic and extrinsic tuneability, via alloy composition and heavy ion irradiation, respectively.

Given the correlated disorder serves to modulate the local crystallographic periodicity, this gives rise to the possibility of a form of disorder-phonon coupling. To investigate this possibility one alloy composition was measured with grazing incidence inelastic x-ray scattering (GI-IXS) and compared with extensive ab-initio modelling [2]. The resulting dispersions are shown in figure 1. We discovered strong disorder-phonon coupling that relaxes degeneracy conditions at the P position, hardens the LA-2/3<111>p mode ubiquitous to monotonic bcc crystals and produces significant phonon linewidth broadening at almost all positions in the 1st Brillion zone [1]. This broadening is almost entirely due to the presence of correlations, and results in a strong reduction of the phononic contribution to thermal conductivity.

Within its conventional role as an advanced nuclear fuel, a proper understanding of the local structure of γ-(U1-xMox) alloys and its behaviour under irradiation is of great interest for accurate modelling efforts, especially those concerning diffusion related properties, and may also shed light on other currently unexplained phenomena such as the apparently contradictory fcc nanobubble lattice that forms from fission gasses. However, more broadly, as similar effects are expected in any system able to host comparable levels of crystallographic conflict we believe this novel form of correlated disorder constitutes a compelling tool for designing disorder into future functional materials.

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Ultrafast manipulation of spin and carrier by a femtosecond pulsed laser in low-dimensional magnetic films

Professor Yongbing Xu, Dr. Bo Liu, Professor Jing Wu, Dr. Xuezhong Ruan, Professor Liang He, Dr. Jian Tu

MC51: Ultrafast Dynamics in Magnetic and Strongly-Correlated Materials XI, August 25, 2022, 4:30 PM - 6:00 PM

In ferromagnetic materials, it has been well demonstrated that, in a strong non-equilibrium state excited by a femtosecond (fs) laser pulse, magnetization can be quenched on a sub-picosecond timescale [1]. It opens up an important research field of femtosecond magnetism, which aims to manipulate spins via light-matter interactions and promote next-generation ultrafast data-storage technologies. In this talk, we will report our recent studies of the spin and carrier dynamics of a few low-dimensional magnetic systems excited by a femtosecond pulsed laser. In a colossal magnetoresistive (CMR) La0.7Sr0.3MnO3 film, we have found that the demagnetization amplitude maps the fourfold symmetry of dx2 − y2 electrons orbits by rotating the sample orientation and the polarization of the probe light [2]. As the LSMO film has strong anisotropic spin-orbit coupling (SOC), the ultrafast demagnetization depends on both the material's orbital orientation and the polarization of the probe light, showing that ultrafast manipulation of magnetism can be achieved by utilizing anisotropic SOC. Topological insulators (TIs) with unique band structures and strong SOC have wide application prospects in the fields of ultrafast optical and spintronic devices. In a prototype magnetic TI system, Cr-doped Bi2Se3, we have found that the concentration of the Cr doping plays a key rule to the bulk and surface spin ordering [3]. Using the time- and angle-resolved photoemission spectroscopy technique, we have studied the relaxation process of the hot carriers in Cr-doped Bi2Se3 under fs laser excitation and found that electronic temperature and chemical potential decrease fast with the increase in the Cr doping concentration [4]. These suggest a mechanism of impurity band-assisted carrier relaxation, where the impurity band within the bulk bandgap introduced by Cr doping provides significant recombination channels for the excited electrons. The recent discovery of intrinsic ferromagnetism in two-dimensional (2D) van der Waals (vdW) crystals has opened up a new arena for spintronics. In a few-layered van der Waals (vdW) 2D magnet Fe3GeTe2, we found that both magnetization and magnetic anisotropy energy (MAE) can be strongly modulated by a femtosecond laser pulse [5]. The light modulation of the magnetization was also observed at room temperature, showing the emergence of light-driven room-temperature (300 K) ferromagnetism in few-layered Fe3GeTe2 whose intrinsic Curie temperature is around 200 K. The light-tunable ferromagnetism is attributed to changes in the electronic structure of Fe3GeTe2 by optical doping. As manifested by the enhancement of both total magnetization and the Curie temperature, we propose that after strong fs laser excitations, the Fermi level moves to a position of much larger electron density of states and the exchange interaction increases. Further spin and carrier dynamic measurements will be discussed.

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Molecular Dynamics Studies of the Conformational Free Energies of Xylan Glycosidic Linkages and the Flexibility of Xylan Chains

Mr Peter Starrs

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Polysaccharide hydrogels, such as those formed by the arabinoxylans (AX) from the seed husk of Plantago ovata, have useful applications in several areas including food structuring (as a healthy replacement for fats and/or gluten) and in drug delivery. These particular AX are of interest due to their unique structure and mechanism of gel formation. They consist of a β-1,4-linked xylose backbone which is densely substituted (on almost every backbone unit) by side chains containing 1 – 3 units of α-arabinose and/or β-xylose. Experiments have indicated that gel formation in water occurs due to hydrogen bonding between AX chains, as opposed to chemical cross-linking typical of AX from other species (e.g., wheats). Furthermore, gels obtained from different extractable AX fractions have very different physical properties, but almost indistinguishable monosaccharide and linkage compositions. This implies that gel properties are sensitive to the specific structure and decoration pattern of the side chains. Understanding this structure-property relationship could allow for the rational design or modification of AX gels (via targeted enzymatic cleavage) towards specific applications.

To approach the atomistic details of AX interactions, we turn to molecular dynamics (MD) simulations on explicitly solvated model systems. To begin with, we have limited our focus to observing how different backbone substitutions affect the conformational freedom of the backbone linkages and therefore the flexibility of the chains. From these simulations we produce plots of the free energy vs the glycosidic dihedral angles Φ and Ψ (i.e., Ramachandran plots). We also obtain the apparent persistence lengths for oligomer systems by using the Kratky-Porod polymer model to fit chain correlation data. Example results for the simple case of xylobiose and for a 14-unit xylan oligomer are given in figure 1. So far, we have noted significant disparity in results between different carbohydrate forcefields, namely GLYCAM06 and CHARMM36. Generally, CHARMM36 produces narrower minima in the glycosidic conformation maps and correspondingly longer persistence lengths (stiffer chains). Both forcefields appear to overestimate persistence lengths relative to experiment (2-3 nm for wheat AX, while our results span from 4-8 nm across substitution patterns tested). However, the different assumptions made in experimental and computational determination of this observable allows for some wiggle room.

To help resolve the dilemma of which forcefield(s) to trust, we are currently working to generate comparisons with continuum solvation (SMD) hybrid Density Functional Theory (DFT) (ωB97X-D3 /def2-TZVP). Building on work by French and co-workers, we have produced an adiabatic Φ/Ψ energy map for xylobiose by performing constrained optimisation at 20°-spaced Φ/Ψ points. Lacking any entropy contributions, this is not directly comparable to the above mentioned free energy maps from forcefield MD. However, we can produce adiabatic maps at the forcefield level by running a series of constrained MD simulations at the same Φ/Ψ points used for DFT. If we assume that the SMD solvation method is accurate (which it has been shown to be for neutral molecules), we may observe which forcefield reproduces the solvated potential energy surface more accurately.

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Sub-gap states in hybrid superconductor-semiconductor single and double nanowire devices

Associate Professor Kasper Grove-Rasmussen

MC21: Bound States in Hybrid Superconductor Nanostructures II, August 22, 2022, 2:00 PM - 3:30 PM

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Co-Authors: A. Vekris[1], J. C. Estrada Saldaña[1], T. Kanne[1], L. Pavešić[2], R. Žitko[2], M. M. Wauters[1], M. Burrello[1], J. Nygård[1] and co-authors in Refs. 1-6.
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We present recent activities on hybrid superconductor-semiconductor double and single nanowire devices, which are of particular interest for studying phenomena related to Yu-Shiba-Rusinov (YSR), Andreev and Majorana sub-gap states. The double nanowire material system consists of two closely grown InAs nanowires covered by an in-situ metalized half/full epitaxially-matched Al shell [1]. We show three types of hybrid double nanowire devices, Little-Parks devices [2], parallel double quantum dot Josephson junctions [3] and superconducting islands [4] with focus on measurements of the two latter devices. Furthermore, we present measurements on a quantum dot (QD)-superconducting island (SI) system defined in single aluminum-InAs nanowires, realizing a spin coupled to a superconductor with tunable charging energy [5]. The YSR sub-gap states can be tuned to the Coulombic limit as the charging energy of the superconducting island is increased. The measurements also reveal the tunable nature of the nanowire SI-QD and even SI-QD-SI system, which is promising for making entangled chains of the QD-SI unit [6].

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DC and microwave transport properties of topological insulator nanoribbon-superconductor hybrid junctions

Thilo Bauch, Ananthu Surendran, Núria Alcalde Herraiz, Gunta Kunakova, Jana Andzane, Donats Erts, Floriana Lombardi

MC21: Bound States in Hybrid Superconductor Nanostructures IX, August 25, 2022, 11:30 AM - 12:30 PM

The study of hybrid material systems with a conventional superconductor in proximity to a strong spin-orbit semiconductor or a Topological Insulator (TI) has lately received a dramatic boost. The potential of such hybrid systems to host exotic phenomena such as Majorana bound states makes them interesting for topological quantum computation architectures [1-2]. In a multimode hybrid TI Josephson junction with two terminal geometry, Majorana physics manifests as peculiar properties of a part of the Andreev bound states carrying the Josephson current. They give rise to an unconventional 4π periodic current phase relation (CPR) coexisting with a 2π periodic CPR resulting from the conventional Andreev bound states. We make use of Al-Bi2Se3-Al junctions fabricated using TI nano ribbons grown by physical vapour deposition. [3-5] To extract the current phase relation (CPR) of our TI-junction, we implemented an asymmetric dc-Superconducting Quantum Interference Device (SQUID) measurement technique. We observe clear deviations from a standard sinusoidal CPR in all our devices pointing towards the presence of highly transparent modes in our TI junctions. To obtain more information about the bound state spectrum we have implemented a microwave rf-SQUID probing scheme for our Al-Bi2Se3-Al hybrid junctions. Here, we embedded a TI Josephson junction-based rf-SQUID in a superconducting coplanar wave-guide resonator. The frequency response of the coupled resonator/junction system to an externally applied magnetic field (phase bias) at various temperatures is used to deduce information about the phase dependence of the bound state spectrum of the junction. We find that the bound state spectrum in our TI Josephson junctions is dominated by highly transparent modes.

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Spintronics with low symmetry materials

Prof. Luis Hueso

Semi-plenary: Professor Luis Hueso, August 23, 2022, 10:00 AM - 11:00 AM

The integration of logic and memory in spin-based devices, as in the recent MESO proposal by Intel [1], could represent a post-CMOS paradigm. A key player in this proposal is the spin Hall effect, which permits to electrically create or detect pure spin currents without using ferromagnetic materials (FM). Understanding the different mechanisms giving rise to SHE allows one to optimize spin-to-charge conversion in heavy metals [2]. Using these mechanisms, we developed a novel and simple nanodevice to readout the magnetic state of the FM electrode using spin Hall effect [3]. The spin-orbit based detection allows us to independently enhance both the output voltage (needed for reading) and the output current (needed for cascading circuit elements) while downscaling the device dimensions, which are necessary conditions for implementing the MESO logic [1]. However, limitations in metallic materials makes the search for other alternatives peremptory.
In the second part of my presentation, I will present a radically different approach to further enhance spin-charge conversion. By using low-symmetry materials, we have been able to both improve the output signals in our devices as well as to create new spin-to-charge conversion effects forbidden in common isotropic materials.
Engineering van der Waals heterostructures which combine graphene with a transition metal dichalcogenides with low crystal symmetry such as MoTe2, SHE is created in novel crystallographic directions [4]. The combination of long-distance spin transport and SHE in the same heterostructure gives rise to an unprecedented spin-charge conversion efficiency, making graphene-based systems excellent candidates for MESO logic [1,3].
Finally, in the last section I will show how a chiral crystal of Tellurium delivers a charge to spin conversion in the direction of the chiral axis by means of the Edelstein effect [5]. Chiral materials are the ultimate broken symmetry systems and open the way to a new way of delivering spintronic and chiralitronic devices.

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Aluminum plasmonics in Casimir-Lifshitz forces and Near-field radiative heat transfer.

Prof Raul Esquivel-sirvent

MC19: Advances in the Casimir Force and Heat Transfer Phenomena VI, August 23, 2022, 4:30 PM - 6:00 PM

We present a theoretical calculation of the near-field radiative heat transfer (NFRHT) and the Casimir-Lifshitz force between Al surfaces. In particular, we are interested in the effect of the oxide layers of AlO2 that forms on the surfaces.
The system consists of two slabs each of an Al layer deposited on a Si substrate. As the Al layer oxidizes the dielectric function changes going from an isotropic function to an anisotropic one giving rise to hyperbolic modes. As the oxidation continues, the oxide layer reaches a percolation point where the Al plasmon response degrades, and the surface phonon modes of Al2O3 become active, thus increasing the spectral radiative heat flux and decreasing the Casimir-Lifshitz force. This occurs when the content of aluminum oxide on the surface approaches 67\% in volume, which corresponds to the percolation threshold according to the Bruggeman effective medium theory.

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Tracking Ultrafast Bound Exciton Formation in Organic Optoelectronic Devices

Marios Maimaris, Allan J. Pettipher, Mohammed Azzouzi, Daniel J. Walke, Xijia Zheng, Andrei Gorodetsky, Yifan Dong, Pabitra Shakya Tuladhar, Helder Crespo, Jenny Nelson, John W. G. Tisch, Artem A. Bakulin

Optoelectronic properties and applications of organic semiconductors are defined by the formation and dynamics of excitons which are electron-hole pairs bound electrostatically, with the energy difference to separated charges known as exciton binding energy. The fundamental mechanisms underlying the exciton binding are complex and its ultrafast sub-200fs timescales impose stringent time-resolution requirements on the experimental technique. Previously, ultrafast optical pump-probe (PP) spectroscopy, two-photon photoemission, photoluminescence, and anisotropy has proved to be a useful tool to capture exciton dynamics, showing a rapid (within 100-fs time resolution) creation of excitons with an ultrafast (<200fs) exciton localisation and charge separation. Although these methods track well the population dynamics of states with specific energies, they do not provide direct access to the binding energy of excitonic states and may not distinguish excitons from other excited species. This lack of bound states sensitivity can be overcome using pump-push-photocurrent (PPPC) techniques. In PPPC, after the initial excitation of the system by the pump, a second pulse, that is the push-pulse, re-excites the bound excited states promoting their dissociation and the push-induced photocurrent originated from the re-excited bound excited states is measured.

Here, we apply a combination of pump-probe (PP) and pump-push-photocurrent (PPPC) spectroscopies with sub-10-fs time resolution to separate and track in time the ultrafast formation of bound excitons in a ‘classical’ conjugated polymer, polyfluorene poly(9,9-dioctylfluorene) (PFO), device. We found that excitons created by near-absorption-edge excitation are intrinsically bound states, or are becoming such within 10 fs after excitation. At the same time, hot excitons with >0.3 eV excess energy do have a chance for spontaneous dissociation and acquire fully bound character only at a 50-fs timescale. Excitation fluence dependent measurements show that the exciton binding does not depend on the density of excited states and that exciton-exciton annihilation contributes to charge dissociation by giving excess energy to the bound exciton. Furthermore, we develop a simple global kinetic model which reproduces PP and PPPC experiments with a compact set of shared parameters, supporting the above conclusions. Finally, we use the non-adiabatic excited state molecular dynamics package (NEXMD) to simulate singlet exciton evolution in an oligomeric model of this polymer. Our simulation confirms that binding energy of the near-band-edge S1 excitons does not evolve significantly beyond the ~20-fs timescale and that these near-band-edge states can be populated through hot exciton states cooling with characteristic time of 50 fs.

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Orientational transitions of discotic columnar liquid crystals in cylindrical pores

Dr Ruibin Zhang

MC13: Topological and Geometrical Effects in Complex Nanostructures II, August 22, 2022, 2:00 PM - 4:00 PM

In cylindrical confinement the columns of discotic liquid crystals can orient either perpendicular or parallel to the long axis of the pore, depending on surface anchoring type, pores size and columns rigidity. However it is not well understood how the hexagonal lattice copes with the curvature inside the confinement. Using X-ray diffraction, we find here that for narrow cylindrical pores the orientation, termed here (100)$\parallel$, is preferred with the columns lying perpendicular to the pore axis z and one of the densely packed {100} planes aligning parallel to z. As the pore diameter increases, a transition occurs from the {100}$\parallel$ to the (100)$\perp$ orientation, in which the hexagonal lattice rotates by 90° so that one of its {100} planes becomes perpendicular to z. Four triphenylene derivatives were used: hexa(hexyloxy)triphenylene (HATO6), HAT07, hexa(hexylthio)triphenylene (HATS6) and a newly synthesised HATO6F8, which is like HATO6 but with a perfluorooctyl segment attached at the end of each alkyl chain. In 60 nm pores the hexagonal lattice of SATO7 shows random orientation and HATO6 shows poor (100)$\parallel$orientation. For HATS6, the replacement of oxygen linkage by sulphur stabilizes the (100)$\parallel$ orientation. The addition of tetranitrofluorenone (TNF) acceptor to HATO6 was also found to stabilize the (100)$\parallel$orientation. The extension of the side chains in HATO6F8 moves the {100}$\parallel$ - (100)$\perp$ transition to larger pores. The results are discussed in the context of previous findings on related materials in a wider pore size range to give a comprehensive picture of confined columnar liquid crystals whose applications critically depends on our ability to align them.

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The Effect of Lithium Concentration on the Radiation Damage in UK Nuclear Waste Glasses

Miss Aine Black, Dr Maulik Patel, Professor Frédéric Blanc, Dr Mike Harrison, Dr Laura Leay

MC38: Controlled Irradiation Disorder in Model Systems: Organisation, Dynamics, and Transformations XI, August 25, 2022, 4:30 PM - 6:00 PM

The glass compositions used in the UK to immobilise the highly radioactive waste arising from the reprocessing of used nuclear fuel are termed 'Calcium Zinc' (CaZn) and 'Mixture Windscale' (MW). In this work, CaZn and MW base glasses are studied with their full and half lithium content to evaluate the impact lithium concentration has on radiation damage in the glass network. Previous studies by others have been carried out to determine the role of lithium in the glass network and the impact lithium has on the aqueous durability of the glass [1][2]. With this knowledge, our work discusses the impact of lithium concentration on the degree of radiation damage caused by gamma rays and its role within the glass network relating to the order/disorder of the connectivity of the glass. This information is fundamental for the long-term evolution of high-level nuclear waste immobilisation in the UK. Gamma irradiations were carried out for all four glass compositions at the Dalton Cumbrian Facility to simulate the effect of gamma radiation on the pristine glass network. Glasses were irradiated with 0.5 MGy and 5 MGy doses at a dose rate of 85 Gy/min. We postulate that since lithium is a network modifier, gamma irradiation-induced changes are more likely to occur in glasses with higher lithium concentration. The relationship between lithium concentration, the disorder of the glass network and the change in connectivity of the glass can be probed by Nuclear Magnetic Resonance (NMR), Raman spectroscopy and thermal analysis. Multidimensional multinuclear Magic Angle Spinning (MAS) NMR and Raman spectroscopies investigations of the glass network were carried out to identify structural changes between pristine and irradiated glasses. Additionally, changes in the local atomic scale structures were correlated with thermal behaviours as obtained from glass transition temperature (Tg) measurements.

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Geometry optimization of quantum devices: spin qubits and topological superconductors

Anton Akhmerov

MC41: Real Space Simulations of Topological Matter and Disordered Materials I, August 22, 2022, 11:30 AM - 12:30 PM

Mesoscopic quantum devices, both topological and conventional, are predominantly made by trial and error. While simulations seem like a useful tool in saving time and optimizing the device performance, the unavoidable disorder and parameter variation limits the usefulness of simulations because it is impossible to build a device as specified.

I will demonstrate how to make device performance simulations useful by using spin qubits and Majorana Josephson junctions as examples. I will demonstrate that despite the large device to device variation in parameters, a simulation may predict performance of a quantum dot device. Further, I will demonstrate how to use a physics-inspired analog of a stochastic gradient descent to optimize the topological gap in a Majorana Josephson junction.

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Study of Experimental Regimes for the Observation of Quantum Many-Body Mixed phase space

Mr Aiden Daniel, Mr Jean-Yves Desaules, Dr Ana Hudomal, Dr Zlatko Papic

MC42: Broken Ergodicity and Localisation in Quantum Many-body Systems VIII, August 24, 2022, 4:30 PM - 6:00 PM

Recently, a yearning for the origin of Quantum Many-Body Scarring, a weak ergodicity-breaking phenomenon that depends heavily on the states studied, has emerged. Through the toolset of the Time-Dependent Variational Principle (TDVP), a correspondence has been found between the presence of this phenomena and a semi-classical mixed phase space in some systems. By expressing our states as matrix product states (MPS), and through the application of TDVP on a given system where we project the system into a manifold of states, one can derive semi-classical equations of motion taken by said quantum states. In cases where the error between TDVP and exact dynamics are small, semiclassical dynamics shadow exact dynamics and states found in regular islands encompassed by a chaotic sea in phase space often display scarring behaviour in the quantum case. This opens up an exciting avenue for probing and understanding quantum many-body scarring. We seek to find a regiment which allows for the experimental observation of this mixed phase space shadow cast on a quantum system. Focusing specifically on the infamous PXP model with chemical potential and choosing TDVP bond dimension $\chi=2$, we first provide an experimentally realisable ansatz that allows one to initialise as any TDVP manifold state with good fidelity. Using the simulation of TDVP, with errors in mind, we then identify regions where the system agrees with and exhibits a semiclassical mixed phase space. More specifically, we identify states found in these ostensible "regular" and "chaotic" regions. Through simulation of exact dynamics, we show that said states indeed take trajectories predicted of the mixed phase space and we then provide experimentally realisable measurements that one could take to show the same. Said measurements include simple observable such as magnetisation of a quantum state or single-site fidelity.

