

The Joint 28th AIRAPT and 60th EHPRG International Conference 2023

Programme

Monday 24 July 2023

Time	Room	Programme
8:15am to 8:45am	Lennox	Registration and Arrival Refreshments
8:45am to 9am	Lennox	Opening Ceremony
9am to 9:50am	Lennox	Plenary I Eva Zurek: Chemically Complex Light-Element Superconductors from First-Principles Theory
9:50am to 10:15am	Lennox	Morning Break
10:15am to 12:15pm	Lennox	Hydrides 1 (Session Chair: Stan Tozer) 10:15am - 10:45am Lilia Boeri: Ab-initio design of high-Tc conventional Superconductors: how far is room-temperature Superconductivity? 10:45am - 11:15am Hanyu Liu: High superconductivity in light-element systems under high pressure 11:15am - 11:30am Taner Yildirim: High-throughput search and discovery of near-room temperature superconductors under extreme pressures 11:30am - 11:45am Siyu Chen: Strong-correlation effects in high-pressure rare-earth superhydrides 11:45am - 12:00pm Lewis Conway: Accelerating the Prediction of High-Pressure Hydrides Using Data Derived Potentials 12:00pm - 12:15pm Changqing Jin: New Polyhydride Superconductors
	Lowther	Phase Diagrams - Ionic Systems (Session Chair: Kamil Dziubek) 10:15am - 10:45am Arthur Haozhe Liu: High pressure phase transitions studies using synchrotron X-ray techniques 10:45am - 11:15am Marion Harmand: Tracking phase transitions of Fe ₂ O ₃ at planetary interiors conditions 11:15am - 11:30am Anja Rosenthal: The densities and phase transformations of subducted hydrous oceanic crust up to the Earth's transition zone: Insights from in-situ x-ray diffraction measurements 11:30am - 11:45am Renata Wentzcovitch: PBE-GGA predicts the B8↔B2 phase boundary of FeO at Earth's core conditions
	Menteith	Multifunctional Materials (Session Chair: Yogesh Vohra) 10:15am - 10:45am Catalin Popescu: Cooling and energy conversion via pressure in barocaloric materials 10:45am - 11:00am Francesco Capitani: Metastable liquid-like CO ₂ confined in a mesoporous Metal-Organic Framework at high-pressure 11:00am - 11:15am Josu Sánchez-Martín: High-pressure Structural Stability of Ni ₃ V ₂ O ₈ and Co ₃ V ₂ O ₈ : Raman and Infrared Spectroscopy (Ni, Co) and X-ray diffraction (Co) studies 11:15am - 11:30am Xiaodong Yao: Anomalous polarization enhancement in a vdW ferroelectric material under pressure