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Time evolution on NISQ Hardware, a Matrix Product State Approach

Kieran Bull, Zlatko Papic, Sonika Johri

MC36: Integrating Quantum Computers in Condensed Matter Physics Simulations V, August 23, 2022, 2:00 PM - 3:45 PM

Noisy intermediate-scale quantum (NISQ) computers suffer from qubit noise, which impacts the performance of deep quantum circuits. We argue there should exist a suitably shallow unitary circuit to simulate time evolution of a many bodied quantum system, providing the system exhibits suppressed entropy growth from certain initial states. For such a scenario, dynamics projected to a manifold of low bond dimension matrix product states should be a good approximation for the full dynamics. By constructing a parametrized unitary matrix product operator which generates states in the low bond dimension manifold and mapping it to a unitary circuit, we can find a shallow depth variational ansatz for dynamics simulations on NISQ hardware. We test this claim by considering two systems, a many bodied quantum scarred model (PXP model) and a low energy quench of the longitudinal Ising model, obtaining hardware results of their time evolution on both IBM and IONQ quantum computers.

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Memory and Many-Body Localization: An Informational Approach

Alex Nico-Katz

MC42: Broken Ergodicity and Localisation in Quantum Many-body Systems IV, August 23, 2022, 11:30 AM - 12:30 PM

Local memory is a widely-touted feature of many-body localized systems in which subsystems retain information about their initial state over time. Despite its value both as a characteristic signature of localization and its potential application in quantum computation, local memory is often explored outside the information-theoretic framework. The emergence of local memory is most often inferred from entanglement growth or correlation functions, both of which fail to fully capture its nature. In this talk we propose the use of tools from the quantum information community to formalize the study of memory, and apply these tools in the context of many-body localization. We start by outlining the main ways local memory is investigated in condensed matter systems and their relative shortcomings. We then introduce an informational standard and several informational quantities which we can use to directly quantify local memory: the amount of information - in bits - a subsystem retains over time. This framework reveals several interesting features of many-body localized systems. We analyze a many-body localized spin chain, revealing that the most widely-used signature of memory erases much of the actual information that is otherwise accessible in the subsystem. Finally we analyze the many-body localization transition in small systems and reveal a simple procedure that improves scaling results; affording us a better grasp on how memory emerges in systems at criticality and a potential glimpse into the thermodynamic limit.

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Exploring the realm of the axion with quantum devices in ADMX

Dr. Chelsea Bartram

MC28: Condensed-matter Quantum Technology on the Hunt for Dark Matter II, August 22, 2022, 2:00 PM - 3:30 PM

The axion is a prime candidate for dark matter. Unique in its ability to solve both the dark matter problem and the strong CP problem, its existence would provide tantalizing clues to physics beyond the Standard Model. The Axion Dark Matter eXperiment (ADMX) searches for axion dark matter using a resonant haloscope consisting of a microwave cavity immersed in a high magnetic field. Recent sensitivities achieved by ADMX were enabled by the advent of quantum amplifiers such as microstrip SQUID amplifiers (MSAs), Josephson parametric amplifiers (JPAs), and Josephson traveling wave parametric amplifiers (JTWPAs). We present the results of recent axion searches, in addition to plans for future data-taking runs. The ADMX collaboration intends to traverse the 1--4 GHz region of the axion parameter space in the coming years. Future iterations of the experiment will power combine the signals from multiple smaller cavities to overcome scaling challenges at higher frequencies. Additionally, the collaboration is considering the potential implementation of new technology to boost the haloscope scan speed, from squeezing to superconducting films. We present progress made on these fronts.

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Matter in non-perturbative cavity QED

David Zueco

MC25: Emerging Trends in Many-Body Cavity Quantum Electrodynamics IX, August 25, 2022, 11:30 AM - 12:30 PM

In this talk, we discuss the theory of a general material system of N particles coupled to a cavity. We focus on equilibrium. We use bounds for the partition function and a a coherent-state path integral formulation. We obtain the exact (non-local) action where the photonic degrees of freedom are replaced by an effective position-dependent interaction between the particles. Besides, in the large-N limit, we show that the theory can be cast into an effective Hamiltonian where the cavity induced interactions are made explicit. We showcase the descriptive power of the formalism with various examples: photon condensation, the 2D free electron gas in a cavity, the modification of quantum magnetism and the engineering of long range interactions. We delve into the example of modifying magnetic interactions discussing our first experimental steps.

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Quantum optomechanics at room temperature: A nanomechanical endeavour?

Pierre Verlot

MC17: Nanomechanical and Electromechanical Systems X, August 25, 2022, 2:00 PM - 3:30 PM

Optomechanics is the field investigating the reciprocal interaction between electromagnetic and mechanical degrees of freedom1. Recently, impressive progress has been accomplished in the field, notably with the demonstration of multiple systems operating in the quantum regime of the optomechanical interaction2–4. This in great part relies on the extreme miniaturization of the mechanical devices, which enables drastic decrease of the thermal noise, at the benefit of quantum effects5,6.
So far however, the quantum regime of the optomechanical interaction has essentially been evidenced at liquid helium temperature or below and remains remote to ambient conditions. In this talk, I will present novel approaches raising the realistic perspective of operating optomechanical systems deep in the quantum regime and at room temperature. I will primarily focus on the fabrication and optomechanical characterization of a novel hybrid carbon nanotube-based approach7–9 which is found to reach a record low thermal force noise at room temperature, while fully preserving sensing capabilities. I will also discuss the role of non-linearities and corresponding sensing limitations for the sensitivity of those devices at ambient temperature. Last, I will introduce recent results on a novel quantum hybrid optomechanical approach, based on the use of gram-scale rare-earth ion doped crystal10,11, which appears very promising as for reaching the quantum regime at room temperature and under very robust conditions12.

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Origin of the Flat Band in Heavily Cs-Doped Graphene

Prof. Alexander Grüneis, Niels Ehlen, Gianni Profeta

MC12: Physics in 2D Nanoarchitectonics IV, August 23, 2022, 11:30 AM - 12:30 PM

A flat energy dispersion of electrons at the Fermi level of a material leads to instabilities in the electronic system and can drive phase transitions. Here we show that the flat band in graphene can be achieved by sandwiching a graphene monolayer by two cesium (Cs) layers [1]. We investigate the flat band by a combination of angle-resolved photoemission spectroscopy experiment and the calculations. Our work highlights that charge transfer, zone folding of graphene bands, and the covalent bonding between C and Cs atoms are the origin of the flat energy band formation. Analysis of the Stoner criterion for the flat band suggests the presence of a ferromagnetic instability. The presented approach is an alternative route for obtaining flat band materials to twisting bilayer graphene and yields thermodynamically stable flat band materials in large areas.

[1] ACS Nano 2020 14 (1), 1055-1069

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One becomes two: non-equilibrium assemblies that split cells across evolution

Prof Andela Saric

MC6: Emergent Phenomena in Driven Soft, Active and Biological Matter IV, August 23, 2022, 11:30 AM - 12:30 PM

The molecular machinery of life is largely created via self-organisation of individual molecules into functional larger-scaled assemblies. Such processes are multi-scale in nature and constantly driven far from thermodynamic equilibrium. Our group develops minimal coarse-grained models to investigate how driven macromolecular assemblies result in living machines, and how such processes can fail, leading to diseases.

Today I will present our research on computational modelling of active elastic filaments that dynamically reshape and cut cells. I will present the comparison of our simulation results to live cell data on reshaping processes across evolution — from cellular trafficking to cell division. I will finish with our recent efforts in computationally evolving assemblies that perform a desired function. Beyond their biological context, our models can help guide the design of artificial structures that are able to mimic life at the nanoscale.

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Tuning between continuous time crystals and many-body scars in long-range XYZ spin chains

Andrew Hallam, Zlatko Papić, Kieran Bull, Ivar Martin

MC42: Broken Ergodicity and Localisation in Quantum Many-Body Systems X, August 25, 2022, 2:00 PM - 3:30 PM

Persistent oscillatory dynamics in non-equilibrium many-body systems is a tantalizing manifestation of ergodicity breakdown that continues to attract much attention. Recent works have focused on two classes of such systems: discrete time crystals and quantum many-body scars (QMBS). While both systems host oscillatory dynamics, its origin is expected to be fundamentally different: discrete time crystal is a phase of matter which spontaneously breaks the Z2 symmetry of the external periodic drive, while QMBS span a subspace of non-thermalizing eigenstates forming an su(2) algebra representation. Here we ask a basic question: is there a physical system that allows to tune between these two dynamical phenomena? In contrast to much previous work, we investigate the possibility of a \emph{continuous} time crystal (CTC) in undriven, energy-conserving systems exhibiting prethermalization. We introduce a long-range XYZ spin model and show that it encompasses both a CTC phase as well as QMBS. We map out the dynamical phase diagram using numerical simulations based on exact diagonalization and time-dependent variational principle in the thermodynamic limit. We identify a regime where QMBS and CTC order co-exist, and we discuss experimental protocols that reveal their similarities as well as key differences.

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Bottom-up fabrication of graphene nanoribbons: from ultra-high-vacuum to device integration

Dr. Gabriela Borin Barin

MC12: Physics in 2D Nanoarchitectonics III, August 22, 2022, 4:30 PM - 6:00 PM

Graphene nanoribbons (GNRs) show exciting properties deriving from electron confinement and related band gap tunability [1]. The ability to tune GNRs' electronic and magnetic properties at the single atom level makes them an ideal platform for a wide range of device applications, from classical transistors to spintronics. In this contribution, I will address the necessary steps to bring GNRs from ultra-high vacuum (UHV) to device integration focusing on our progress on the characterization and transport measurements of armchair graphene nanoribbons. After the UHV bottom-up growth, GNRs were transferred using a polymer-free [2] and/or an electrochemical delamination method [3]. GNRs transferred onto graphene/SiC (G/SiC) substrates allowed us to image transferred GNRs, for the first time, with scanning tunneling microscopy (STM) resolution as well as observe 9-AGNRs' frontier orbitals on G/SiC.
We strongly rely on Raman spectroscopy to investigate the structural quality and the length of GNRs after substrate transfer. Our Raman study demonstrates that a length-dependent, Raman-active low-energy vibrational mode is present in all families of AGNRs and provides information on their length as well as overall structural integrity of the ribbons and their interaction with technologically relevant substrates [4]. Additionally, we designed and synthesized a precursor molecule with a single halogen substituent to selectively grow short 7-AGNRs with a single length. The successful growth is observed by STM and the characteristic length-dependent Raman mode. Further, I will discuss the unique zig-zag/armchair aspect ratio that allowed us to use these structures as a testbed to investigate the reactivity of this molecule using Raman spectroscopy [5].
Finally, armchair GNRs were integrated in different device architectures and their transport properties were characterized. 9-AGNRs were integrated in narrow finger-gate devices that allowed the gating of these GNRs separately from the source and drain electrodes. Low-temperature transport spectroscopy measurements reveal quantum dot (QD) behavior with rich Coulomb diamond patterns, suggesting that the GNRs form QDs that are connected both in series and parallel [6]. In a different device architecture, 9-AGNRs were integrated with Pd electrodes and a double-gate (DG) structure. 9-AGNR- field effect transistors showed high Ion/Ioff up to 10^5, excellent, highest to date, Ion = 12 µA and device yields up to 80-90% [7].

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Fermion-Parity-Based Computation and its Majorana-Zero-Mode Implementation

Campbell Mclauchlan, Benjamin Béri

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Majorana zero modes (MZMs) promise a platform for topologically protected fermionic quantum computation. However, creating multiple MZMs and generating (directly or via measurements) the requisite transformations (e.g., braids) pose significant challenges. We introduce fermion-parity-based computation (FPBC): a measurement-based scheme, modeled on Pauli-based computation, that uses efficient classical processing to virtually increase the number of available MZMs. Given the input of so-called magic states, FPBC operates without the need to perform any unitary transformations such as braids. FPBC requires all MZM parities to be measurable, but this conflicts with constraints in proposed MZM hardware. We thus introduce a design in which all parities are directly measurable and which is hence well suited for FPBC. This poster is based on Phys. Rev. Lett. 128, 180504 (2022).

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Extreme conditions science using the new ID27 beamline at the fourth generation EBS-ESRF

Gaston Garbarino, Mohamed Mezouar, Wolfgang Morgenroth, Anna Pakhomova, Tomasz Poreba, Bjorn Wehinger, Hemann Muhammad

MC46: Matter Under High Pressure III, August 22, 2022, 4:30 PM - 6:00 PM

The new EBS-ESRF light source allows a great improvement of our fundamental understanding of materials under high compression due to the unprecedented characteristiques of the generated X ray beams. The array of techniques, in the early days restricted to structural measurements using X-Ray diffraction, is now extended and includes many others such as Inelastic X-ray Scattering, Nuclear Inelastic Scattering, X ray absorption and emission spectroscopy, X ray magnetic circular dichroism, X-ray Compton scattering and X-ray magnetic scattering. As a direct consequence, many scientific breakthroughs have been achieved across fields ranging from fundamental physics to Earth and planetary sciences, chemistry and materials research, and extending into biophysics and biochemistry including questions concerning life and biological function under extreme conditions. The investigation of matter under extreme conditions is one of the pillar scientific cases to exploit the new fourth generation EBS-ESRF. In this presentation, we will introduce the ambitious and innovative modernization project to upgrade ID27 to a long beamline with unique photon flux and focusing, time resolution and coherence capabilities. This ‘high-flux nano-XRD’ beamline is optimized for the needs of the geo- and materials-science community for in-situ XRD and XRF studies under extreme conditions. The details of this project as well as the status of the high pressure activity at the ESRF beamlines and the on-site high pressure preparation dedicated laboratories will be presented.

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New iontronics devices using electric double layer electrets

Dr. Shimpei Ono, Mr. Kazumoto Miwa

MC10: Nanodevice Iontronics VIII, August 24, 2022, 4:30 PM - 6:00 PM

Electric field control of materials properties is one of the longstanding issues in solid-state science. The uniqueness of this approach is that carrier concentration can be modified without chemical doping which is inherently associated with the disorder. In recent decades, a different route for carrier doping which relies on an electrochemical concept has been extensively investigated to control materials properties with an electric field. It is well known that when a voltage is applied to an electrolyte, a huge electric field of the order of 10 MV/cm is generated at the solid/liquid interface due to the formation of an electric double layer (EDL). Owing to this extremely high electric field, EDL gating has the unique capability to push the charge density accumulation that is well beyond the limitations of any solid gate dielectric. In this talk, we are going to explore this window of extreme electric fields using “an electric double layer electret (EDLE)” which is a second-generation EDL gating allowing for the control of novel states of matter. The EDLE is formed by anchoring the motion of ions inside the IL gel after the formation of the EDL, and it can sustain the EDL without any external bias-voltage source. Simply sticking the EDL electrets containing the gate array on top of the semiconductor, we can modulate the electric states of the materials.

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Cooling nano-electronic devices to ultra-low temperatures

Jonathan Prance

MC24: Quantum Electronics at Ultra-low Temperatures VII, August 24, 2022, 2:00 PM - 3:30 PM

Experimental breakthroughs over the past five years have demonstrated new techniques to cool the conduction electrons in micro- and nano-scale devices and materials below 1 millikelvin [1-5]. As well as the exciting possibility of studying electronic systems in a new regime, cooling far below the current standard of ~10 millikelvin may have immediate practical benefits such as enhancing the performance of quantum technologies, metrological standards and sensors.

One challenge to reaching on-chip electron temperatures in the microkelvin regime is the need to work below the base temperature of dilution refrigerators. Some suitable refrigeration techniques exist but they are not generally available and remain largely confined to specialist labs. The second challenge is creating a strong thermal link between the refrigerant and the system of interest. This is particularly difficult for very small and cold objects where the thermal links between different subsystems within materials become extremely weak and heat capacities are small. Solutions that have been recently demonstrated include immersion cooling of samples in liquid helium, demagnetisation refrigeration of electrical contacts and on-chip demagnetisation refrigeration. This talk will review the current state-of-the-art in cooling nanoelectronic devices and discuss possible ways to make the techniques more broadly applicable.

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Taking the temperature of a pure quantum state

Prof John Goold, Prof. Mark Mitchsion, Prof. Alessandro Silva, Dr. Marlon Brenes, Dr. Archak Purkayastha

MC20: Recent Advances in Quantum Thermodynamics with a Focus on Many-body Interactions VI, August 23, 2022, 4:00 PM - 6:00 PM

Temperature is a deceptively simple concept that still raises deep questions at the forefront of quantum physics research. The observation of thermalisation in completely isolated quantum systems, such as cold-atom quantum simulators, implies that a temperature can be assigned even to individual, pure quantum states. Here, we propose a scheme to measure the temperature of such pure states through quantum interference. Our proposal involves interferometry of an auxiliary qubit probe, which is prepared in a superposition state and subsequently decoheres due to weak coupling with a closed, thermalised many-body system. Using only a few basic assumptions about chaotic quantum systems -- namely, the eigenstate thermalisation hypothesis and the emergence of hydrodynamics at long times -- we show that the qubit undergoes pure exponential decoherence at a rate that depends on the temperature of its surroundings. We verify our predictions by numerical experiments on a quantum spin chain that thermalises after absorbing energy from a periodic drive. Our work provides a general method to measure the temperature of isolated, strongly interacting systems under minimal assumptions.

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Quantum optics with molecules

Claudiu Genes

Coherent light, either classical or quantum, as in the case of optical cavities, has the power to strongly modify and eventually enhance material properties. Different competing theoretical approaches are currently emerging to describe photon-electron interactions in the presence of vibronic coupling. I discuss progress we have recently made in developing a quantum Langevin equations approach to quantum optics with molecules. At the level of a single or a few molecules, this method can analytically describe effects such as polariton cross-talk, Purcell modification of branching ratio and incoherent FRET (Förster resonance energy transfer) migration of energy [1,3]. In the mesoscopic limit, where many molecules are coupled to a single cavity mode, I discuss strategies for incorporating frequency and orientational disorder, near field couplings and vibrational relaxation in an analytical model showing the degradation of the VRS (Vacuum Rabi splitting) at high densities [2].

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Boosting 2D materials with molecules:

multi-responsive and high-performance opto-electronic devices

Paolo Samorì

MC10: Nanodevice Iontronics X, August 25, 2022, 2:00 PM - 3:30 PM

Two-dimensional materials exhibit exceptional physical and chemical properties which can be further enhanced and enriched via their controlled interfacing with molecules and (supra)molecular assemblies. In my lecture I will introduce the importance of functionalization of 2D materials to engineer hybrid systems with ad hoc characteristics. I will show how non-covalent and covalent approaches can offer viable solutions to impart new functions to 2D semiconductors rendering them multiresponsive, to leverage the dimensionality for enhanced electronic transport in 2D semiconductors and to develop highly-sensitive pressure sensors for health monitoring. The presented modular strategies offer a simple route to generate multifunctional coatings, foams and nanocomposites with pre-programmed properties to address key global challenges in electronics, sensing and energy applications.

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Emergent magnetism triggered by ionic liquid gating at the metal insulator transition in SrIrO3 ultrathin films

Juan I. Beltrán, Fernando Gallego, Javier Tornos, Andrea Peralta, Federico Monpean, Mar García, Carlos León, Jacobo Santamaría, Maria del Carmen Muñoz

MC10: Nanodevice Iontronics XII, August 26, 2022, 9:00 AM - 10:00 AM

Emergent magnetism triggered by ionic liquid gating at the metal insulator transition in SrIrO3 ultrathin films

Juan I. Beltrán1, Fernando Gallego1, Javier Tornos1, Andrea Peralta1, Federico Mompean2, Mar Garcia Hernandez2, Carlos León1,2, Jacobo Santamaría1,2, Carmen Muñoz3

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Abstract:

Ultrathin iridate films resembling properties of the Ruddlesden Popper series, Srn+1IrnO3n+1, have gathered large attention from the condensed matter community due to the wide range of exhibited phenomena such as metal-insulator transitions, weak antiferromagnetism, topological phases, etc. [1,2]. In these oxides, different types of interactions, including Coulomb repulsion, kinetic energy and spin-orbit coupling have comparable energy scales and thus have comparable importance in determining electronic and magnetic properties. Particularly interesting is an emergent magnetic state, at temperatures below the metal insulator transition, in ionic liquid gating experiments on SrIrO3 films with thickness less than 2nm grown on SrTiO3 [3]. In this work we employ ab-initio simulations at SrIrO3-SrTiO3 heterostructures to reveal the possible role of an external electric field in modulating the magnetic phase. When reversing the electric field direction we find an asymmetric effect in the system properties establishing an abrupt transition between an antiferromagnetic-insulator and a paramagnetic-metal phase. The antiferromagnetism is intimately linked to the atomic structure, e.g. to the octahedral arrangement, which through Dzyaloshinskii-Moriya interaction gives rise to a weak out-of-plane ferromagnetic moment. This magnetic order is the result of a restored symmetry due to the interplay between electric field and thin film symmetry breaking. The effect of inversion symmetry breaking is enhanced by flipping the external electric field, resulting in a metallic paramagnetic state. Our results suggest there is a complex interplay between atomic structure, electronic properties and magnetism. This interplay explains the experimental data obtained from X-ray diffraction and magnetotransport measurements.

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Figure 1 Caption. Band dispersion for 3 SIO ML on STO (panels (a), (b), (c)). Different colors correspond to projections of bands on the different IrO2 planes in the structure (blue, red and green correspond respectively to the first, second and third closest IrO2 plane to the STO interface). Calculations are under external electric fields E=-0.1 eV/Å (a), E=0 (b) and E=+0.1 eV/Å

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Universal features in finite-time quantum critical machines

Victor Mukherjee

MC20: Recent Advances in Quantum Thermodynamics with a Focus on Many-body Interactions IV, August 23, 2022, 11:30 AM - 12:30 PM

Finite-time quantum machines operating close to phase transitions may exhibit several universal features in their output, owing to diverging length and time scales close to criticality. I will discuss the operation, control and fluctuations of quantum engines and quantum batteries operating close to quantum phase transitions; I will show how one can harness the universality associated with quantum critical points to develop high-performing many-body quantum machines.

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“Chiralized” Cu and Ni deposits obtained via Electroless deposition.

Claudio Fontanesi, Aldo Girimonte, Andrea Martini, Roberto Giovanari, Walter Giurlani, Massimo Innocenti

MC10: Nanodevice Iontronics VII, August 24, 2022, 2:00 PM - 3:30 PM

“Chiralized” Cu and Ni deposits obtained via Electroless deposition.
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The influence of physical constraints in the field of “chiral-electrode”|solution interfaces is the sub-ject of rapidly growing scientific and applicative interest in electrochemistry.1,2 In physics (and biol-ogy too), the concept of chirality, and the relevant involvement of physical interactions ruling chiral-systems is a fascinating field of science: Maxwell equations, light polarization to mention a few (in biology, the homochirality dilemma). Besides pure scientific aspects, chirality means applications: asymmetric synthesis and enantioselectivity/enantio-recognition (sensors). Within the area of chirali-ty, it was shown that chiral systems are able to interact selectively with spin-polarized electrons3 act-ing also as spin-filtering systems.4 Then, the implementation of the chiral spin-selectivity in electro-chemistry, lead to SDE (spin-dependent electrochemistry).5 Recently, electrodes functionalized with chiral molecules shown better charge transfer properties if compared with structurally similar achiral compounds.6 Moreover, bulk “chiralized” electrodeposited nickel and electropolymerized aniline (PANI), showed both good enantioselectivity as well as spin filtering (magnetoresistance) proper-ties.7–9 In this paper we are studying “chiralized” metals by electroless co-deposition of a suitable metal (here Cu and Ni) with an enantiopure chiral molecule: asymmetry inducer. This aiming to de-posit a chiral conductive (metallic and possibly ferromagnetic) surface on a non-conductive material, in view of applications in both energy (photovoltaic) and spintronics (spin-valve) applications. At present, in our laboratory the electroless deposition of both Cu and Ni was successfully carried out using Ag nanoparticles as the catalyzer, Figure 1. Co-deposition in the presence of enantiopure chiral organic compounds is under investigations.

Figure 1. Cu electroless deposition using Ag nanoparticles.
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Electrolyte-Gated Transistors Biosensors for Healthcare Applications

Matteo Sensi, Marcello Berto, Carlo Augusto Bortolotti, Fabio Biscarini

MC10: Nanodevice Iontronics VIII, August 24, 2022, 4:30 PM - 6:00 PM

Electrolyte-gated transistors (EGTs) based on organic semiconductors and graphene derivates are emerging in the field of biosensing because they are ultrasensitive, label-free, can be fabricated on flexible substrates at low cost and interfaced with biological samples.[1,2] We show some examples to demonstrate the possibility to use this technology to develop biosensors for different healthcare applications, by just selecting the most effective device architecture and material.
All the presented devices share a common transistor architecture, consisting of two interdigitated electrodes, source and drain, covered with an active material, in contact with a gate electrode through an electrolyte. The biosensing event takes place at the gate/electrolyte interface, by functionalization of the gold gate with a biorecognition moiety, and it is amplified by the active material channel thanks to the high-capacitance electrical double-layers formed at the gate/electrolyte and electrolyte/channel interfaces.
We fabricated EGTs biosensors for ultrasensitive detection of biomarkers by using different materials in the channel, namely ambipolar Reduced-Graphene Oxide, organic p-type semiconductor TIPS-Pentacene and poly(3,4-ethylenedioxythiophene)polystyrene sulfonate (PEDOT:PSS) polymer mixture.
Thanks to tailored gate functionalization, we realized a disposable rGO-EGT immunosensor for the detection of anti-Infliximab antibodies, which are produced by patients upon treatment with the immunotherapeutic drug Infliximab and can make the therapy ineffective. Furthermore, we developed an Electrolyte-Gated Organic Field-Effect Transistor (EGOFET) immunosensor for the detection of anti-Nivolumab antibodies, based on the organic semiconductor TIPS-pentacene, showing fM theoretical Limit of Detection (LOD).[3]
We also successfully employed an organic electrochemical transistor (OECT) genosensor for the detection of oligonucleotides, thanks to a facile functionalization process based on polydopamine.[4] Finally, we demonstrated the possibility to use EGOFET for the specific detection of transcription factors, by using the consensus DNA sequence as biorecognition element.
We conclude that EGTs biosensors show promising performances for the future application at the Point-of-Care but also for fundamental studies on macromolecules interactions.

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Beyond Batteries: Reimagining the role of ions in electronics

Prof. Susan Fullerton

MC10: Nanodevice Iontronics X, August 25, 2022, 2:00 PM - 3:30 PM

The interplay between ions and electrons governs processes as common as the biochemistry essential for life and the performance of devices as ubiquitous as batteries. The energy that powers our smart phones and laptops is stored by ions. Yet when we peer past the battery and examine the device-scale electronics, mobile ions are nowhere to be found. This is a missed opportunity because the coupling between ions in electrolytes and electrons/holes in novel semiconductors is strong. For example, in two-dimensional (2D) materials this coupling has uncovered exciting phenomena such as spin polarization, photogalvanic current, current-induced circularly polarized electroluminescence, and superconductivity. Remarkably, these demonstrations have relied on electrolytes that were not designed for investigating semiconductor physics, but instead for energy storage (e.g., solid polymer electrolytes and ionic liquids). Our group is reimagining how ions can be used in electronics when the electrolyte is custom designed to provide a specific functionality or unlock a new mechanism to control transport. For example, we have developed a “monolayer electrolyte” that is a single molecule thick and is designed for bistability. We have custom-synthesized a single-ion conductor and used it as an electric double layer (EDL) gate on 2D FETs to control strain via field-effect. Together with our collaborators we have develop several new types of “locking” electrolytes that can lock and unlock EDLs via multiple external triggers. Our development of these and other new ion-conductors is grounded in fundamental materials science and driven by applications in the electronics community including non-volatile memory, low-power logic, hardware security, and neuromorphic computing. In this talk I will highlight our most recent developments on ion conductors with an eye towards application.

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Ion-gating of individually contacted quasi 1-D metal-oxide semiconductor core-shell heterojunctions

Valeria Demontis

MC10: Nanodevice Iontronics VII, August 24, 2022, 2:00 PM - 3:30 PM

Metal oxide (MOx) semiconductors are very attractive materials owing to their favorable electronic and optical properties, abundance, high stability, non toxicity, and simple preparation methods, which make them highly promising for applications in optoelectronic devices, solar cells, photodetectors, and sensors [1]. In this context, the possibility to effectively tune the electronic properties of these materials is key requirement for exploring novel functional devices. To this regards, ionic gating has been demonstrated as a very powerful tool to control the electronic properties of different classes of materials, such as oxides [2], organic semiconductors [3] and III-V semiconductor nanowires [4-5].
In this work we investigated multi-contact devices based on individual MOx nanowires, featuring a radial p-n heterojunction (p-type Cu2O or Co3O4 shell and n-type ZnO core). The device architecture allowed to investigate the heterostructure electric transport properties in multiple configurations, i.e. core-core, shell-shell, and core-shell. The architecture also allowed to operate the system in a dual gate configuration, using a conventional back gate and the ionic gate. The core-core current-voltage characteristics showed an ohmic behavior, as expected for ZnO nanowire devices. The current-voltage characteristic in core-shell configuration demonstrated a rectifying behavior typical of p-n junction devices, while in shell-shell configuration, the output characteristics were compatible with those of a semiconductor device with Schottky contacts. The experimental curves were fitted using a diode equation for the core-shell configuration and with a current voltage model for double Schottky barrier devices [6] for the shell-shell configuration, in order to extract relevant device parameters including diode ideality factor and barrier heights. Our results shine light on the nanoscale building blocks of very promising nanostructured platforms for energy conversion and harvesting as well as photodetection.
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A Heat Driven Iontronic Nanotransistor

Alessia Colosimo

MC10: Nanodevice Iontronics VIII, August 24, 2022, 4:30 PM - 6:00 PM

Heat is one of the most abundant naturally occurring resources and can be exploited for many aims, e.g., energy harvesting or nano-microscale sensing in biological systems. Recently, research efforts on heat transport are being boosted by the spread of novel thermoelectric materials and new tools to exploit thermal budgets at the nanoscale. Among these, ion-based soft-matter systems (such as polyelectrolytes) are rapidly emerging as an ideal platform for the exploitation of thermoelectric phenomena for heat-to-energy conversion and heat sensing.
In this work, combining the versatility of solid-state nanoelectronic devices together with the promising physio-chemical properties of polyelectrolytes, thermally driven field-effect control of a nanowire-based device is achieved. Such thermal gating mechanisms are generated by thermodiffusion (Soret effect [1]) of ions occurring in a droplet of poly(ethylene oxide) functionalized with Na+ ions, coupled with a single InAs nanowire field-effect transistor [2]. The heat-driven rearrangement of ions of the polyelectrolyte causes an accumulation of the charged species at the electrolyte/nanowire interface, allowing for the observation of heat driven modulation of the electronic transport in the nanowire via the mechanism of the formation of the electric double-layer [3, 4]. We realize a novel architecture of heat driven nanotransistor, characterizing the device operation in its parameter space at room temperature. Resorting to multiscale molecular dynamics simulations and finite element analysis, we relate operational regimes and hysteretic behaviors observed in our devices to microscopic parameters of the polyelectrolyte. Our work reports for the first time novel insights on the microscopic parameters of novel soft thermoelectric materials and the achieved results will be fundamental for the design of innovative polyelectrolytes for the next generation thermoelectric generators and sensors.

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Classical to quantum transport crossover in InAs nanowires enabled by electrolyte gating

Domenic Prete

MC10: Nanodevice Iontronics XI, August 25, 2022, 4:30 PM - 6:00 PM

Electrolyte gating is emerging as a promising tool to control the electronic properties of semiconducting nanostructures both in the classical and quantum regimes [1, 2]. Indeed, the possibility to access electric fields featuring unprecedented intensity had been exploited to observe the rise of superconductivity [3,4] by inducing high carrier concentration in functional materials. Nonetheless, to date the applications of electrolyte gating for applications in quantum technologies is limited to devices employing the technique to enhance the carrier concentration to induce exotic phenomena, while the use of the intense electric fields - made accessible by the ionic accumulation at the electrolyte/nanostructure interface - to generate confinement potentials designing quantum systems remains unexplored.
In this work, we exploit for the first-time electrolyte gating to confine charge carriers in an InAs nanowire and realize a device which allows to observe a transition from classical transport to the quantum realm on the same nanostructure. Clear evidence of one-dimensional transport features are observed in an otherwise classical nanostructure, ascribable to the confinement electrical field generated by the ionic layer formed at the interface between the nanowire and an ionic liquid. We perform bias spectroscopy and magneto-transport measurements, finding a reduced effective diameter of the conduction channel coherent with the confinement of the charge carriers being confined away from the surface of the nanowire. This work provides the first demonstration of a novel approach enabling the realization of quantum devices featuring high performance and extreme flexibility for the development of quantum technologies.
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Spinorial states and spin-orbit coupling in nanowires under strong anisotropic radial electric fields

Guido Goldoni, Andrea Vezzosi, Andrea Bertoni

MC10: Nanodevice Iontronics XI, August 25, 2022, 4:30 PM - 6:00 PM

Controlling spin-orbit coupling (SOC) in nano-fabricated semiconductors is critical to engineer scalable spintronic
devices. In quasi-1D systems this is also associated to the Majorana physics. As SOC is induced by inversion symmetry breaking of the electronic system, external fields can be effectively employed to modulate spin splitting via the Rashba mechanism. In this perspective iontronics envisions ad additional path in terms of control of the intensity and symmetry of external fields. In doped samples, however, external fields are screened by electron/hole cloud, which therefore is an essential ingredient for predictive modelling.
We use a k · p theory to explore gate-controlled Rashba-induced spinorial conduction and valence band structure
in large, n- or p-doped III-V semiconductor nanowires, possibly including radial heterostructuring. Wires of different material classes, size and doping are investigated under the influence of back-gates and/or global gates which can be independently driven in a field-effect configuration (see figure).
We show that, in high carrier density, SOC has a nonlinear electric field susceptibility, due to large reshaping of the quantum states, and we analyze recent experiments in light of our calculations [1]. Radial heterostructures turn out to add a valuable degree of freedom as barrier materials may allow for a stronger symmetry breaking inducing specific interface-related contributions to SOC [2]. Gate potentials, breaking the native symmetry of the nanocrystal, also couples to the magnetic field (either axial or normal to the wire) at sufficiently high gate potential and expose the vectorial character of SOC [3,4].

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Ionic liquid gating of CVD-growth WS2-based field effect transistors

Leonardo Martini

MC10: Nanodevice Iontronics XII, August 26, 2022, 9:00 AM - 10:00 AM

The research in two-dimensional (2D) materials has attracted great interest in recent years, for electronic, spintronic and optoelectronics applications. One class of 2D materials of particular interest is transition metal dichalcogenides (TMDs), where one layer of transition metal atoms is packed between two layers of dichalcogenides atoms [1]. TMDs possess a bandgap which changes from indirect to direct when the thickness goes from bulk to monolayer [2]. Specifically, particular interest is devoted to tungsten disulphide (WS2) [3], due to the presence of a direct bandgap in the visible range (around 2 eV) making it suitable for electronics and optoelectronics applications. Hence, controlling the growth process in order to obtain highly crystalline WS2 with appreciable electronic and optical properties is of primary importance. Furthermore, the employment of CVD-growth would be desirable for the transition from lab scale to mass production of commercial devices.
In this work, we address the transport properties of field effect transistors based on CVD-growth WS2 by resorting to non-conventional gating techniques, in order to explore novel features inaccessible with standard solid state gating[4].
In order to optimize electrical performance of WS2 for the realization of functional devices, we first undergo the material to annealing procedures, employing both electrical and thermal techniques. We then characterize the electrical performance, contact resistance and extract carrier mobility for both the pristine and treated sample. We also discuss the improvement of the performance by measuring the transfer characteristics upon conventional back gate as well as ionic liquid gate operation. Finally, by exploiting ionic liquid gating, we probe electronic transport properties in a dual-gated device configuration, exploring doping regimes inaccessible with conventional techniques.
We believe that the demonstration of the liquid-gating techniques combined with CVD-growth TMDs could allow the study of exotic electrical properties in a variety of technologically relevant materials, with possible implications for industrial applications provided by the scalability of our approach.
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Leonardo Martini1, Valeria Demontis2, Domenic Prete2, Domenica Convertino1,3, Simona Pace1,3, Paolo Paletti1,3, Camilla Coletti1,3, Francesco Rossella4
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Global Sensing and Its Impact for Quantum Many-Body Probes

Abolfazl Bayat

MC20: Recent Advances in Quantum Thermodynamics with a Focus on Many-body Interactions VI, August 23, 2022, 4:00 PM - 6:00 PM

Quantum sensing is one of the key areas that exemplify the superiority of quantum technologies. Nonetheless, most quantum sensing protocols operate efficiently only when the unknown parameters vary within a very narrow region, i.e., local sensing. Here, we provide a systematic formulation for quantifying the precision of a probe for multiparameter global sensing when there is no prior information about the parameters. In many-body probes, in which extra tunable parameters exist, our protocol can tune the performance for harnessing the quantum criticality over arbitrarily large sensing intervals. This significantly enhances the performance of the probe even when the interval of interest is so large that the precision is bounded by the standard limit. We also apply our mechanism for global quantum thermometry which leads to find optimal probes which can measure temperature over several orders of magnitude. We observe the emergence of different phases for such optimal probes as the temperature interval is increased. In addition, we show how the best approximation of optimal global probes can be realized in spin chains, implementable in ion traps and quantum dots.

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Realizing a minimal Kitaev chain in coupled quantum dots

Di Xu, Tom Dvir, Guanzhong Wang, Nick van Loo, Chun-Xiao Liu, Grzegorz Mazur, Alberto Bordin, Sebastiaan ten Haaf, David van Driel, Francesco Zatelli, Filip Malinowski, Ji-Yin Wang, Xiang Li, Sasa Gazibegovic, Ghada Badawy, Erik Bakkers, Michael Wimmer, Leo Kouwenhoven

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Majorana bound states constitute one of the simplest examples of emergent non-Abelian excitations in condensed matter physics. A toy model proposed by Kitaev shows that such states can arise on the edges of a spinless p-wave superconducting chain. Practical proposals for its realization require coupling neighboring quantum dots in a chain via both electron tunneling and crossed Andreev reflection simultaneously. Here we demonstrate for the first time the simultaneous presence of all necessary ingredients for an artificial Kitaev chain: two spin-polarized quantum dots in an InSb nanowire strongly coupled by both elastic co-tunneling and crossed Andreev reflection. Our system can be further fine-tuned to a sweet spot where a pair of Majorana bound states is predicted to appear. In this sweet spot, the transport characteristics satisfies all accessible theoretical predictions for a Majorana bound state platform for the first time, including pairwise correlation, zero charge and the expected phase diagram. While the simple system presented here can be scaled to simulate a full Kitaev chain with an emergent topological order, it can also be used imminently to study the physics of Majorana bound states and non-abelian anyons.

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Direct measurement of the Andreev Bound State spin during the Singlet-Doublet transition

Di Xu, David van Driel, Guanzhong Wang, Nick van Loo, Grzegorz P. Mazur, Francesco Zatelli, Alberto Bordin, Sasa Gazibegovic, Ghada Badawy, Erik P. A. M. Bakkers, Leo P. Kouwenhoven, Tom Dvir

MC21: Bound States in Hybrid Superconductor Nanostructures VI, August 23, 2022, 4:30 PM - 6:00 PM

Majorana bound states appearing at the edge of a 1-dimensional topological superconductor have distinct signatures in spin and charge. An Andreev bound state (ABS) is expected to similarly show both charge and spin reversal at the singlet-doublet quantum phase transition. These properties are inaccessible in conventional two-terminal spectroscopy. Here we employ a three-terminal setup consisting of a proximitized InSb nanowire coupled to a quantum dot on one side and a tunnel junction on the other side. The application of a magnetic field turns the quantum dot into an effective spin detector, which in combination with the other tunnel probe, allows us to study the spin and charge degrees of freedom of the hybrid system. We observe fully spin-polarized ABSs that reverse their spin-polarization and charge when undergoing a quantum phase transition. We propose that these techniques can be applied in the future to study topological superconductivity.

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Successive Electronic Topological Transitions in the Antiferromagnet UPd2Al3

Dr. Alexandre Pourret, Dr. Georg Knebel, Pr. Dai Aoki, Dr. Gabriel Seyfarth, Pr. Gertrud Zwicknagl

MC50: Fermi Surface Topological Transitions - Effects of Interactions VII, August 24, 2022, 2:00 PM - 3:30 PM

Metamagnetic transitions correspond to a sudden and strong increase of the magnetization as a function of an external magnetic field. They are observed in localized antiferromagnetic systems with a rather strong magnetic anisotropy due to spin-flop transitions as well as in paramagnetic systems of itinerant electron systems into a ferromagnetic system. The magnetic character at low field of the systems can be very different indicating the complexity of a common understanding. Only recently is has been stressed that these metamagnetic transitions eventually appear together with a topological Fermi surface transition corresponding to a Lifshitz transition.
Here we report successive anomalies at low temperature in the magnetic field dependence of the thermoelectric signal in the heavy-fermion compound UPd2Al3 inside the antiferromagnetic state up to the metamagnetic transition at HM=18 T. Based on renormalisation perturbation theory and the partitioning of the f orbitals into localized and delocalized parts, our analysis attributes these anomalies to complex topological changes occurring on the Fermi surface driven by Zeeman effect. The observation of a sudden change of sign both in the thermoelectric power and in the Hall coefficient at HM in addition to the appearance of large quantum oscillations in the thermoelectric power coefficient above HM indicate a strong Fermi surface reconstruction at the metamagnetic transition due to the unfolding of the electronic bands.