	Lammermuir	<p>Ice, Water and Clathrates (Session Chair: John Loveday)</p> <p>10:15am - 10:45am Katrin Amann-Winkel: Water & amorphous ice: using X-rays to map the phase diagram</p> <p>10:45am - 11:15am Rachel J. Husband: XFEL heating of low Z materials: a new pathway to superionic ice</p> <p>11:15am - 11:30am Fernando Izquierdo-Ruiz: Molecular replacement in Clathrate Hydrates</p> <p>11:30am - 11:45am Ciprian Pruteanu: Non-random fluid mixtures, present and future: the case of methane and water</p> <p>11:45am - 12:00pm Gunnar Weck: Phase diagram of hot dense superionic ice probed by synchrotron X-ray diffraction</p> <p>12:00pm - 12:15pm Choong-shik Yoo: Superionic Phases of H₂O and H₂O-He at High Pressure-Temperature Conditions: Structure, Bonding and Transition Mechanisms</p>
	Moffat	<p>Magnetic Materials 1 (Session Chair: Jing Song)</p> <p>10:15am - 10:45am Wenli Bi: High-pressure effect on candidate Dirac materials EuMnPn₂ (Pn = Sb, Bi)</p> <p>10:45am - 11:00am Shiyu Deng: Pressure tuning and Evolution of Structural, Magnetic and Electronic Properties in TMPX₃ van-der-Waals Compounds</p> <p>11:00am - 11:15am Mohamed Zayed: Neutron scattering study of SrCu₂(BO₃)₂ under high pressure</p> <p>11:15am - 11:30am Angel M. Arevalo-lopez: High-pressure ilmenite-type MnVO₃: crystal and spin structures in the itinerant-localized-covalent regimes</p> <p>11:30am - 11:45am Zheng Deng: Giant Exchange Bias Induced by Few Oersteds in a High-Pressure Stabilized Double Perovskite Y₂NiIrO₆</p>
12:15pm to 2pm	Lennox	Lunch
1pm to 2pm	Lowther	<p>Meeting: "Women Under High Pressure" group</p> <p>Shanti Deemyad will lead this session, introducing the goals and direction of "Women in high pressure".</p> <p>Then successful scientists will share with the audience about their trajectories: Sakura Pascarelli, Chrystele Sanloup, Eva Zurek, Laura Henry. Followed by an open discussion</p>
2pm to 4pm	Lennox	<p>Cores of Terrestrial Planets (Session Chair: Guillaume Morard)</p> <p>2:00pm - 2:30pm Chris McGuire: In-situ X-ray diffraction of laser-shock compressed binary compounds at Megabar pressures</p> <p>2:30pm - 2:45pm Anatoly Belonoshko: Experimental evidence for the high-PT body-centered cubic Fe</p> <p>2:45pm - 3:00pm Efim Kolesnikov: Development of strength and texture in hexagonal Fe-Si-C alloy at planetary cores conditions</p> <p>3:00pm - 3:15pm Tetsuya Komabayashi: Chemical thermodynamics of Earth's core materials under high pressure</p> <p>3:15pm - 3:30pm Susanne Müller: Effect of carbon on sound velocities of iron alloys and compounds at Earth's inner core conditions</p> <p>3:30pm - 3:45pm Ian Ocampo: In situ x-ray diffraction of iron oxides dynamically loaded to multi-megabar pressures</p> <p>3:45pm - 4:00pm Jac Van Driel: Composition of the Martian Core</p>

	Lowther	<p>Chemical Bonding 1 (Session Chair: Paul Attfield)</p> <p>2:00pm - 2:30pm Stefano Racioppi: Core-Electrons Chemical Bonding. Redefining the Chemistry of the Elements at High Pressure</p> <p>2:30pm - 3:00pm Hussien H. Osman: Mechanism of electron-rich multicenter bonding in elemental crystals under pressure</p> <p>3:00pm - 3:15pm Francisco Javier: High pressure studies in compounds with multicenter bonds</p> <p>3:15pm - 3:30pm Madhavi Dalsaniya: Theoretical investigation on the reactivity of fluorine and bromine at high pressure: emergence of novel bromine fluorides</p> <p>3:30pm - 3:45pm Michael Pravica: Inner shell chemistry at extreme conditions</p> <p>3:45pm - 4:00pm Alhaddad Toni: Exceptional phonon point versus free phonon coupling in Zn-based semiconductor mixed crystals under pressure</p>
	Menteith	<p>Nitrides, Borides and Carbides 1 (Session Chair: Dominique Laniel)</p> <p>2:00pm - 2:30pm Maxim Bykov: High-pressure synthesis of binary and ternary polytrides in laser-heated diamond anvil cells</p> <p>2:30pm - 3:00pm Florian Trybel: Ultra-high complexity of synthesized meta-stable nitrides</p> <p>3:00pm - 3:15pm Julio Pellicer-Porres: BN under high pressure revisited</p> <p>3:15pm - 3:30pm Altair Soria Pereira: Exploiting the reduction of Si melting temperature for the production of boron carbide-based composites under high pressure</p> <p>3:30pm - 3:45pm Hitoshi Yusa: High-pressure synthesis of light lanthanide dodecaborides (RB₁₂) : Synthesis condition, valence fluctuation and bulk moduli</p> <p>3:45pm - 4:00pm Matteo Ceppatelli: Synthesis of single-bonded cubic AsN from the high-pressure and high-temperature chemical reaction of arsenic and nitrogen</p>
	Lammermuir	<p>Developments at XFELs & Lasers (Session Chair: Jon Eggert)</p> <p>2:00pm - 2:30pm Laura Robin Benedetti: Progress in Time-Resolved X-ray Diffraction with Laser Compression at the National Ignition Facility (NIF)</p> <p>2:30pm - 3:00pm R. Stewart McWilliams: Design of Static High Pressure Experiments at Free Electron Lasers</p> <p>3:00pm - 3:15pm Samantha Clarke: In situ X-ray diffraction of TATB on NIF</p> <p>3:15pm - 3:30pm Nicolas Jaisle: Finite Element Method applied to MHz X-ray diffraction in Diamond Anvil Cell</p> <p>3:30pm - 3:45pm James McHardy: Exploring hard X-ray free electron laser energy deposition through target imprinting</p> <p>3:45pm - 4:00pm Orianna Ball: Dynamic Optical Pyrometry of Static High-Pressure Targets under X-ray Free Electron Laser Radiation</p>
	Moffat	<p>Ceramics and Composites (Session Chair: Shrikant Bhat)</p> <p>2:00pm - 2:30pm Bo Xu: Heterogeneous Diamond-cBN Composites with Superb Toughness and Hardness</p> <p>2:30pm - 2:45pm Fang Peng: Study on Stress, Strain and Densification of Superhard Materials and Ceramics during High Pressure Sintering</p> <p>2:45pm - 3:00pm Tao Liang: Mechanical properties of high-pressure synthesized hexagonal silicon</p> <p>3:00pm - 3:15pm Volodymyr Svitlyk: Extreme Zr-based synthetic phases for the safe disposal of nuclear waste</p>
4pm to 4:30pm	Lennox	Afternoon Break