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Restoring the strange metal phase in underdoped cuprated via suppression of Charge Density Wave

Floriana Lombardi

MC31: The Physics of Cuprates X, August 25, 2022, 2:00 PM - 3:30 PM

The “strange metal” phase of High Critical Temperature Superconductors (HTS) is one of the most striking manifestations of the strong electron-electron correlation in these materials. It manifest at optimal doping as a linear temperature dependence of the resistivity that persists to the lowest T when superconductivity is suppressed. This behavior is fundamentally different from that observed in more conventional metals, where a T-linear dependence of the resistivity is found, only at high temperatures, where phonon scattering dominates the transport. For underdoped cuprates this behavior is lost below the pseudogap temperature T*, where Charge Density Waves (CDW) together with other intertwined local orders characterize the ground state of the material. The association between the departure from the T-linear resistivity and the occurrence of the pseudogap phenomenon has long been speculated. However, there is no consensus on the physics at play. To address the origin of the T-linear dependence departure in the underdoped regime we have tuned the ground state of underdoped the HTS by using the geometric modification of the unit cell under the strong strain induced by the substrate. We show that the T-linear resistivity of highly strained, nm thick and underdoped $YBa_2Cu_3O_{7-\delta}$ (YBCO) films is restored when the CDW amplitude, detected by Resonant Inelastic X-ray scattering, is suppressed [1]. This observation points towards an intimate connection between the onset of CDW and the departure from the strange metal behaviour in underdoped cuprates, a link which was unclear up to now. At the same we observe that the superconducting temperature onset and the upper critical field H_{c2} are enhanced at dopings where the CDW is suppressed which supports the competition between charge order and superconductivity. These effects demonstrate how strain control and nanoscale dimentions allow to manipulate the ground state of HTS which is crucial to understand the complex physics of these materials.
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Higgs collective mode in superconductors probe by Raman spectroscopy

Marie-aude Méasson

We explore the mechanism of observability that makes the Higgs mode of the superconducting state detectable by Raman spectroscopy based on the interplay between the charge-density-wave and superconducting states.
We show that, by reaching a region of coexistence of both states in transition metal dichalcogenides 2H-MX2, , we unravel an intense and narrow sub-gap superconducting mode, attributed to a Higgs mode, coexisting with the expected incoherent Cooper-pair breaking signature. By application of high pressure, we follow the behaviors of the collective modes of both states that are consistent with theoretical calculations.

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QUEST-DMC: Simulation studies for the detection of sub-GeV
dark matter with a superfluid Helium-3 calorimeter.

Dr Paolo Franchini

MC28: Condensed-matter Quantum Technology on the Hunt for Dark Matter II, August 22, 2022, 2:00 PM - 3:30 PM

Several independent observations suggest that there is more mass in the Universe than has been directly observed. Dark matter is a hypothetical new form of matter that does not interact with the electromagnetic field and has a very weak interaction with ordinary baryonic matter. WIMPs (Weakly Interacting Massive Particles) are a dark matter candidate currently widely investigated in experiments, but most experiments are constrained to spin-independent interactions in the 10-100 GeV/c^2 mass range. QUEST-DMC will use superfluid Helium-3 as a dark matter collision target, aiming to reach the world-leading sensitivity to spin-dependent interactions of 0.1-1 GeV/c^2 mass dark matter candidates.

Here we discuss a simulation of the superfluid ^{3}He bolometer's impact energy sensitivity, and argue that recoil energy of <10 eV can be detected using nanomechanical resonators. We also investigate the sources of radioactive background at and above this region and their relative importance using the Geant4 particle physics simulations toolkit.
We aim to report on the development of a dark matter bolometer based on these studies.

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Quantum simulation with ultracold atoms – emergent Hilbert-space fragmentation

Monika Aidelsburger, Sebastian Scherg, Thomas Kohlert, Bharath Hebbe Madhusudhana, Pablo Sala, Frank Pollmann, Immanuel Bloch

MC20: Recent Advances in Quantum Thermodynamics with a Focus on Many-body Interactions V, August 23, 2022, 2:00 PM - 3:30 PM

Well-controlled synthetic quantum systems, such as ultracold atoms in optical lattices, offer intriguing possibilities to study complex many-body problems relevant to a variety of research areas, ranging from condensed matter to statistical physics. In particular, out-of-equilibrium phenomena constitute natural applications of quantum simulators, which have already successfully demonstrated simulations in regimes that are beyond reach using state-of-the-art numerical techniques.

This enables us to shed new light on fundamental questions about the thermalization of isolated quantum many-body systems. While generic models are expected to thermalize according to the eigenstate thermalization hypothesis (ETH), violation of ETH is believed to occur mainly in two types of systems: integrable models and many-body localized systems. In between these two extreme limits, there is, however, a whole range of models that exhibit more complex dynamics, for instance, due to an emergent fragmentation of the many-body Hilbert space. A versatile platform that paves the way towards studying this rich variety of ergodic-breaking phenomena is the 1D Fermi-Hubbard model with a strong linear potential.

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Observation of long-range TGBA phase, polar order and thermochromic behaviour in a chiral bent-shaped liquid crystals

Ms. Vidhika Punjani, Dr. Golam Mohiuddin, Ms. Supreet Kaur, Mr. Raj Kumar Khan, Dr. Sharmistha Ghosh, Dr. Santanu Kumar Pal

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

In the molecular self-assembly of liquid crystalline systems, chirality is crucial. It induces a variety of unusual mesophases to emerge, including the blue phase (BP) and twist grain boundary phase (TGB). The liquid crystal analogue of the Abrikosov vortex state in type-II superconductors is the complicated TGB phase. This complicated mesophase is found between an isotropic or chiral nematic (N*) and smectic A (SmA) or smectic C (SmC) phase due to competition between the chiral packing requirement for the formation of a spiral macrostructure and the requirement for the formation of a stable lamellar structure.

The interaction of bent-core systems' chiral superstructures with the molecular chirality provided by cholesterol's stereogenic centres is investigated in this paper. We present a series of cholesterol-based bent-shaped materials with the direct attachment of cholesterol moiety to the central core on one arm and attachment of 4-n-alkoxy-2-hydroxybenzaldehyde via Schiff base to the central core on the other arm. By altering the terminal chain of these bent-shaped compounds, a variety of unique mesophases such as BPIII, BPI/II, Ncyb*, TGBA, SmA, SmAPA, and SmX was detected. This molecular design allows the TGBA phase to be enantiotropically stabilised over a wide temperature range. To the best of our knowledge, this is one of the fewest reports of bent-shaped liquid crystals stabilising TGBA phase in long temperature range [1,2]. Interestingly, the lower homologue of the series showed thermochromic behaviour. Moreover, one of the higher homologue of the series showed spontaneous formation of polar order in the SmA phase (Ps ~ 61 nC/cm2) which is quite rare in cholesterol-based bent-shaped systems.

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Arrays of optical tweezers and dressed Rydberg atoms for quantum simulators of electron-phonon interaction and multi band effects.

James Hague, Calum MacCormick, Pavel Kornilovitch, Leon Petit

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

We calculate Hubbard parameters for arrays of optical tweezers, and discuss how dressed Rydberg atoms (DRAs) in such arrays can be used to make quantum simulators for electron-phonon interaction and multi band effects. Arrays of optical tweezers are highly flexible: both depth and shape of individual lattice sites can be controlled dynamically. Our goals are to understand how (1) Hubbard parameters differ between arrays of optical tweezers and standard optical lattices (2) quantum simulators can be used to emulate quantum materials in the weak- and intermediate-coupling regimes where multiple bands interact and the basis is not localised and (3) quantum simulators built from arrays of optical tweezers can be used for other key interactions such as electron-phonon coupling.

We determine expressions for the hopping and Hubbard U of arrays of optical tweezers finding that strongly correlated systems with arbitrary structures can be simulated, including those with a multiple-site basis and impurities. Quantum simulators of Hubbard models with (1) arbitrary basis are required to represent many real materials of contemporary interest, (2) broken translational symmetry are needed to study impurity physics (3) dynamical lattices are needed to investigate strong correlations out of equilibrium. We consider experimental parameters for quantum simulation of Hubbard models with an arbitrary basis. Finally, we discuss the onset of charge transfer insulating states in ionic Hubbard models.

We describe a quantum simulator for the Hubbard-Holstein model (HHM), comprising two DRA species held in a monolayer by independent arrays of optical tweezers, predicting that boson-mediated preformed pairing and Berezinskii-Kosterlitz-Thouless (BKT) transition temperatures are experimentally accessible. Zeros in the ac Stark shift allow independent control of two Rydberg atom species. We predict sufficient tunability to probe (1) both HHMs and unconventional phonon-mediated repulsions (2) the competition between intermediate-strength phonon- and Coulomb-mediated interactions (3) BKT transitions and preformed pairing that could be used to examine the pseudogap. We discuss phonon-mediated pairing and condensation.

As proof of concept, density-functional calculations are made for the bandstructure for a ‘graphene’ quantum simulator made from arrays of optical tweezers. Optical tweezers must be well separated to reproduce Dirac points. Sinusoidal lattices cannot reproduce band structure. Light DRAs with small linewidth of intermediate state offer best properties. Sufficient hops to reach equilibrium are possible within Rydberg lifetimes and heating times, but the simulator is at the limit of current cold atom technology.

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Light bipolarons and other pairing in UV models of BCC and FCC lattices

Dr Ganiyu Adebanjo, James Hague, Dr Pavel Kornilovitch

MC35: Collective Effects and Non-Equilibrium Phenomena in Quantum Gases and Superconductors VIII,
August 24, 2022, 4:30 PM - 6:00 PM

The fulleride superconductors with face-centred-cubic (FCC) or body-centred-cubic (BCC) structure have unusually high transition-temperature to kinetic-energy ratios. We discuss how small light pairs can be realised on BCC and FCC lattices. We calculate pair mass, radius, and binding conditions, and use these to compute transition temperatures. We demonstrate that, within UV models (extended Hubbard models with onsite interaction U and inter-site interaction V) with a large and repulsive Hubbard U, paired fermions in FCC lattices have qualitatively different properties than pairs in other three-dimensional cubic lattices. Our results show that strongly bound, light, and small pairs can be generated in FCC lattices across a wide range of the parameter space. Even if the lattice constant is large (as in the fullerides) we estimate that such pairs can Bose condense at high temperatures [1]. Small light pairs are more difficult to realise on BCC lattices. We discuss how in the dilute limit, 6Li in body-centered-cubic (BCC) optical lattices could be used to realise cold-atom quantum simulators of this pairing. Local pairs form in such lattices with large binding energies (and thus binding temperatures). Small and light pairs form when the onsite U and inter-site V have similar sizes and are attractive, and these are estimated to form a Bose–Einstein condensate below around 10 nK [2]. Finally we examine bipolaron pairs in these lattices using path integral quantum Monte Carlo techniques.

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Self-organization in polarised tissues due to feedback between cell- and macroscopic-scale forces

James Hague

MC2: Self-Organisation in Living Systems VIII, August 24, 2022, 4:30 PM - 6:00 PM

Extracellular matrix (ECM) is an important component of living tissues that needs to be included in biophysical models alongside cells. It is typically a viscoelastic substance made up of polymers such as collagen, and provides structure as well as mediating forces between cells. Our goal is to introduce a microscopic biophysical model for self-organization and reshaping of lab grown polarised tissues, and to validate the model and determine the parameters by comparing with artificially grown tissues. The purpose of the model is to simulate the interactions between large numbers of cells and the ECM using a microscopic (rather than continuum) model to allow the tracking of individual cells and the ECM separately, more like the situation within real tissues. The self-organisation within the model is co-driven by microscopic active forces between cells and an extracellular matrix (ECM), and macroscopic forces that develop on tissue length-scales. When large numbers of cells act together these forces drive, and are affected by, macroscopic-scale self-organization and reshaping of tissues in a feedback loop. We want to understand the active feedback between cells and the extracellular matrix, and its relationship to macroscopic self-organization and reshaping of tissue. Our microscopic biophysical model consists of a contractile network representing the ECM, that interacts with a large number of cells interacting via dipole forces, which we use to describe the macroscopic self-organization and reshaping of tissue. We solve the model using simulated annealing, finding close agreement with experiments on artificial neural tissue. We discuss the calibration of model parameters. We conclude that feedback between microscopic cell-ECM force-dipole interactions and tissue-scale forces is a key factor in driving macroscopic self-organization of cells and reshaping of tissue. Finally, we discuss recent extensions to the model to examine the role of disorder in the model.

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Study of surface enhanced Raman spectroscopy effect on surface reconstructed Al2O3 substrate

M.sc Ephraim Thomas Mathew, Dr Weronika Andrzejewska, M.sc Zygmunt Miłosz, Prof dr hab Maciej Wiesner

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Surface enhanced Raman spectroscopy (SERS) effect increases the Raman scattering signals of very low analyte concentration on surfaces. A single crystal M - plane Al2O3 was thermally annealed in air to form a corrugated, saw-tooth pattern (1). A thin layer of Au (12 nm) was deposited on the corrugated Al2O3 using a PREVAC ultra-high vacuum electron beam evaporation system. Structural analysis of the sample by atomic force microscopy revealed ordered growth of Au deposition along the corrugation as in the Figure. Furthermore molecules of human IgG were immobilized onto the Au coated substrates by UV light assisted technique(2). The SERS effect measured by microRaman spectroscopy with laser wavelength λ =758 nm showed an optical enhancement of three orders of magnitude for immobilized human IgG molecules. An anisotropy of propagation of optical phonon in the IgG was observed. Intensities of peaks related with the IgG depended on relative orientation of the laser beam polarization and corrugation direction.

Acknowledgments

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Modelling Crystallisation in Polymers

Rasha Algethami, Nigel Clarke

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

We are developing phase-field models in which the molecular detail is coarse-grained into an order parameter that describes the local density of crystal or liquid. The phase-field model is then coupled to the Stokes equation of motion for fluid flow, assuming low Reynold's number. We are using a new approach to the modelling, known as fluid-particle dynamics, in which we treat the crystal as a high viscosity liquid rather than a solid. A set of two-dimensional numerical simulations of single crystals were performed in order to study the effect of crystal shape, aspect ratio and shear rate on the rotation behaviour of the crystal in the flow. Additionally, comparative investigations were carried out to examine the rotation behaviour due to the melt–crystal interface in rhombus crystals, similar to those observed in single crystals of polyethylene, at different values of interfacial energies, interfacial thickness and angle between faces of the rhombus shape. These simulations show that crystal rotation is almost proportional to the shear rate, but it decreases with an increase in the aspect ratio of the crystal.

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Nanoscale Electrochemical charge transfer kinetics investigated quantitively by Electrochemical Microwave Microscopy

Mohamed Awadein, Maxwell Sparey, Simon Grall, Ferry Kienberger, Nicolas Clement, Georg Gramse

MC17: Nanomechanical and Electromechanical Systems XI, August 25, 2022, 4:30 PM - 6:00 PM

The ability to probe the local reactivity of an electrode with GHz frequency has become available owing to the heterodyne capacitive sensing method. This method opens a new perspective on the comprehension of electrochemical reactivity at the nanoscale using electrochemical microwave microscopy with unprecedented sensitivity in the range of attoampere corresponding to only few hundreds of molecules. The electrochemical microwave microscopy provides electrochemical information on the nanoscale i.e. cyclic voltammetry and electrochemical impedance spectroscopy. The former was achieved by measuring the change of the interfacial capacitance corresponding to linear potential sweep, whereas, the latter was achieved by adding a modulation spectrum within the range of kHz under bipotentiostatic control. Exemplified here with the localized relaxation processes of an electrode modified with self-assembled monolayers immersed in an electrolyte. A capacitive analysis presented here enables a clean mapping of kinetic faradic characteristics and the parasitic contributions (nonfaradaic) to be spectrally resolved and subtracted. In particular, this methodology reveals an undistorted assessment of accessible redox site density of states associated with faradic capacitance, fractional surface coverage and electron transfer kinetics at the nanoscale. These direct observations of nanoscale electrochemistry enable advances in nano-electrochemistry.

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Exploring novel semiconductor/superconductor hybrids

Erik Bakkers

Majorana zero modes are expected to appear at the surface of a topological superconductor. One way to induce topological superconductivity is by coupling a superconductor to a semiconductor, which has strong spin-orbit coupling and a large g-factor. The field has mainly been concentrated on III-V semiconductors, like InSb and InAs, connected to Al as the superconductor. The zero modes obtained so far are likely trivial states, which are induced by disorder in the devices. In this study, we explore new fabrication routes to reduce disorder and novel material combinations, which have more extreme properties. One of our routes comprises in-situ device fabrication under ultra-high vacuum, using shadow deposition, such that interfaces are clean. In parallel, we explore novel materials such as SnTe, which is a topological insulator, PbTe, which is a semiconductor with an extremely high dielectric constant, and PbSnTe ternary compounds to tune the carrier density. We show first results on the growth of these materials and first transport results, revealing the effects of the high dielectric constant. We discuss challenges to be addressed in future studies.

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Exploring new semiconductor/superconducting hybrid material

Erik Bakkers

MC21: Bound States in Hybrid Superconductor Nanostructures II, August 22, 2022, 2:00 PM - 3:30 PM

Signatures of Majorana Zero Modes have been collected over the last decade, but there is no definitive proof of the existence of these states. Most likely the level of disorder in these devices succeeds the energy scale of that associated with the topological gap. Disorder may be present within the semiconductor, at the surface of the semiconductor, or at the semiconductor/superconductor interface. In this work, we explore new hybrid combinations, which should lead to larger topological gaps, and a better screening of charged defects and impurities. We study the growth of PbTe, which is a trivial semiconductor but with strong spin orbit coupling, and SnTe, a material that has been predicted to be a topological crystalline insulator, and combinations of these two, ternary alloys. This system can be combined with Pb and Sn as superconductors, resulting in a new materials platform, which we envision to be promising for realizing topological superconductivity.

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Hydrodynamic interactions induce microphase separation in active systems

Zhan Ma, Renato Assante, Cesare Nardini, Joakim Stenhammar, Davide Marenduzzo, Alexander Morozov

MC6: Emergent Phenomena in Driven Soft, Active and Biological Matter II, August 22, 2022, 2:00 PM - 3:30 PM

Free of the constraints of equilibrium statistical physics, active matter systems exhibit a variety of unexpected phenomena. Their origin lies in the detailed balance being broken by the self-propulsion and interactions between active particles at the microscopic level. Such systems can often be classified as either 'dry' or 'wet' active matter when dominated by friction with their surroundings and long-ranged hydrodynamic interactions, respectively. Manifestations of broken detailed balance often comprise novel phases that are absent in equilibrium. In dry active matter, an archetypal example is given by the motility-induced phase separation, while in wet active matter, the same role is played by 'bacterial turbulence' - large-scale collective motion of a dilute suspension of motile organisms.

In this talk we introduce a model that simultaneously includes long-range hydrodynamic interactions between microswimmers and microscopic ingredients necessary for the formation of motility-induced clusters. We demonstrate that the model yields a variety of new phases. Most importantly, we find that the growth of motility-induced clusters is arrested by hydrodynamic interactions leading to microphase separation. We discuss its mechanism and propose a phase diagram for such systems.

Z.M. and A.M. acknowledge financial support from EPSRC New Horizons programme (grant number EP/V048198).

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Novel Non-equilibrium Phenomena in Quantum Fluids of Light

Marzena Szymanska

MC25: Emerging Trends in Many-Body Cavity Quantum Electrodynamics XI, August 25, 2022, 4:30 PM - 6:00 PM

Driven-dissipative quantum fluids of light, experimentally realised in for example semiconductor microcavities, circuit or cavity QED systems, provide a unique testbed to explore new non-equilibrium quantum phenomena. I will review recent progress in this field. In particular, we show that polariton quantum fluid can exhibit a non-equilibrium order, where superfluidity is accompanied by stretched exponential decay of correlations. This celebrated Kardar-Parisi-Zhang (KPZ) phase has not been achieved before in any system in 2D and even 1D realisations are not conclusive. I will then discuss how these systems can undergo other unconventional phase transitions and orders, and display flow properties connected but distinct from conventional superfluidity. Finally, when placed in strained honeycomb lattice potentials, polariton fluids can condense into a rotating state, the lowest Landau level, forming a vortex array and spontaneously breaking time reversal symmetry.

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A holographic model for surface plasmon-polaritons

Ulf Gran

MC31 : The Physics of Cuprates XI, August 25, 2022, 4:30 PM - 6:00 PM

In recent years the dynamical charge response of the strange metal phase in high temperature superconductors have become experimentally accessible. We construct a holographic model for the interface between a strange metal and a dielectric and study the collective modes. We focus on the surface plasmon-polariton and present preliminary results regarding its dispersion relation and discuss the possible connection to experiments.

582

Coherent control of protein structural dynamics with X-ray crystallographic observation

Professor Jasper Van Thor, Dr Christopher Hutchison, Dr James Baxter, Dr Ann Fitzpatrick, Dr Gabriel Dorhliac, Dr Alisia Fadini, Dr Samual Perrett, Dr Karim Maghlaoui, Dr Salomé Bodet Lefèvre, Dr Violeta Cordon-Preciado, Dr Josie Ferreira, Dr Volha Chukhutsina, Dr Douglas Garratt, Dr Jonathan Barnard, Dr Gediminas Galinis, Dr Flo Glencros, Dr Marc Morgan, Dr Sian Stockton, Dr Ben Taylor, Dr Letong Yuan, Dr Matthew Romei, Dr Chi-Yun Lin, Prof Jon Marangos, Prof Marius Schmidt, Dr Viktoria Chatrchyan, Prof Tiago Buckup, Dr Dmitriy Morozov, Dr Jaehyun Park, Dr Sehan Park, Dr Intae Eom, Dr Minseok Kim, Dr Dogeun Jang, Dr Hyeongi Choi, Dr HyoJung Hyun, Dr Gisu Park, Prof Eriko Nango, Dr Rie Tanaka, Dr Shigeki Owada, Dr Kensuke Tono, Dr Takanori Nakane, Dr Daniel DePonte, Dr Sergio Carbajo, Dr Matt Seaberg, Dr Andy Aquila, Dr Sebastien Boutet, Dr Anton Barty, Prof So Iwata, Prof Steven Boxer, Prof Gerrit Groenhof

MC47: X-ray Free Electron Lasers for Condensed Matter & Materials Physics (XFELs for CMMP) II, August 22, 2022, 2:00 PM - 4:00 PM

We address the assignment of ultrafast structural dynamics that are measured using TR-SFX under typical pump-probe conditions. The femtosecond time scale motions of a fluorescent protein that undergoes photoisomerisation have both electronic ground state and excited state contributions, and require a wavepacket analysis to assign the dynamics. We apply the analysis of impulsive stimulated Raman spectroscopy and coherent control methodology to the real-space observation of low frequency vibrational dynamics and displacements, that we have measured by ultrafast X-ray crystallography. Using the 'Tannor-Rice' coherent control method it is shown that ultrafast motions can be strongly amplified. This demonstrates that the conventional pump-probe measurements, without application of optical control, are dominated by electronic ground state displacements that are unrelated to the reactive photoisomerisation coordinate. We present the first application of coherent control using X-ray crystallography in combination with coherence theory that has application to the real space wavepacket observation.

583

Novel theoretical prediction of physical properties of Fe(n+1)CdC(n) and Mn(n+1)SiC(n) (n=1, 2 and 3): ab-inition calculations.

Mr Fouad Keramsi

In this work, we have studied the magnetic stability, structural, electronic, elastic, magnetic, and thermodynamic properties of the Fen+1CdCn and Mnn+1SiCn. To realize this study, we used the linearly augmented plane wave method (FP-LAPW) based on density functional theory implanted in Wien2k code. The exchange–correlation potential is treated with the local density approximation LSDA. The formation energies were calculated for the three compounds and showed that these compounds are thermodynamically stable in a ferromagnetic spin configuration. Further analysis was done to check the mechanical and dynamical stability based on Born criteria and phonon spectra. The result shows that the increase in the stacked layer increases the rigid layer mode and the metallicity of the compounds. To understand such behavior, both analysis based on electron density and topological analysis of electron density was done. Additionally, we show that the total magnetic moment increases while the number of layers increases. The study also used the quasi-harmonic method to predict some relevant thermal properties of the three stable compounds.

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Fermion-boson interacting systems in InQuanto software package

Maria Tudorovskaya

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

To be added later

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Tunable superconducting coupling of quantum dots via Andreev bound states

Michael Wimmer, Chun-Xiao Liu, Guanzhong Wang, Tom Dvir

MC21: Bound States in Hybrid Superconductor Nanostructures I, August 22, 2022, 11:30 AM - 12:30 PM

Semiconductor quantum dots have proven to be a useful platform for quantum simulation in the solid state. However, implementing a superconducting coupling between quantum dots mediated by a Cooper pair has so far suffered from limited tunability and strong suppression. We propose to mediate tunable effective couplings via Andreev bound states in a semiconductor-superconductor nanowire connecting two quantum dots. We show that in this way it is possible to individually control both the coupling mediated by Cooper pairs and by single electrons by changing the properties of the Andreev bound states with easily accessible experimental parameters. In addition, the problem of coupling suppression is greatly mitigated. We also propose how to experimentally extract the coupling strengths from resonant current in a three-terminal junction. This proposal paves the way to implementing a minimal Kitaev chain experimentally.

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Application of Density Matrix Wigner Transforms for Ultrafast X-ray Crystallography

Sam Perrett, Jasper van Thor

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

With the advent of 4th generation light sources (XFELs), Time-Resolved Serial Femtosecond Crystallography (TR-SFX) has been a powerful tool in capturing structural molecular movies of many light-initiated processes. (1) Femtosecond optical pump, X-ray probe has allowed a new regime of coherent dynamics to be explored. The difference electron density obtained from pump-probe TR-SFX contain contributions from both ground and excited states, and are not separable as in spectroscopy. Additionally, in the sub-picosecond regime it is known from the Raman literature that coherent motion is generated in both ground and excited states, upon excitation in the Franck-Condon regime. (3) The extent to which this vibrational coherent motion is observed in difference electron density maps is unclear. (3)
Here we present a theoretical work, to model the various population and coherent dynamics of a system. The non-perturbative density matrix simulation describes the response of a system upon excitation. It is tuneable according to the parameters of the system (energy levels, dephasing, population decay...) and the conditions of the excitation (carrier frequency, pulse energy…). A Wigner Transform of the time-dependant density matrix evolving under Liouville-von Neuman equation converts to a phase space distribution (position and momentum) showing the coherent dynamics. These phase space Wigner distributions are analogous to the difference electron density maps obtained by SFX and thus can be used to ascribe the experimental observed signals.
A series of TR-SFX in the sub-picosecond regime experiments in a Tannor-Rice (pump-dump) control scheme, were used to investigate excited and ground state coherence contributions in the difference electron density maps of a fluorescent protein. It was found that a stimulated emission dumping interaction within the vibrational dephasing time drastically increased the observed signals. (4) A density matrix simulation using the proteins experimentally measured parameters, assigned the observed signals to ground state coherence enhanced by the stimulated emission dumping. Further multi-pulse excitation conditions are explored and predict the amplification of SFX signals.
Shorter optical and X-ray pulse durations (>50 fs) and increasingly more exotic pulse regimes are becoming available at FELs. Combined with high repetition of the latest FELs, improving the signal-to- noise-ratio and will allow vibronic motion to be observed on the sub-Angstrom level. Wigner transforms of the density matrix will allow analysis and assignment of the complex motion observable with developing capabilities of XFEL instruments.

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Electrical Bandgap Tuning and Spin Transport in Fully Encapsulated Bilayer Graphene Devices: Steps Towards 2D Spin Logic

Dr Christopher Anderson, Dr Victor Guarochico-Moreira, Mr Noel Natera Cordero, Mr Jesus Jesus Toscano Figueroa, Prof Irina Grigorieva, Dr Ivan Vera-Marun

MC14: Beyond Charge Transport in Nanostructures and 2D Materials via Geometric Design VII, August 24, 2022, 2:00 PM - 3:30 PM

The state variable in digital devices has been realised, to date, by measurement of charge. Spintronics offers a new paradigm to improve performance, whereby the quantum spin states of one or more electrons could be used as an alternative state variable. Improvements in transport and control of spin information are necessary for spin logic to be fully realised in graphene devices. Bilayer graphene (BLG) offers the opportunity to electrically control its bandgap[1][2][7] (Figure 1) and, as a result, the spin transport in the channel; thereby potentially enabling fabrication of a graphene based spin field effect transistor.

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Figure 1 Graphene channel resistivity as a function of carrier density and perpendicular electric field, at low temperature. Insets adapted from [1].
Figure 2 Optical image of the BLG device and schematic of its cross-section.

BLG spin transport measurements are conventionally made[3][4][7] using invasive 2D contacts which interface over the width of the graphene channel and, as such, modify the properties of the channel. This type of contact has been shown to cause spin relaxation[5] and inhomogeneous doping[6]. In contrast, our devices incorporate fully encapsulated, high quality BLG with non-invasive contacts, enabled by 1D edge contact technology (Figure 2). These only make contact with the edge of the graphene, preserving the channel's electronic properties. Figure 1 shows the resistivity change at low temperature, afforded by a perpendicular electric field (D) applied via a top gate, thus revealing the bandgap opening. Spin transport in a non-local spin valve arrangement, has been achieved in the same device and measured as a function of carrier density, revealing signals (ΔRnl) of the order of an ohm at low temperature. Similar measurements at room temperature have also been achieved. The status of our research is presented, along with an outline of future steps paving the way to electrical control of spin transport in a high quality, 1D edge contacted BLG device.

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Signatures of the nonlocal Josephson effenct in Andreev-molecules

Mátyás Kocsis

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Andreev molecules – Josephson junctions positioned closely enough to each other for entangled Andreev bound states to arise – have received much attention recently as they could have applications in quantum technologies. Such a system can be formed in InAs nanowires covered with epitaxial Al, by etching away the Al to form the junctions. In this realization quantum dots will form in the junctions, that can be tuned by local gates. As the Andreev bound states hybridize, tuning the parameters of the first junction (such as the gate voltage of the dot), we can influence the current phase relation of the second junction. This is the nonlocal Josephson effect.
We calculate what the signatures of the nonlocal Josephson effect are, what parameter regimes should be examined to observe the most robust signatures. These results will prove useful for the experimental characterization of such devices.

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Characterization of Topological Defects and Phase Transitions in Nanocrystals Ferroelectrics using coherent diffraction imaging

Dr. Xiaowen Shi, Dr. Dmitry Karpov, Dr. Wonsuk Cha, Dr. Ross Harder, Prof. Edwin Fohtung

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Topological defects are important phenomena in a wide range of research fields such as biology, physics, and materials science. The ability to control and manipulate the topological states will profoundly impact nanotechnology in general, particularly for the design and characterization of the next-generation spintronic devices, quantum computation, and information storage. High-resolution non-invasive three-dimension (3D) imaging is critical for a better understanding of their fundamental mechanisms. Conventional high-resolution electron microscopy methods perform sub-atomic resolution 3D imaging on a routine basis, however, invasive slicing/milling is needed, as a result, that might induce excessive strain on the systems, so that the specimens' native state of the energy landscape might be significantly influenced. This adds difficulties in preserving the specimens' native chemical environments. On the other hand, X-rays have a high penetration depth that allows accessing 3D volumetric information with non-invasive nature. Moreover, the non-interference of the X-rays (electromagnetic waves in general) with electric and magnetic fields enables the performance of in situ and operando imaging. Here, we will show how Bragg coherent diffractive imaging (BCDI), supplemented with Landau phase-field theory, can be implemented to study the evolution of domains with ferroelectric origin, polar vortices [1], and 1D strings [2] in individual single crystals under external electric fields. Our results demonstrate the feasibility of modulations of the topological structures with the crystallographic structural phase change primarily driven by an external electric field in ferroic materials. Reconstructions of the domain morphology, vortex core, and the corresponding energy landscape suggests the important roles topological excitations might play in manipulating and controlling both structural and electronic properties in ferroics systems. We envisage our methods can be applied to study a variety of solid state nanomaterials systems and next-generation electronic devices in which large-scale topological textures are expected to be playing major roles[3,4].

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Optically active self-organised quantum dots in marginally twisted MoSe2/WSe2 and MoS2/WS2 bilayers

Vladimir Falko

MC16: Spin Control in Twisted Van Der Waals Heterostructures V, August 23, 2022, 2:00 PM - 3:30 PM

Moiré superlattices in twistronic heterostructures are a powerful tool for materials engineering. In marginally twisted (small misalignment angle, θ) bilayers of nearly lattice-matched two-dimensional (2D) crystals moiré patterns take the form of domains of commensurate stacking, separated by a network of domain walls (NoDW) with strain hot spots at the NoDW nodes. Here, we show that, for type-II transition metal dichalcogenide bilayers MoX2/WX2 (X=S, Se), the hydrostatic strain component in these hot spots creates quantum dots for electrons and holes. We investigate the electron/hole states bound by such objects, discussing their manifestations via the intralayer intraband infrared transitions. The electron/hole confinement, which is the strongest for θ <0.5o, leads to a red-shift of their recombination line producing single photon emitters (SPE) broadly tuneable around 1.2eV by misalignment angle. These self-organised dots can form in bilayers with both aligned and inverted MoX2 and WX2 unit cells, emitting photons with different polarizations. We also find that the hot spots of strain reduce the intralayer MoX2 A-exciton energy, enabling selective population of the quantum dot states.

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Interfacial structure of the ionic liquid 1-octyl-3-methylimidazolium dicyanamide on molybdenum disulfide under an applied potential: a combined experimental and molecular dynamics study

Ms Audrey Steinberger, Ms Layla Bou Tannous, Mr Zheng Gong, Mr Paul-Henri Haumesser, Mr Anass Benayad, Mr Agilio Padua

MC10: Nanodevice Iontronics XI, August 25, 2022, 4:30 PM - 6:00 PM

Room temperature ionic liquids (ILs) can create a strong accumulation of charges at solid interfaces by forming a very thin electric double layer (EDL). They offer in addition remarkable properties such as a wide electrochemical window, a high thermal stability, a low vapor pressure, and a tunable viscosity, making them very interesting electrolytes for novel electronic devices [1,2].

Efficient field-effect transistors have been built with a 2D semiconductor channel (namely molybdenum disulfide MoS_2) gated using an ionic liquid in a configuration called an IL-FET [3]. In these devices, the charge carrier density and gating speed directly depend on the structure and dynamics of the EDL. It is therefore necessary to understand how the EDL structure evolves under an applied potential as a first step to understand the IL-FETS properties, in the aim of drawing guidelines on how to choose the IL for optimum performance.

We have studied the interfacial structure of 1-octyl-3-methylimidazolium dicyanamide ([C8C1im][DCA]) on a MoS_2 interface using atomic force microscopy (AFM) experiments and polarizable molecular dynamics (MD) simulations. This IL was chosen due to its low viscosity and large electrochemical window, making it a good candidate for FETs enhancement, and because experiments and simulations could be interestingly combined on this system. Both AFM force-distance measurements and MD simulations were performed at open circuit potential and under applied potential, and yield the number and thickness of the ionic layers in the EDL. Moreover, the experiments provide informations on the force necessary to rupture the layers, while the simulations allow a further insight into the composition of the layers and the spatial orientations of the anions and cations [4].

In this presentation, we will show and discuss our results, and conclude with an opening toward complementary X-ray photoelectron spectrometry (XPS) measurements.

Acknowlegments:
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Coherent Transport of Quantum Solitons in Superconducting Circuits

Mr Ben Blain, Dr Giampiero Marchegiani, Dr Juan Polo, Prof. Dr Luigi Amico

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Superconducting junctions constitute a promising platform for future implementation of quantum processors. Arrays of Transmon qubits naturally implement the Bose-Hubbard model, with negative (attractive) on-site interaction. Source-to-drain transport has recently been experimentally characterised in an array of Transmon qubits. In this work, we demonstrate that the transport near the ground state of such systems occurs as transmissions of a bright quantum soliton. We analyse how the transport involves specific collective bosonic excitations. Implications for the actual experimental realisations are discussed, with a focus on experimental feasibility.

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Interfacial ferroelectricity in marginally twisted 2D semiconductors studied via KPFM

Dr Elisa Castanon, Dr Astrid Weston, Dr Vladimir Enaldiev, Dr Fabio Ferreira, Dr Shubhadeep Bhattacharjee, Dr Shuigang Xu, Mr Yunze Gao, Dr Wendong Wang, Dr Matthew Hamer, Ms Harriet Read, Dr Laura Fumagalli, Dr Andrey Kretinin, Dr Hector Corte-Leon, Dr Zefei Wu, Dr Nicholas Clark, Dr Alex Summerfield, Dr Teruo Hashimoto, Professor Sarah Haigh, Dr Olga Kazakova, Professor Sir Andre Geim, Professor Vladimir Fal'ko, Professor Roman Gorbachev

MC16: Spin Control in Twisted Van Der Waals Heterostructures V, August 23, 2022, 2:00 PM - 3:30 PM

The twist (i.e. rotation) angle stablished between adjacent layers of 2D crystals has attracted a great deal of attention in recent years. By modifying the rotation between the layers, new periodicities can be obtained serving as a way to manipulate the interlayer coupling, and leading to the production of heterostructures with novel functionalities that cannot be achieved on their isolated forms [1]. With respect to the widely studied transition metal dichalcogenides (TMDCs), a recent study by Weston et al. [2] demonstrated that lattices reconstruct at small twist angles ($\theta < 2°$). In particular, twisted bilayers with the 3R stacking polytype reconstruct to form a tessellated pattern of triangular domains separated by a network of partial dislocations for twist angles between 0 and 2°(i.e. $0 < \theta < 2°$).

Here, we present our most recent results revealing that such 3R stacked twisted bilayers host spatially separated domains of opposite polarity leading to stable room temperature ferroelectricity in a material with nanometre-scale thickness [3]. We study the physical properties of the ferroelectric domains formed in 3R-MoS2 bilayers by employing two-pass phase modulated Kelvin probe force microscope (PM-KPFM) in high vacuum environments (~10^-6 mbar). PM-KPFM is a technique that allows the characterization of the contact potential difference (V_CPD) of a sample in a non-destructive and non-invasive manner, achieving spatial and electronic resolutions down to 20 nm and 20 mV, respectively. Here, as shown in figure 1 (See supporting document), no major features are observed in the topography map, while the contact potential difference map shows the presence of ferroelectric domains on top of the 3R-MoS2 homo-bilayer. Different patterns can be seen, from the triangular commensurate region highlighted in green as an inset, to areas with more irregular patterns. These differences are attributed to variations of the twisting angle between the regions as a result of the fabrication process. Besides imaging the domain structure, we employed this data to calculate quantitatively the potential difference between the domains, which resulted to be $2\Delta V = 100 \pm 20$ mV, in agreement with the theoretical calculations. Finally, manipulation of the ferroelectric domains was demonstrated by imaging with KPFM while applying varying back-gate voltages.

These results demonstrate that it is possible to fabricate and manipulate nanometre-thick heterostructures featuring room-temperature ferroelectricity, which could potentially lead to the development of novel devices with combined optoelectronic and memory functions. Furthermore, this study highlights the potential of SPM as a crucial technique to unravel and understand the physical properties of 2D materials and their related heterostructures.

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Rapid Enhancement in Spin Decoherence Due to Strong Electron Interactions and Quantum Memory Effects

Mr Tobias Boorman, Dr Bernd Braunecker

MC51: Ultrafast Dynamics in Magnetic and Strongly-Correlated Materials XI, August 25, 2022, 4:30 PM - 6:00 PM

We theoretically investigate the effect of strong electron interactions on the short time build-up of entanglement between a quantum spin and a correlated metal. Specifically, we consider the free induction decay of the spin embedded in its metallic environment as the central process of a magnetic resonance, such as NMR or EPR. The entanglement arises through non-Markovian dynamics at short initial times as the result of coherent correlations between the spin and environment, and is manifested through a rapid initial decay in the spin's expectation values. We investigate the impact of strong electron interactions within a robust analytical framework, allowing us to extract explicitly each elementary many-body decay channel for the archetypical example of a strongly correlated system, a Luttinger liquid. Within this framework we confirm the established modification of the Korringa relation, over timescales where thermal fluctuations are the dominant feature. In addition, we can cover the full range of dynamics, extending to a concise description of shorter timescales where quantum memory effects dominate. Such information could be useful for devising more appropriate quantum error correction schemes, taking into account the fast, interaction-dependent initial slip.

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Exploring possible materials for mobile qubits

Bertrand Dupé

Afternoon Break and Posters I, August 22, 2022, 3:30 PM - 4:30 PM

Although topology took a major role in the development of particle Physics, its use in condensed matter physics arrived quite recently. It was only in 2016 that Aldane, Kosterlitz and Thouless were awarded a Nobel Price in Physics for the discovery of topological phase transitions and topological phases of matter. These concepts are now in the forefront of research and are unveiling new possibilities to store and process information, transport electrical charge and spins [1].
Skyrmions are non-collinear, localized magnetic states. Their chiral properties are not only resulting in their stabilization but also at create an emergent magnetic field that exhibits a non-zero Chern number. When this emergent field is coupled to a s-type superconductor, a Majorana state may emerge in the superconductor [2,3]. In that case, the presence of the Majorana state in combination with the high skyrmion mobility allow quantum computing operations. Here, we use density functional theory (DFT) calculations to explore interplay between surface magnetism created by 3d elements and 4d/5d superconducting substrate. We project the DFT band structure on Wannier functions that we use to parametrize s a s-d tight-binding Hamiltonian [4]. Previously, we have identified the presence of in Co/Ru(0001) [5]. We use this methodology to further explore the presence of Majorana states in this system.

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623

Quantum computing: prospects and challenges

Dr. Vivien Kendon

MC36: Integrating Quantum Computers in Condensed Matter Physics Simulations IV, August 23, 2022, 11:30 AM - 12:45 PM

Quantum computing promises more efficient computation for some important types of problems, such as simulation of quantum systems, non-convex optimisation, and (famously) factoring large semi-primes. However, the first useful quantum computers will be limited in what they can do.
Applying them to bottlenecks that are hard for classical computers is key to extracting the best performance out of combined classical and quantum hardware. Interfacing different types of hardware brings many challenges, including mismatched timescales, incompatible data formats, and more complicated logic in the programme flow. The basic concepts that make quantum computing an exciting near term prospect will be explained for non-experts (avoiding the current hype), and some of the opportunities explored.

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Molecular Quantum Circuit Design

Dr. Jakob Kottmann

MC36: Integrating Quantum Computers in Condensed Matter Physics Simulations IV, August 23, 2022, 11:30 AM - 12:45 PM

A lot of effort is spend in order to identify useful design principles for the construction of parametrized quantum circuits capable of preparing good approximations to ground states of electronic systems.
This talk will introduce circuit design principles based on high-level concepts in Chemistry. In particular we will leverage information from chemical graphs by connecting them to molecular orbitals, and their representation as unitary operations. This allows the targeted construction of comparably shallow and local low-parametrized quantum circuits suitable for variational optimization and provides a promising route towards fully automatized approaches.

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Practical error mitigation by verification

Prof. Dr. Thomas O'Brien

MC36: Integrating Quantum Computers in Condensed Matter Physics Simulations V, August 23, 2022, 2:00 PM - 3:45 PM

Quantum error mitigation is an essential last step in the path towards a useful application of a quantum computer. Post-selection and purification techniques are a promising part of the error mitigation zoo. In this talk I will outline two of these techniques, symmetry verification and echo verification, and discuss their performance and practical limitations.

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The Hubbard model – Open Questions

Prof. Emanuel Gull

MC36: Integrating Quantum Computers in Condensed Matter Physics Simulations V, August 23, 2022, 2:00 PM - 3:45 PM

The Hubbard model is the simplest model of interacting fermions on a lattice and is of similar importance to correlated electron physics as the Ising model is to statistical mechanics or the fruit fly to biomedical science. Despite its simplicity, the model exhibits an incredible wealth of phases, phase transitions, and exotic correlation phenomena. While analytical methods have provided a qualitative description of the model in certain limits, numerical tools have shown impressive progress in achieving quantitative accurate results over the last years. This talk will give an introduction to the model, illustrate the progress that has been achieved over the last years in revealing various aspects of the correlation physics of the model, and delineate open physics questions

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High-resolution SPM imaging of molecules with a functionalized probe

Pavel Jelínek

MC18: Developments at the Frontiers of High-resolution Scanning Probe Microscopy I, August 22, 2022, 11:30 AM - 12:30 PM

High-resolution AFM/STM/IETS imaging of molecules acquired functionalized tips [1] created a lot of excitement among researchers from many fields including material science, physics and chemistry. Here we will briefly describe a common underlying mechanism responsible for the unprecedented AFM/STM/IETS submolecular contrast [2]. The first results were obtained using CO-tips, which became very widespread due to easy handling and the high spatial distribution. However, these tips show a weak electrostatic signal and do not allow the acquisition of magnetic contrast. Recently, other alternatives have also been used, such as a metallocene tips, which allows for magnetic contrast [3,4]. Another interesting alternative is tip functionalization with a single Xenon atom, which, thanks to its strong polarization, allows us to image the anisotropic distribution of the atomic charge [4]. We will provide some more theoretical insight into the imaging mechanism of these probes too.

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Manipulating Exciton Polariton Condensates at Room Temperature

Prof. Qihua Xiong

Semi-plenary: Professor Qihua Xiong, August 25, 2022, 10:00 AM - 11:00 AM

Recently, microcavity exciton polariton research has attracted considerable interests in a number of excellent optical gain materials that demonstrate unique properties compared with conventional III-V or II-VI semiconductor quantum wells and organic semiconductors. Those materials include transition metal dichalcogenides (TMDs), and certain halide perovskite semiconductors. Particularly, those materials exhibit large exciton binding energies (much larger than thermal fluctuation energy ~ 26 meV), large oscillator strength and peculiar electronic band structures such as valley polarization or encoded chiroptical responses. In this talk, we will discuss our recent effort in manipulating exciton polariton condensates in halide perovskite semiconductors microcavities, for instance using artificial lattices to engineer the strong optical responses including topological properties, and their ultrafast propagation. Finally, we will briefly discuss the nonlinear optical properties in monolayer TMD microcavities, by a pump-probe transient spectroscopy at momentum space. Our results demonstrate a promising perspective of polaritonics in a wide range of ultrafast optical and photonic applications at room temperature.

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Dynamics of charges, spins and phonons captured by ultrafast scanning tunneling microscopy

Sebastian Loth

MC18: Developments at the Frontiers of High-resolution Scanning Probe Microscopy II, August 22, 2022, 2:00 PM - 3:30 PM

Combining the advantages of ultrafast spectroscopy and atomic-resolution scanning probe microscopy into one tool has been a dream for quite some time. Technological progress in picosecond electronics and reliable femtosecond laser sources has now turned this dream into reality. Two methods that drastically boost the time resolution of scanning tunnelling microscopes appear particularly promising: all-electronic excitation and optical excitation by THz light. I will introduce how these methods can resolve collective dynamics of charge, spin and phonons on surfaces.
All-electronic excitation offers a versatile platform in which microwave frequency sources or arbitrary waveform generators can be used to measure stochastic [1] or coherent spin dynamics [2] at the speed of the intrinsic electron-spin scattering on surfaces. THz pump-probe spectroscopy on the other hand circumvents any bandwidth limits of cabling and directly excites the STM's tunnel junction [3]. This enables extremely high time resolution in the femtosecond range and resolves molecular vibrations [4] and phonon propagation in thin films [5].
These ultrafast STM-based techniques give direct access to fundamental processes in matter at their intrinsic time and length scale.

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Bias-induced suppression of tip relaxation and atom manipulation

Filipe Junqueira, Yi-Ying Sung, Brian Kiraly, Philip Moriarty

MC18: Developments at the Frontiers of High-resolution Scanning Probe Microscopy II, August 22, 2022, 2:00 PM - 3:30 PM

The tunnel current in the junction of a scanning tunnelling microscope (STM) is routinely exploited to drive a variety of manipulation processes at the atomic and (sub)molecular levels, generally via inelastic channels such as vibrational heating [1]. We report here instead an intriguing suppression of both atom deposition and tip relaxation induced by the application of a bias voltage during the manipulation process.

A combined STM-qPlus atomic force microscope (Unisoku USM-1300) operating at 4.2 K was used to deposit single gold atoms and small two-dimensional (typically dimers)/three-dimensional clusters on Au(111) by gentle indentation of the oscillating Au-coated tip. The tip was moved towards the surface by approximately 300 pm from the z value defined by tunnel current feedback in dynamic STM mode (i.e. with an oscillating tip; an oscillation of ~ 100 pm was used throughout). Although initial indentation events tend to produce clusters of variable size, the tip typically evolves towards a “steady state” whereby there is a high probability of single atom deposition. The inset to Fig. 1(A) shows an example of a set of atoms deposited in this way, with Fig. 1(A) itself showing an example of a Δf(z) curve that resulted in the deposition of an atom. (Other more sophisticated and artistic examples of the application of this type of technique can be found at the Nanosurf lab (Jelinek et al.) website [2].)

At a bias of -110 mV, the tip was ramped towards the surface resulting in the Δf(z) curves shown in the inset to Fig. 1(B). There is very little hysteresis for the ingoing and outgoing frequency shift curves. No change was observed in the tip state or the sample surface following this z ramp. Reducing the bias to 400 microvolts [3] leads to a significant amount of hysteresis. The form of the hysteresis was entirely reproducible down to the 100 mHz level over the course of tens of z ramps of this type.

The origin of the suppression effect will be discussed in the context of the field-driven atomic manipulation processes described in the early STM literature [4,5]. Use of qPlus AFM provides new insights into field-induced relaxation/reaction not possible via STM manipulation alone. In addition, prospects for 3D assembly of nanoclusters using this approach will be outlined.

Fig. 1(A) Inset: STM image of sixteen atoms deposited from a Au-coated STM/qPlus AFM tip onto a Au(111) surface. The graph shows the difference between the ingoing (blue) and outgoing (orange) frequency shift signals for an atom deposition event. (B) Application of a bias voltage (in this case, -110 mV, see inset) suppresses the tip relaxation seen for lower voltages.

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Multilayered Artificial Spin-Vortex Ice for Beyond-2D Reconfigurable Magnonics

Dr Jack C. Gartside, Mr Kilian Stenning, Dr Alex Vanstone, Dr Troy Dion, Ms Holly Holder, Dr Will Branford

MC44: New Perspectives in Magnonics, from 2D to 3D Systems III, August 22, 2022, 4:30 PM - 6:00 PM

Strongly-interacting nanomagnetic arrays including artificial spin ice are finding increasing use as model host systems for reconfigurable magnonics. The strong inter-element coupling allows for stark spectral differences across a broad microstate space due to shifts in the dipolar field landscape.
Recently, 'Artificial Spin-Vortex Ice' (ASVI) was demonstrated - using bistable islands which can assume macrospin and vortex states. These two magnetic textures have very different magnonic behaviours, field dispersions and resonant frequencies, with mode shifts of 3.8 GHz available between textures.

Reconfigurable magnonics is beginning to surpass the constraints of purely 2D systems and exploit the enhanced flexibility and microstate space available by exploring the z plane. ASVI is an ideal model system for this exploration. We demonstrate nanoislands with 16 possible states, and a huge field-programmable 16^N microstate space in an N-island array.

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Microwave spectroscopy of interacting spins in Andreev bound states

Mr Jaap J. Wesdorp, Mr. Arjen Vaartjes, Mr. Francisco Matute-Cañadas, Dr. Lukas Grünhaupt, Dr. Tom Laeven, Mr. Sebastiaan Roelofs, Dr. Lukas J. Splitthoff, Ms. Marta Pita-Vidal, Mr. Arno Bargerbos, Dr. David van Woerkom, Prof. Dr. Leo P. Kouwenhoven, Prof. Dr. Alfredo Levy-Yeyati, Dr. Christian K. Andersen, Dr. Bernard van Heck, Dr. Gijs de Lange

MC21: Bound States in Hybrid Superconductor Nanostructures IV, August 23, 2022, 11:30 AM - 12:30 PM

Andreev bound states are fermionic states localized in weak links between superconductors and can be occupied with spinful quasiparticles. Microwave experiments using superconducting circuits with InAs/Al nanowire Josephson junctions have recently enabled probing and coherent manipulation of a single spin-1/2 quasiparticle occupying a bound state but have remained limited to zero or small fields. Here we use a field-compatible superconducting circuit to perform spectroscopy of spin-polarized Andreev bound states in external magnetic fields up to ≈ 250 mT. We identify singlet and triplet states of two quasiparticles occupying different Andreev bound states through their dispersion in magnetic field. These states are split by the exchange interaction and couple via the spin-orbit interaction, analogous to two-electron states in quantum dots. We also show that the magnetic field allows to drive a direct spin-flip transition of a single quasiparticle when it is trapped in the junction. Finally, we measure a gate- and field-dependent anomalous phase shift of the Andreev spectrum, of magnitude up to ≈ 0.7π. Our observations demonstrate new ways to manipulate Andreev states in a magnetic field and reveal the presence of a spin-polarized triplet component in the supercurrent

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2.6 Tesla Cryogen Free Mu3e system

Dr Roger Mitchell

MC24: Quantum Electronics at Ultra-low Temperatures VII, August 24, 2022, 2:00 PM - 3:30 PM

Cryogenic Ltd has manufactured a large bore cryogen-free magnet system to enable investigations of the lepton-flavour violating decay of muons into an electron and two positrons. The magnet is installed at the Paul Scherrer Institute in Villigen, Switzerland.
The cryostat has a 1 metre room temperature bore and houses a 2.6T magnet with a base homogeneity of <0.12% over a 1.3m central region. The NbTi magnet comprises four separately powered windings. Varying the current in the windings permits subtle changes to the field profile as well as establishing a shallow gradient field along the bore.
The magnetic stray field is limited to 5mT at 1m by encasing the cryostat in a 27 tonne passive shield with overall dimensions of 2.1m diameter x 3.4m long. Access to 1m bore tube is via semicircular swing doors each weighing 0.5 tonnes.
The magnet cold mass is 1.5 tonnes and is cooled to 3.5K using four 1.5W Gifford McMahon two-stage cryocoolers. The magnet operated to full field without training. To ensure safety in operation the magnet is magnetically balanced within the iron shield using a series of load cells to monitor relative displacements between the cryostat and the shield.
The overall system footprint was subject to severe spatial restrictions imposed by the beamline architecture. Careful optimisation was necessary to achieve the critical specifications within the dimensional constraints.
The room temperature bore will house a purpose-built detector developed at PSI which is inserted via a rail system attached to the bore wall.

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Water confined in nanopores: What do we know about it and what is it good for?

Prof. Dr. rer. nat. Patrick Huber

MC7: Exploring Liquid Properties in Confined Geometry (Up To Mesoscopic Scales) VII, August 24, 2022, 2:00 PM - 3:30 PM

Water confined in pores a few nanometers across plays a dominant role in many natural and technological processes ranging from clay swelling, frost heave, and catalysis via colloidal stability and protein folding to transport across artificial nanostructures and bio-membranes. In nanoporous media the geometrical confinement and pore wall-fluid interactions as well as complex pore morphologies may significantly alter water's physico-chemical equilibrium and non-equilibrium properties, causing, for example, the molecular structuring of the fluid, huge negative Laplace pressures in the liquid and changed shear viscosities.

In the first part of my talk I will present optofluidic, X-ray and neutron scattering experiments on capillarity-driven transport, self-diffusion dynamics of water and aqueous electrolytes in nanoporous solids [1, 2] as well on the interplay of water's capillarity with the confining solids' elasticity [3, 4]. The observations on the effective, porous-medium scale will be related to the single-nanopore fluid properties [2], also by resorting to computer simulations. In the second part of my talk I will exemplify that exploiting water's peculiar nanofluidics in combination with self-organized porosity in solids offers an entirely novel design space for sustainable, active integrated materials with functional diversity. In particular, I will present porous materials with electrically switchable wettability and hydraulic permeability [5] as well as large electrochemo-mechanical actuation for potential applications in Lab-on-a-Chip fluidics, sensorics, water filtration and energy conversion [5,6,7].

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Figure : Laser-ultrasound experiment on water-infiltrated nanoporous silicon.

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Flocking fluids

Prof. Dr. Denis Bartolo

MC7: Exploring liquid properties in confined geometry (up to mesoscopic scales) VIII, August 24, 2022, 4:30 PM - 6:00 PM

We are active matter. We can walk jump and swim without relying on external drives to actuate our body. Beyond the specific case the human body, the term active matter now refers to any self-organized structure assembled from living or synthetic units independently driven far from equilibrium. In particular, inspired by the dazzling dynamics of animal groups, physicists and chemists have successfully engineered active fluids driven from within by flocks of self-propelled particles. In my talk, I will show how nearly pristine laminar flows emerge in fluids made of flocks of colloidal particles confined in microfluidic devices. Combining experiments simulations and theory, I will explain the generic mechanism that allow flocking matter to heal their topological singularities [1] and discuss the robustness of their spontaneous flows in heterogeneous environments [2].

Picture of a two-dimensional colloidal active fluid. The fluid self-organises its flow to eventually form a pristine vortex pattern. During the transient dynamics typical bow-tie patterns precedes vortical motion. Credits: A. Chardac and D. Bartolo

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The role of interstitial fluid accumulation and relocalization for embryonic axis formation in zebrafish

Ms Karla Huljev, Prof. Carl-Philipp Heisenberg

MC3: Tissue Dynamics: From in Vivo Experiments to in Silico Modelling IX, August 25, 2022, 11:30 AM - 12:30 PM

Accumulation of interstitial fluid (IF) between embryonic cells is a common phenomenon in vertebrate embryogenesis. IF has long been speculated to play a role in embryo patterning and morphogenesis, but direct evidence supporting such functions is still sparse. Here we show that the relocalization and accumulation of IF ahead of the migrating anterior axial mesendoderm (prechordal plate, ppl) is critical for ppl cell protrusion formation and migration, a key process in embryonic axis formation. We further show that ppl cell migration and IF accumulation are engaged in a positive mechanical feedback loop, where internalized ppl tissue, moving in between the epiblast and yolk cell, compress the overlying epiblast tissue, causing IF to relocate from the epiblast surface to the epiblast-yolk cell interface directly ahead of the advancing ppl. This accumulation of IF, in turn, facilitates ppl cell protrusion formation and migration by opening up the space into which the ppl moves, and thus the ability of the ppl to trigger the relocalization of IF by pushing against the overlying epiblast. Thus, embryonic axis formation relies on a positive mechanical feedback loop between tissue movement and IF relocalization.

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Collective mechanisms for cell motility in monolayers and stratified epithelia

Prof. Dr. Lisa Manning

MC3: Tissue Dynamics: From In Vivo Experiments to In Silico Modelling X, August 25, 2022, 2:00 PM - 3:30 PM

In epithelial monolayers, the collective behaviour of cells often changes over time. One example is changing tissue fluidity, where a tissue alternates between a fluid-like state where cells move and exchange neighbours rapidly and a second solid-like state where cell motion is arrested and neighbour exchange stops. An open question is how cells are altering their individual properties to achieve this collective behaviour. Several recent works have demonstrated that in some fully 3D tissues, density and rigidity percolation transitions drive the collective behaviour. Here, I will highlight our recent work suggesting that a different, cell-shape-based transition is driving collective behaviour observed in several in vivo and in vitro epithelial model systems, and discuss the different origins of the shape-based vs. density-based types of transitions. Finally, I will discuss our new work modelling stratified epithelia using shape-based methods in order to predict how heterotypic interfacial tensions interact with tissue fluidity to drive compartmentalisation and regulate self-renewal.

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Vertex model characterization of active contraction pulses in epithelial cells

Ms. Fernanda Pérez Verdugo, Prof. Dr. Rodrigo Soto

MC3: Tissue Dynamics: From In Vivo Experiments to In Silico Modelling X, August 25, 2022, 2:00 PM - 3:30 PM

Several models have been proposed to describe the dynamics of epithelial tissues undergoing morphogenetic changes driven by apical constriction pulses, which differ in where the constriction is applied, either at the perimeter or in the medial regions. To help discriminate between these models, we analyse the impact of where constriction is applied on the final geometry of the active contracted cell, using the two-dimensional vertex model. We find that medial activity, characterized by a reduction in the reference area, generates anisotropic cell shapes, whereas isotropic cell shapes are produced when the reference perimeter is reduced. When plas- ticity is included, sufficiently slow processes of medial contractile activity, compared with the characteristic times of elasticity and plasticity, cells can achieve less elongated shapes. Similarly, for perimeter activity, the highest level of contraction is achieved. Finally, we apply the model to describe the apical contractile pulses observed within the epithelial enveloping cell layer during the pre-epiboly of the annual killifish Austrolebias nigripinnis. The analysis of the cell shape changes allowed a global fit of all parameters of the vertex model, with the pulses being quantitatively captured using perimeter activity and area plasticity.

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In vitro morphogenesis of cellular tornadoes

Mr Aurélien Roux

MC3: Tissue Dynamics, From in Vivo Experiments to in Silico Modelling XI, August 25, 2022, 4:30 PM - 6:00 PM

Tissues acquire function and shape via differentiation and morphogenesis. Both processes are driven by coordinating cellular forces and shapes at the tissue scale, but general principles governing this interplay remain to be discovered. Here, we report that self-organisation of myoblasts around integer topological defects, namely spirals and asters, suffices to establish complex multicellular architectures. In particular, these arrangements can trigger localised cell differentiation or, alternatively, when differentiation is inhibited, they can drive the growth of swirling protrusions. Both localised differentiation and growth of cellular vortices require specific stress patterns. By analysing the experimental velocity and orientational fields through active gel theory, we show that integer topological defects can generate force gradients that concentrate compressive stresses. We reveal these gradients by assessing spatial changes in nuclear volume and deformations of elastic pillars. Altogether, we propose integer topological defects as mechanical organising centres controlling differentiation and morphogenesis.

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Returning to a vital planet: using thermodynamics to define sustainability.

Prof. Henrik Nordborg

Semi-plenary: Professor Henrik Nordborg, August 23, 2022, 5:30 PM - 6:30 PM

In 1615, Galileo Galilei wrote a remarkable letter bemoaning the church's attempt to control science. Today, roughly 400 years later, this letter is more relevant than ever. The current state of the world is a result of politicians ignoring science and scientists allowing themselves to be ignored. As a result, everybody is talking about sustainability without ever defining what is meant by it. Here, we give a thermodynamic definition of sustainability, introduce the concept of a vital planet, demonstrate that our planet is dying, and discuss the options for returning to a vital planet.

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Electronic topology driven by strong correlations

Prof. Dr. Silke Buehler-Paschen

Semi-plenary: Professor Silke Bühler-Paschen, August 26, 2022, 10:00 AM - 11:00 AM

Quantum matter has traditionally been classified by (quantum) phase transitions between different ordered states [1]. The past decade, however, has seen a wealth of developments in what we now call topological quantum matter. Here, the topological nature of the state – a global characteristic (e.g. a Chern number) – takes the role of the local order parameter. Whereas much progress has been made on topological insulators and on noninteracting topological semimetals, a just emerging field are strongly correlated gapless topological phases.

I will report on the recent discovery of the first such materials class, Weyl-Kondo semimetals, and the material – the heavy fermion compound Ce3Bi4Pd3 – that coined this notion [2-4]. It exhibits giant signatures of electronic topology [2,3], which are attributed to Weyl nodes pinned to the immediate vicinity of the Fermi level, giving rise to quasiparticles with ultraslow velocity [2-4]. In this system, genuine topology control can be achieved by magnetic field tuning, leading to the annihilation of Weyl nodes at moderate fields [5]. I will also discuss design strategies for further correlation-driven topological semimetals, ranging from symmetry considerations [6] to the possible role of quantum criticality and emergence [7,8].

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Realizing a minimal Kitaev chain in coupled quantum dots

Di Xu, Tom Dvir, Guanzhong Wang, Nick van Loo, Chun-Xiao Liu, Grzegorz Mazur, Alberto Bordin, Bas ten Haaf, David van Driel, Francesco Zatelli, Filip Malinowski, Jiyin Wang, Xiang Li, Sasa Gazibegovic, Ghada Badawy, Erik Bakkers, Michael Wimmer, Leo Kouwenhoven

MC21: Bound states in hybrid superconductor nanostructures VIII, August 24, 2022, 4:15 PM - 6:00 PM

Majorana bound states constitute one of the simplest examples of emergent non-Abelian excitations in condensed matter physics. A toy model proposed by Kitaev shows that such states can arise on the edges of a spinless p-wave superconducting chain. Practical proposals for its realization require coupling neighboring quantum dots in a chain via both electron tunneling and crossed Andreev reflection simultaneously. Here we demonstrate for the first time the simultaneous presence of all necessary ingredients for an artificial Kitaev chain: two spin-polarized quantum dots in an InSb nanowire strongly coupled by both elastic co-tunneling and crossed Andreev reflection. Our system can be further fine-tuned to a sweet spot where a pair of Majorana bound states is predicted to appear. In this sweet spot, the transport characteristics satisfies all accessible theoretical predictions for a Majorana bound state platform for the first time, including pairwise correlation, zero charge and the expected phase diagram. While the simple system presented here can be scaled to simulate a full Kitaev chain with an emergent topological order, it can also be used imminently to study the physics of Majorana bound states and non-abelian anyons.

Refs. arXiv:2206.08045, arXiv:2205.03458, arXiv:2110.05373, arXiv:2203.00107

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A quantum computing future for condensed matter physics

Dr Matthias Troyer

Plenary: Professor Matthias Troyer, August 23, 2022, 9:00 AM - 10:00 AM

While still in early development, quantum computing is already overturning our notions of computing. Quantum computers will be able to solve certain problems that are intractable on any imaginable classical computer. While this potential is real, quantum computers are best viewed as special purpose accelerators for specific problem classes. I will present guidelines for the most promising applications, which include quantum simulations. They promise to revolutionize condensed matter physics and materials science by allowing accurate simulation of complex strongly correlated quantum systems and the predictive modeling of materials.

Diving deeper into these applications I will review quantum algorithms for these problems and their requirements on quantum hardware. First academic simulations of quantum dynamics can be done with tens of thousands of high quality qubits. Other applications will be to finding exact ground and excited states of strongly correlated systems, and to sign-problem-free quantum Monte Carlo simulations. Realistic simulation of strongly correlated molecules or materials with a precision that is not achievable classically will require more than a million fast and high quality qubits. I will also discuss that disruptive quantum breakthroughs in computational materials science require conceptual and classical algorithmic advances in addition to the development of large-scale quantum computers.

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Slow liquid dynamics can facilitate fast equilibration of glasses

Prof. Dr. Simone Napolitano

MC7: Exploring Liquid Properties in Confined Geometry (up to mesoscopic scales) X, August 25, 2022, 2:00 PM - 3:30 PM

Thermodynamic equilibrium is rarely encountered in nature. Most of the systems with which we interact during our everyday life are, in fact, out of equilibrium and, upon time, they spontaneously evolve towards less energetic states. Importantly, such nonequilibrium kinetics are intimately coupled to molecular motion. Equilibration of supercooled liquids typically follows the structural relaxation, a process exhibiting a superArrhenius temperature dependence, with an activation energy which increases upon cooling. Theoretical frameworks merely based on the segmental relaxation cannot, however, explain how materials can fast-equilibrate when held below the glass transition temperature. In such temperature regime the equilibration mediated by the structural relaxation would, indeed, require geological times.
In this regard, a growing number of experimental observations indicate the presence of a different equilibration pathway with invariant activation energy (~ 100kJ/mol).
Here we provide strong experimental evidence on the occurrence of slow Arrhenius processes (SAPs) in the liquid response of polymers and other materials. For each system investigated a process with a constant thermal activation energy show up at timescales exceeding by far those of the structural process in the liquid state. Importantly, the activation energy of the SAPs matches that of the Arrhenius equilibration processes, which hint at a common molecular origin. Finally, we show that SAP is intimately connected to high temperature flow and drive melts and glasses towards more stable, less energetic states.

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Thermal orientation in fluids and soft matter

Prof. Dr. Fernando Bresme

MC7: Exploring Liquid Properties in Confined Geometry (Up To Mesoscopic Scales) XI, August 25, 2022, 4:30 PM - 6:00 PM

External and electromagnetic fields induce a range of non-equilibrium effects in complex fluids consisting of nanoparticle suspensions (e.g. Soret, Seebeck, Peltier effects), which can be exploited in energy conversion (thermoelectrics), analytical devices for detection of biomolecules, or nanoparticle transport and assembly. The combination of Non-Equilibrium multiscale simulations and theory has paved the way to elucidate the physical behaviour of complex fluids under external fields, showing that their response is much richer than previously anticipated. I will discuss novel thermal orientation effects in molecular liquids and suspensions, which emerge from coupling internal degrees of freedom of molecules and nanoparticles with external thermal fields. These effects open a route to manipulate particles in suspensions and induce electrostatic fields in polar fluids using heat dissipation processes.

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Ionic Gating of 2D Semiconductors

Alberto Morpurgo

MC10: Nanodevice Iontronics IX, August 25, 2022, 11:30 AM - 12:30 PM

In my talk I will discuss different classes of experiments performed in my group, in which we apply ionic gating to different 2D semiconductors. First, I will discuss in detail how ionic gating can be used as a precise quantitative spectroscopic technique, to measure band gaps of 2D semiconductors, as well as band offsets between different atomically thin materials. I will then present very recent experiments in which we succeeded to realize double gated ionic transistors, providing independent control of the accumulated charge density and of the applied perpendicular electric field. These devices allow an electric field to be applied perpendicularly to atomically thin 2D semiconductors that is so large (in excess of 3 V/nm) to completely quench the 1.6 eV band gap of bilayer WSe2. Our measurements show that, in the presence of such a large field, the conductance and valence band overlap, transforming the semiconductors in a semimetal (and possibly –according to theory –in a quantum spin Hall system). Depending on time, I will also discuss in some detail the use and the performance of solid state electrolytes for ionic gating.

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Controlling the hot electrons cooling in graphene with ionic liquid gating

Eva Pogna

MC10: Nanodevice Iontronics X, August 25, 2022, 2:00 PM - 3:30 PM

Ionic liquid gating uniquely enables one to achieve large carrier densities injection (up to ~1014cm-2) by applying relatively moderate (~V) gate voltages. Here, we apply it to tune the Fermi energy EF of large area (~1cm2) CVD grown single-layer graphene (SLG) in the range -650 to 250 meV and demonstrate unprecedented control of its ultrafast optical response [1].
The out-of-equilibrium optical properties as a function of EF are characterized by performing a transient absorption study in the near-infrared range (NIR) of an ionic liquid gated top-gate field effect transistor (FET), see Fig.1a. The pump pulse (0.8eV photon energy) photoexcites the SLG by instantaneously inducing an out-of-equilibrium charge carrier distribution which rapidly (in less than 100 fs) thermalize to hot Fermi-Dirac distributions (FD) at an elevated electronic temperature Te (~1000K). The cooling dynamics of the hot charge carriers is traced by monitoring the differential transmission (ΔT/T) of a broadband NIR probe pulse (0.729-1.240 eV photon energy) as a function of the pump-probe time delay, see Fig.1b. Our study reveals that the cooling dynamics of hot electrons can be significantly slowed down by increasing the doping, see Fig. 1b. We explain this effect by the quenching of the emission of optical phonons which is an intrinsic relaxation mechanism dominating the cooling also in high quality, low defect SLG [2]. Moreover, ionic liquid gating enables one to demonstrate that, for doping levels exceeding the Pauli blocking threshold for interband transition, SLG photoexcitation results in photoinduced absorption, causing a change of sign of the ΔT/T signal, see Fig. 1b.
The ultrafast charge carrier dynamics of SLG is crucial for its optoelectronic applications, including photodetectors, saturable absorbers, modulators and light emitters [3]. The electrostatic control of the recovery dynamics and of the sign of differential transmission, opens intriguing perspectives for applications of SLG as a tunable saturable absorber to provide tunable pulse durations or alternatively act as optical limiter.

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Integrated Proton-gated Bioelectronic Circuits using Nanowires and Nanoscale Patterned Ion-gating Elements

Adam Micolich

MC10: Nanodevice Iontronics XI, August 25, 2022, 4:30 PM - 6:00 PM

One of the central endeavours in the fields of bioelectronics and neuromorphic computing is the development of logic elements that can transduce and process ionic and electronic signals. Semiconductor nanowires have seen considerable interest for electronic device applications recently and their high surface-to-volume ratio and highly exposed conduction channel means they are very effectively gated by mobile ions external to the nanowire, e.g., a dissociable salt in a hydrated polymer matrix [1] or an ionic liquid [2]. A key challenge in such devices is scale and patterning. Nanowires have a diameter < 100 nm and typical channel length of a few □m, while most ion-gating approaches are unconstrained or at best patterned to ~100 □m using conventional approaches in organic electronics [3].

We previously demonstrated that the dominant polymeric material for ionic gating of devices, LiClO4-doped poly(ethylene oxide), can be patterned at the nanoscale using direct-write electron-beam lithography, i.e., it functions as a negative electron-beam lithography resist [4]. We used this approach to demonstrate low sub-threshold swing gating of both n-InAs [4] and p-GaAs [5] nanowire transistors, the latter within 25% of the room temperature thermal limit [5].

Motivated by the bioelectronic signal transduction challenge, we started developing nanoscale complementary circuit architectures for ion-to-electron signal transduction featuring n-InAs and p-GaAs nanowires as the electronic elements and electron-beam patterned poly(ethylene oxide) as the ionic element [6]. The transistors were on separate chips, formed into a circuit via external wiring, with gain < 1 and signal fidelity loss above 50 Hz.

To improve on this, we recently moved to Nafion as the ion-gating material, which we selected due to its high protonic conductivity. We show a method for nanoscale patterning of Nafion-gate structures with linewidths down to 125 nm that enables fully monolithic ion-to-electron transducers with DC gain > 5 and frequency response up to 2 kHz for sine wave signals. We will also discuss work to understand how the electron-beam patterning process impacts on Nafion water uptake and the resulting ionic conductivity of the patterned structures.

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Impact of ionic-gating on the memory operation of InAs nanowire FETs

Valeria Demontis, Faella Enver

MC10: Nanodevice Iontronics XI, August 25, 2022, 4:30 PM - 6:00 PM

Ion gating is emerging as a very powerful tool for tuning the electronic properties of semiconducting nanostructures and enables unique device performances when compared to conventional gating techniques, opening the way to novel applications in several fields including nanoelectronics [1,2], bioelectronics [3] and energy harvesting [4]. In this context, the study of the interaction between an electrolyte and the semiconductor nanostructure is fundamental to understand device operation and to boost the design of novel functional devices employing ion gating.
In this work, we report the impact of ionic liquid [EMIM-TFSI] on the electrical transport properties of InAs nanowires used as memory components, by employing dual gated field effect transistors (DG-FETs). To this aim, we probe the nanostructure in several ionic gate regimes by exploiting standard back-gating techniques at 150 K, when the ionic liquid is frozen and any crosstalk between the ionic gate and the back gate is ruled out. We observe a systematic shift of the threshold voltage in our DG-FETs after the immersion of the nanowire in the ionic liquid, ascribable to the adsorption of ionic species on the surface of the semiconductor. This effect, which can be further manipulated by rearranging the ionic distribution of the ionic liquid, is also found to have a strong impact on the hysteretic features observed in the transfer curves of the devices. By combining the effects on the threshold voltage and hysteresis on single nanowires, we observe that the ionic environment surrounding the nanostructure may induce noticeable improvement in the on/off ratios and level retention times in InAs nanowire-based memories (Figure 1).

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Mechanical characterisation of migrating monolayers:

a kinematic and dynamic study of Stokes flow.

Ms. Hélène Delanoë-Ayari, Ms. Mélina Durande, Mr. Guillaume Duprez, Ms. Sham Tlili, Mr François Graner, Ms. Alice Nicolas

MC3: Tissue Dynamics: From in Vivo Experiments to in Silico Modelling XII, August 26, 2022, 9:00 AM - 10:00 AM

Confluent monolayers of cells are able to polarize and flow, either under an artificial symmetry breaking (wound healing) or spontaneously when confined under certain geometries.
We propose an extensive mechanical study of such flows, and show how we can infer the rheological properties of the monolayer by simple kinematics analysis [1]. Then, we will focus on stresses measurements inside the monolayers trying to separate passive and active stresses as was proposed recently [2]. We will show that these measurements provide information on how migrating epithelia regulate their mechanical interaction with their environment.

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Figure : Stokes flow experiment for an epithelial cell monolayer on a racetrack.

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Tunable critical Casimir forces counteract Casimir–Lifshitz attraction

Falko Schmidt, Agnese Callegari, Abdallah Daddi-Moussa-Ider, Battulga Munkhbat, Ruggero Verre, Timur Shegai, Mikael Käll, Hartmut Löwen, Andrea Gambassi, Giovanni Volpe

MC19: Advances in the Casimir Force and Heat Transfer Phenomena VI, August 23, 2022, 4:30 PM - 6:00 PM

In developing micro- and nanodevices, stiction between their parts is a well-known problem [1]. It is caused by the finite-temperature analogue of the quantum electrodynamics Casimir–Lifshitz forces [2,3], which are normally attractive [4]. Repulsive Casimir–Lifshitz forces have been experimentally realized [5-9] but their reliance on specialized materials severely limits their applicability and prevents their dynamic control. Here, we experimentally demonstrate that repulsive critical Casimir forces, which emerge in a critical binary liquid mixture upon approaching the critical temperature [10,11], can be used to counteract the stiction due to Casimir–Lifshitz forces and actively control microscopic and nanoscopic objects with nanometer precision [12]. Our experimental demonstration, conducted on a microscopic gold flake suspended above a flat, gold-coated substrate immersed in a critical binary mixture, can foster the development of micro- and nanodevices by preventing stiction as well as by providing active control and precise tunability of the forces acting between their constituent parts.

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Vibrational Properties Beyond Debye Model

Dr. Dehong Yu

MC7: Exploring Liquid Properties in Confined Geometry (up to mesoscopic scales) IX, August 25, 2022, 11:30 AM - 12:30 PM

The vibrational density of states (VDOS, denoted g(ω)) is a fundamental property of solid materials, determining the specific heat and thermal transport. For over 100 years, theDebye model has served the fundamental law for our understanding of the vibrational properties of bulk solid materials which show a low energy relationship of $g(\omega) \propto \omega^2$, where ω is the frequency and g(ω) is the number of modes within an energy/frequency interval. In this presentation, I will report the recent discoveries on systems where the Debye model failed based on experimental observations using inelastic neutron scattering.

Upon the transition from solid to liquid phase, the conventional stable phonon vibration modes in solid phase are replaced by more complex instable vibrational modes, called instantaneous normal modes (INM) at the liquid state. The INMs are consequences of the intrinsic anharmonic interaction potentials among the atoms in liquid phase. Due to the complicated potential landscape, it has been very difficult to analytically describe the vibrational phonon density of states (VDOS) of liquids until very recently. Zaccone and Baggioli [1] have recently developed a theoretic model based on overdamped Langevin liquid dynamics. Distinct from the Debye law, $g(\omega) \propto \omega^2$, for solids, the model for liquids reveals a linear relationship, $g(\omega) \propto \omega$, in the low-energy region. With inelastic neutron scattering, we confirmed this model on real liquid systems including water, liquid metal, and polymer liquids. We have applied this model and extracted the effective relaxation rate for the short time dynamics for these liquids [2].

Contrastingly, when the crystalline materials are confined in nanometre scale with reduced degrees of freedom, a crossover from the Debye ω^2 scaling to an ω^3 behaviour is discovered through measurement of the VDOS of amorphous ice confined inside graphene oxide membranes using inelastic neutron scattering. The experimental observation is well reproduced by molecular dynamics simulations. Theoretically, it is shown that the ω^3 behaviour results from the geometric constraints on the momentum phase space induced by confinement along one spatial direction [3].

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Acknowledgments: DHY would like to acknowledge all coauthors listed in the references [2,3] on which the talk is based.

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Temperature and pressure effects on phase stability from theoretical modelling: application to the tin-sulphide phase space

Miss Ioanna Pallikara, Dr Joseph Flitcroft, Dr Jonathan Skelton

MC46: Structure, Dynamics and States in Matter under High Pressure VI, August 23, 2022, 4:30 PM - 6:00 PM

Computational materials modelling using first-principles techniques such as density-functional theory (DFT) is an important part of contemporary materials science. However, routine DFT calculations tend to focus on the equilibrium geometry, with additional methods required to incorporate pressure and temperature effects into theoretical models.

The phonon frequencies from the harmonic approximation (HA) enable calculation of the temperature-dependent Helmholtz free energy to predict thermal phase transitions. The presence or absence of imaginary harmonic modes in the phonon spectrum can identify “soft-mode” phase transitions where high-temperature phases are crystallographic averages over lower-symmetry minima. Finally, the quasi-harmonic approximation (QHA) includes the volume dependence of the lattice energy and phonon frequencies to calculate the Gibbs free energy as a function of temperature and pressure and enable derivation of p/T phase diagrams.

In this talk we will discuss the application of lattice-dynamics modelling to the tin sulphide system. The tin sulphides are well-known optoelectronic materials with applications including as photovoltaics, photocatalysts, and thermelectrics. The phase space is comparatively rich, comprising five known or proposed SnS monochalcogenide phases, a disulphide SnS2 and a sesquisulphide Sn2S3. This poses a challenge to experiments, as phase impurities can for example affect the performance of SnS-based PV devices.

Comparing DFT lattice energies yields an initial convex hull, providing a stability ordering of the monochalcogenides and predicting Sn2S3 to be unstable with to disproportionation. The Helmholtz energies correctly predict the experimental phase transition between the orthorhombic Pnma and Cmcm phases of SnS and identify the π-cubic phase to be a low-lying metastable phase. The phonon dispersion of Cmcm SnS shows imaginary modes, indicating a soft-mode-driven phase transition. The equilibrium rocksalt phase has imaginary modes that are found to harden under pressure. The zincblende phase of SnS proposed in several experimental studies is found to be a high-energy structure with a high proportion of imaginary modes in the phonon density of states. Finally, free energy calculations show that Sn2S3 is selectively stabilised at finite temperature due to its having a larger vibrational entropy.

A QHA study of the four (meta)stable SnS phases shows that the p/T phase diagram of SnS features only the Pnma and Cmcm phases. Pressure is found to stabilise the Cmcm phase, reducing the Pnma → Cmcm phase transition temperature, and at pressures around 11.5 GPa the imaginary modes harden to make this phase both thermodynamically and dynamically stable.

Overall, this work highlights the utility of lattice-dynamics modelling in understanding the effects of temperature and pressure on materials with complex phase spaces, and for providing theoretical predictions to inform the experimental synthesis of phase-pure samples.

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Characterising Triplet States in Organic Photovoltaic Materials

Prof Dr. Tracey Clarke

MC48: Multi-modal Characterisation of Thin Film Optoelectronics for Energy Applications V, August 23, 2022, 2:00 PM - 3:30 PM

Organic photovoltaics (OPV) are close to reaching a landmark 20% device efficiency. One of the proposed reasons that OPVs have yet to attain this milestone is their propensity toward triplet formation. However, the observation of significant triplet populations in high-performing blends suggests that the influence of triplet states may not be so simple. I will discuss two systems in which triplets are, respectively, a hindrance and a help.

Small molecule donor DRCN5T can achieve OPV efficiencies of over 10%, but it generates an unusually high population of triplets. These triplets are primarily formed in amorphous regions via back recombination from a charge transfer state, and also undergo triplet-charge annihilation. As such, triplets have a dual role in DRCN5T device efficiency suppression: they both hinder free charge carrier formation and annihilate those free charges that do form. Using microsecond transient absorption spectroscopy under oxygen conditions, this triplet-charge annihilation (TCA) is directly observed as a general phenomenon in a variety of DRCN5T:fullerene and non-fullerene blends.

Efficient charge photogeneration in conjugated polymers typically requires the presence of a second component to act as electron acceptor. A novel low band-gap conjugated polymer (PCPDT-sFCN) with a donor / orthogonal acceptor motif is examined, where the role of the orthogonal acceptor is to spatially isolate the LUMO from the HOMO. This allows for negligible exchange energy between electrons in these orbitals and minimises the energy gap between singlet and triplet charge transfer states. We employ ultrafast and microsecond transient absorption spectroscopy to demonstrate that, even in the absence of a separate electron acceptor, PCPDT-sFCN shows efficient charge photogeneration in both pristine solution and film. This efficient charge generation is a result of an isoenergetic singlet/triplet charge transfer state equilibrium acting as a reservoir for charge carrier formation. Remarkably, the free charges that form via the charge transfer state are extraordinarily long-lived with millisecond lifetimes, due to the stabilisation imparted by the spatial separation of PCPDT-sFCN's donor and orthogonal acceptor motifs. The efficient generation of long-lived charge carriers in a pristine polymer paves the way for single-material applications such as organic photovoltaics and photodetectors.

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Machine Learning in Scanning Probe Microscopy

Prof. Dr. Adam Foster

MC48: Multi-modal Characterisation of Thin Film Optoelectronics for Energy Applications IV, August 23, 2022, 11:30 AM - 12:30 PM

Machine learning methods are increasingly being applied to data challenges in Scanning Probe Microscopy (SPM). In particular, the success of deep learning in image recognition tasks has led to their application to the analysis of SPM images, especially in the context of surface feature characterisation and techniques for autonomously-driven SPM [1]. In this work, we explore the potential for using deep learning to aid in the interpretation of high resolution Atomic Force Microscopy (AFM) images, while also introducing methods to automate tip preparation and atomic manipulation.

AFM with molecule-functionalized tips has emerged as the primary experimental technique for probing the atomic structure of organic molecules on surfaces [2]. Most experiments have been limited to nearly planar aromatic molecules, due to difficulties with interpretation of highly distorted AFM images originating from non-planar molecules [3]. Here we develop a deep learning infrastructure that matches a set of AFM images with a unique descriptor characterising the molecular configuration, allowing us to predict the molecular structure directly in a few seconds on a laptop [4]. We apply this methodology to resolve several distinct adsorption configurations and conformations of molecules based on low-temperature AFM measurements. In general, we find high success rates in predicting the atomic and chemical structure of molecules, and the method can also be used for quantitative predictions of electrostatic properties [5]. This approach opens the door to apply high-resolution AFM to a large variety of systems for which routine atomic and chemical structural resolution on the level of individual objects/molecules would be a major breakthrough.

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Molecular spins as a tool for multimodal characterisation and energy-saving technologies

Prof. Dr. Sandrine Heutz

MC48: Multi-modal Characterisation of Thin Film Optoelectronics for Energy Applications VI, August 23, 2022, 4:15 PM - 5:45 PM

Polyaromatic molecules play a key role in next-generation energy devices. In addition to the low thermal budget involved in processing, their applications range from energy-harvesting in e.g. flexible solar cells, to low-energy operation in e.g. organic light emitting devices and unconventional computing. The performance of the devices is intimately linked to the structure, morphology, and spectroscopic properties of the molecular thin films. Therefore, multimodal materials characterization is paramount to developing molecular-based technologies.
This presentation will focus on using the spin of molecular thin films as both a tool to developing new technologies and as a probe for multimodal materials characterization. First, we will explore how spin can be introduced and controlled in the purely organic material pentacene, an archetypal molecular semiconductor, through photoexcitation that generates triplet excitation. Using novel thin film growth methodologies that rely on the dilution of the pentacene in a wide bandgap matrix [1], the spins can be tuned to either decay via phosphoresence, or interact to undergo fission, a process that generates two singlet excitons and can be used to increase the efficiency in solar cells. Fission, and the interaction between the spins, relies on the precise arrangement of the molecules next to one another. Using electron paramagnetic resonance (EPR) spectroscopy, it was found that while this process is most efficient for parallel molecules, longer-lived triplet-triplet interaction through the formation of quintets is obtained in herringbone conformations. [2, 3] Second, the spin in paramagnetic molecules phthalocyanines will be used as a probe for molecular orientation and aggregation in complex structures used for solar cells, where traditional diffraction techniques are not informative. [4] The potential of those materials as building-blocks in spintronic devices will also be explored.[5]

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Observation of the inverse Shapiro steps in nanoscale superconducting wires

Rais Shaikhaidarov, Kyung Ho Kim, Jacob Dunstan, Ilya Antonov, Sven Linzen, Mario Ziegler, Dmitry Golubev, Vladimir Vladimir Antonov, Evgeni Il'ichev, Oleg Astafiev

MC22: Nanoscale Fabrication of Superconducting Devices and Their Applications X, August 25, 2022, 2:00 PM - 3:30 PM

We observe sharp and clearly visible current steps In=2efn on the current voltage characteristic of the nanoscale superconducting wire exposed to microwave radiation of frequency f. The effect has been theoretically predicted more than thirty years ago, but it was elusive for the experimentalists. The current steps originate from the quantum coherent tunnelling of the so-called phase slips through the nanowire. A phase slip event occurs when a single superconducting vortex crosses the nanowire. The effect resembles that of the well-known voltage Shapiro steps in Josephson junctions, which are currently used in voltage standards. The mathematical similarity between the two effects indicates that the current standard based on phase slips can be realised in the same way as the usual voltage standard based on Shapiro steps. We discuss physics of the effect and condition for observation of the current quantisation.

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Characterising conjugated polymers by high-resolution STM imaging

Dr. Stefania Moro, Dr. Simon Spencer, Prof. Dr. Michael Sommer, Dr. Rawad Hallani, Prof. Dr. Iain McCulloch McCulloch, Prof. Dr. Giovanni Costantini

MC48: Multi-modal Characterisation of Thin Film Optoelectronics for Energy Applications VI, August 23, 2022, 4:15 PM - 5:45 PM

Conjugated polymers (CPs) are promising materials for modern organic electronics, combining structural and electronic adaptability to deliver efficient and low-cost devices.[1] The molecular-scale characterisation of conjugated polymers is, however, still unsatisfactory, as analytical techniques that can provide high-resolution information on polymers are scarce, are averaging ensemble methods and are often limited by the strong tendency towards aggregation of CPs.[2]

In this context, we report here an innovative approach to study CP, i.e. the combination of ultrahigh vacuum (UHV) electrospray deposition (ESD) with low-temperature scanning tunnelling microscopy (LT-STM).[3] This method allows for intact deposition of thermally fragile macromolecules and their characterisation molecule-by-molecule at the ultimate spatial resolution of UHV-STM, revealing the self-assembly, length distribution, sequence, and exact chemical structure of the materials.

In this talk I will demonstrate the power and versatility of ESD-STM for a variety of different systems, where the information obtained from our images has been used to investigate fundamental problems in the microscale behaviour of CPs, as to directly compare the efficiency of different polymerisation techniques, to understand the effect of different side chains on the assembly and packing of materials, and to fully characterise CPs where conventional techniques as nuclear magnetic resonance or gel chromatography cannot be fully trusted. These results show how ESD-STM can push beyond the conventional analytical limits and grants access to materials that could not have been characterised before with high levels of detail.

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Stark Discrete Time Crystal

Yevgeny Bar Lev

MC42: Broken Ergodicity and Localisation in Quantum Many-body Systems VIII, August 24, 2022, 4:30 PM - 6:00 PM

[No abstract was submitted. The conference organisers have added a list of the author's recent references]

[1] Chaos enhancement in large-spin chains
Yael Lebel, Lea F. Santos, Yevgeny Bar Lev [arXiv:2204.00018]

[2] Circular Rosenzweig-Porter random matrix ensemble
Wouter Buijsman, Yevgeny Bar Lev
SciPost Phys. 12, 082 (2022) [arXiv:2111.08031]

[3] Transport in Stark Many Body Localized Systems
Guy Zisling, Dante M. Kennes, Yevgeny Bar Lev [arXiv:2109.06196]

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Superconductivity in Magic-angle Graphene Family

Yuan Cao

MC16: Spin Control in Twisted Van Der Waals Heterostructures VI, August 23, 2022, 4:30 PM - 6:00 PM

The discovery of correlated states and superconductivity in magic-angle twisted bilayer graphene (MATBG) established a new platform to explore interaction-driven and topological phenomena. However, while multitudes of correlated phases have been observed in moiré systems, robust superconductivity has been the least common of all, only found in MATBG and more recently in magic-angle twisted tri-layer graphene (MATTG). Here, we report the experimental realisation of superconducting magic-angle twisted 4-layer and 5-layer graphene, hence establishing alternating-twist magic-angle multilayer graphene as a robust family of moiré superconductors. This discovery suggests that the flat bands shared by the members play a central role in the superconductivity. Moreover, our measurements in parallel magnetic fields, in particular the investigation of Pauli limit violation and spontaneous rotational symmetry breaking (nematicity), reveal a clear distinction between the MATBG and other structures with more than two layers, consistent with the discrepancy in their orbital response to the magnetic field. Our results expand the emergent family of moiré superconductors, providing new insight with potential implications for the design of novel superconducting materials platforms.

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Multi-modal Surface Imaging: Combining Raman, Photoluminescence and Photoluminescence Lifetime

Dr. Stephen McGurk

MC48: Multi-modal Characterisation of Thin Film Optoelectronics for Energy Applications V, August 23, 2022, 2:00 PM - 3:30 PM

Raman and fluorescence spectroscopy are frequently thought of as opposing techniques; however, both provide unique and complimentary data which can be combined to obtain greater understanding of the sample. For studies utilising the autofluorescence properties of the sample measuring both the spectral and temporal autofluorescence allows for better discrimination between endogenous fluorophores. The Raman spectrum can then be used to improve interpretation of the fluorescence data by fully resolving the chemical composition of the sample. This results in a non-destructive label-free tool which can be applied for a wide range of applications. Despite the benefits of this technique, experiments are often not performed in tandem on the same instrument or even within the same study, meaning that crucial information can be missed. Thanks to the flexible design of the RMS1000 Raman Microscope it is now possible to carry out Raman mapping, Photoluminescence (PL) mapping, and Fluorescence Lifetime Imaging (FLIM) on the same area of the sample with ease. These images can then be overlayed to generate a data rich hyperspectral image stack, where every pixel in the image contains a Raman spectrum, a PL spectrum and a lifetime decay. This can also be combined with conventional imaging methods (darkfield/ brightfield) resulting in the most comprehensive image of the sample. Using our software package Ramacle, analysis of all data types can be performed in a streamlined process allowing for rapid interpretation of these complex multi-modal data sets. In this talk we will introduce the instrumentation and software required to achieve this multi-modal data and present results on a range of materials, including 2D semiconductors, plant tissue and mineral inclusions.

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Strongly correlated states and tuneable moiré bands in TMD heterostructures

Prof. Dr. Mauro Brotons I Gisbert

MC16: Spin Control in Twisted Van Der Waals Heterostructures I, August 22, 2022, 11:30 AM - 12:30 PM

Two-dimensional materials provide a highly tunable platform to investigate strongly correlated electronic states. Their unique physical properties, combined with the ability to stack unlimited combinations of atomic layers with arbitrary crystal angle, has unlocked a new paradigm in designer quantum materials. For example, when two different monolayers are brought into contact to form a heterobilayer, the electronic interaction between the two layers results in a spatially periodic potential-energy landscape: the moiré superlattice. The moiré superlattice can create flat bands and quench the kinetic energy of electrons, giving rise to strongly correlated electron systems. In atomically thin transition metal dichalcogenides (TMDs), the wide range of highly tunable many-body interactions can be probed optically: strongly bound excitons can i) probe their immediate dielectric environment and ii) be immersed in a Fermi-sea to form Fermi-polarons affected by charge order and density (e.g. Wigner crystals and Mott insulating states). In the first part of the talk, I will briefly show the magneto-optical behaviour of excitons dressed by a Fermi sea localised by the moiré superlattice of a $MoSe_2/WSe_2$ twisted hetero-bilayer, in which we observe the ordering of both electrons and holes into stable correlated electronic states at a multitude of fractional fillings of the moiré lattice, leading to extraordinary Zeeman splittings of the exciton-polarons. In the second part of the talk, I will show the optical signatures of exciton-polarons in the presence of correlated states in a hetero-trilayer bilayer WSe_2/monolayer $MoSe_2$ moiré heterostructure, in which the energetic ordering of the moiré bands is shown to be highly tunable with applied vertical electric field, leading to the demonstration of hole transfer between correlated states in K- and Γ-derived moiré bands.

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Stiffening of an active solid

Dr Mario SANDOVAL

MC6: Emergent Phenomena in Driven Soft, Active and Biological Matter II, August 22, 2022, 2:00 PM - 3:30 PM

This work deals with the mechanical properties of an active elastic solid defined as a two-dimensional network of active stochastic particles interacting by nonlinear hard springs. It is numerically found that when activity in the system is turned on, the active solid stiffens. Interestingly, the active forces individually acting along the solid are stochastic; thus no preferred direction is imposed. This effect could be potentially used to construct novel active materials whose mechanical properties could be tuned according to their needs.

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Measuring the change in reactivity of a single molecule: Does The Bottom Effect The Top?

Jack Henry, Dr Adam Sweetman, Dr Phil Blowey

MC18: Developments at the Frontiers of High-resolution Scanning Probe Microscopy II, August 22, 2022, 2:00 PM - 3:30 PM

Decades of surface science studies on adsorbed molecules have shown the surface a molecule is adsorbed on can affect the molecule's electronic and geometric structure [1]. However, the change in reactivity of a single molecule induced by the presence of a surface has not been rigorously investigated.

The influence of molecule-substrate bonding on the interactions experienced by a scanning probe microscope (SPM) tip was investigated by studying C60 molecules adsorbed on the Cu(111) surface, using simultaneous non-contact atomic force microscopy (NC-AFM) and scanning tunnelling microscopy (STM). C60 can form distinctly different structures when adsorbed on the Cu(111) surface [2][3], two of which were utilized in this work. In the first structure, the Cu(111) surface remains relatively unperturbed. In the second, the presence of the C60 induces a reconstruction of the underlying Cu(111) surface, with the C60 molecules occupying a 7 atom vacancy. Despite this, both configurations adopt a (4x4) periodicity. This provides an ideal system to probe the effect the molecule-substrate bonding has on the physico-chemical properties of the molecule. As the molecules adsorb in the same orientation in both structures, any difference in the interaction between the SPM tip and the C60 molecules can be attributed to differences in the molecule-substrate bonding. The difference in the molecular-substrate bonding caused by the Cu(111) surface reconstruction has been well documented, through both experimental and computational studies [2][4][5][6].

In this work, the physico-chemical properties of C60 molecules (in different adsorption structures) were investigated using NC-AFM force spectroscopy, through comparing the minima in collected force spectra. Complementary ab initio simulations of the spectra were performed DFT in to gain a deeper understanding of the experimental results.

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Self-Propulsion, Evaporation, and Encapsulation Dynamics of an Aqueous Micro-drop over a Deformable Viscoelastic Liquid Film

Mr Sri Ganesh Subramanian, Prof Sunando DasGupta

MC7: Exploring liquid properties in confined geometry (up to mesoscopic scales) VIII, August 24, 2022, 4:30 PM - 6:00 PM

The process of evaporation is ubiquitous in nature and is relevant to several engineering applications. Specifically, the fundamental aspects of droplet evaporation have been studied for over a century, yet our understanding of the complex attributes pertaining to the evaporation of an aqueous droplet atop a viscoelastic liquid substrate remains nebulous. Herein, the dynamics of a liquid droplet evaporating on a viscoelastic liquid film is presented. The study explores the self-propulsion of the droplet, encapsulation of a minute quantity of water by the polymer and the associated wrinkling of the polymeric film. We will discuss how the coupling between evaporation and viscoelasticity drives droplet self-propulsion and present a model of the evaporation-induced, dynamic variation in both the radius and contact angle of the droplet. Finally, we will describe how the crumpling of the polymeric film and encapsulation are a result of the complex interplay between capillary forces and the viscoelasticity of the substrate. We conjecture that the present study would serve as a fundamental basis for the development of novel droplet-based systems which could find applications in precision drug delivery, spray painting, and lab-on-a-chip systems, to name a few.

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Flexible, stretchable and healable bioelectronics

fabio Cicoira

MC10: Nanodevice Iontronics VII, August 24, 2022, 2:00 PM - 3:30 PM

Organic electronics, based on semiconducting and conducting polymers, have been extensively investigated in the past decades and have found commercial applications in lighting panels, smartphone and TV screens using OLEDs (organic light emitting diodes). Many other applications are foreseen to reach the commercial maturity in future in areas such as transistors, sensors and photovoltaics. Organic electronic materials, apart from consumer electronics, are playing a central role in a myriad of novel applications that are becoming ubiquitous in our society, such as artificial muscles, electronic skin, prosthetics, smart textiles, rollable/foldable displays and biomimetics. Progress in these fields comes after decades of intense research and development in materials science and engineering, which have resulted in materials combining properties that are often mutually exclusive. For instance, materials showing high flexibility/stretchability, self-healing electronic/ionic conductivity, enhanced optoelectronic performance are now a reality. Another flourishing field is that of organic bioelectronics, where devices such as conducting polymer electrodes are used for recording and stimulating neural, muscular and nerve activity. In such applications, organic polymers are very attractive candidates due to their distinct properties of ionic/electronic conduction, which leads to a lower impedance at the electrode/tissue interface, oxide-free interfaces, tunable mechanical properties, which allow films to be deposited on irregular surfaces and tunable surface chemistry, which permits to promote or hinder the adhesion of biomolecules. These features can be particularly useful for enhancing the performance and the biocompatibility of implantable electrodes and other biomedical or wearable devices. My talk will deal with processing and characterization of conducting polymer films and hydrogels and devices for flexible, stretchable and healable electronics as well as for implantable electrodes. I will particularly focus on micro-patterning of conducting polymer films for flexible and stretchable devices, on processing strategies to fabricate stretchable and self-healing conductors, on the fabrication and characterization, in vitro and in vivo, of electrodes for deep brain stimulation, electromyography and electrocardiogram .[1-9]

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Ionic Gating for Clean Quantum Phases in 2D Materials

Jianting Ye

MC10: Nanodevice Iontronics XII, August 26, 2022, 9:00 AM - 10:00 AM

Ionic gating has been an effective way to dope high-density carriers that can then induce quantum phase transition like gate-induced superconductivity. Especially, the combination of a strong gating effect with the unique band structure in TMDs gives rise to rich physical phenomena. High field measurements have established both Ising superconductivity [1] and insulating phases at high gating due to gate-induced inhomogeneities [2]. Recently, we have worked on the opposite side of the story, namely, by using the same method of ionic gating for low-density doping to create a high mobility 2DEG that could be promising for observing the quantum Hall effect (QHE). This talk will briefly introduce the recent methodology for accessing high mobility carriers using techniques such as photo-assisted ionic doping [3]. Furthermore, we can demonstrate the clean quantum state that could be accessed as a clean superconducting state with a mean free path longer than the coherent length [4] and the QH states of 2DEG in TMDs approaching the quantum limit.

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RF reflectometry of a graphene Josephson junction

Christian Schoenenberger, Roy Haller, Gergö Fülöp, David Indolese, Joost Ridderbos, Lukyi Cheung, Jann Ungerer, Pauli Virtanen, Rainer Kraft, Detlev Beckmann, Romain Danneau, K Watanabe, T aniguchi

MC23: Superconducting Circuits for Quantum Technologies III, August 22, 2022, 4:30 PM - 6:00 PM

Gate-tunable Josephson junctions embedded in a microwave environment provide a promising platform to in-situ engineer and optimize novel superconducting quantum circuits. The key quantity for the circuit design is the phase-dependent complex admittance of the junction, which can be probed by sensing an rf SQUID with a tank circuit. Here, we investigate a superconductor-graphene-superconductor junction as a prototype gate-tunable Josephson junction (JJ). The JJ is embedded in a SQUID loop that is inductively coupled to a superconducting resonator operating at 3 GHz. With a concise circuit model that describes the dispersive and dissipative response of the coupled system, we extract the phase-dependent junction admittance corrected for self-screening of the SQUID loop. We decompose the admittance into the current-phase relation and the phase-dependent loss and as these quantities are dictated by the spectrum and population dynamics of the supercurrent-carrying Andreev bound states, we gain insight to the underlying microscopic transport mechanisms in the junction. We theoretically reproduce the experimental results by considering a short, diffusive junction model that takes into account the interaction between the Andreev spectrum and the electromagnetic environment, from which we estimate lifetimes on the order of 10 ps for out-of-equilibrium populations.

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Quantum Computing for Chemistry and Materials Science: Outlook and Opportunities

Dr Phalgun Lolur

MC36: Integrating Quantum Computers in Condensed Matter Physics Simulations VI, August 23, 2022, 4:30 PM - 6:00 PM

As we approach the limitations of conventional computing, quantum computing offers a hope for an alternate and more efficient way of solving certain types of problems. From the very onset of the field, quantum computing is expected to provide an advantage in simulating many body physics of quantum systems. This is of interest to several problems within physics, chemistry, materials science, and beyond. I will introduce the National Quantum Computing Centre (NQCC) and its application discovery program SparQ, aimed at uncovering and developing early use-cases for quantum computing. You will hear how you can engage with the NQCC in driving research and innovation forward. I will also highlight the prospects of quantum computing for chemistry and materials science simulations, along with the limitations in the current noisy intermediate-scale quantum (NISQ) computing era.

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