4:30pm to 6:30pm	Lennox	<p>Hydrides 2 (Session Chair: Eva Zureck)</p> <p>4:30pm - 5:00 pm Ion Errea: Superhydrides on a quantum energy landscape</p> <p>5:00 pm - 5:30 pm Stanley Tozer: A substituted La-based 556 K Tc superhydride superconductor</p> <p>5:30 pm - 5:45 pm Graeme J Ackland: Hydrogen molecules in competition with superconductivity</p> <p>5:45 pm - 6:00 pm Hongbo Wang: High-Tc superconductivity in clathrate calcium hydride CaH₆</p> <p>6:00 pm - 6:15 pm Mikhail Kuzovnikov: Synthesis of novel rubidium superhydrides under high pressure</p> <p>6:15 pm - 6:30 pm Tomas Marqueno: Na-W-H and Na-Re-H ternary hydrides at high pressures</p>
	Lowther	<p>Chemical Bonding 2 (Session Chair: Paul Attfield)</p> <p>4:30 pm - 5:00 pm Kuo Li: Threshold distance of topochemical polymerization</p> <p>5:00 pm - 5:15 pm Samuel Dunning: Diamond Nanothreads: Controlling Solid-State Reactivity via Reaction-Directing Heteroatoms</p> <p>5:15 pm - 5:30 pm Abdelmajid Elmahjoubi: High-pressure Raman scattering and X-ray diffraction study of the highly-mismatched ternary semiconductor alloy Cd_{1-x}BexTe (x≤0.11)</p> <p>5:30 pm - 5:45 pm Alvaro Lobato: Enhancing thermoelectric power in skutterudites by tuning chemical interactions under pressure</p> <p>5:45 pm - 6:00 pm Piotr Rejnhardt: Deuteration-enhanced Negative Thermal Expansion and Negative Area Compressibility in a 3-Dimensional Hydrogen Bonded Network</p> <p>6:00 pm - 6:15 pm Szymon Sobczak: Structural and Electronic Insights Into the Role of Anagostic Bonds in Metal Dithiocarbamate Complexes</p>
	Menteith	<p>Minerals Under High Pressure (Session Chair: Tetsuya Komabayashi)</p> <p>4:30pm - 5:00pm Samu Ishizawa: Melting experiment of MgO under high pressure by in situ time-resolved X-ray diffraction measurement with Bayesian estimation method</p> <p>5:00pm - 5:15pm Yanbin Wang: Simultaneous measurements of ruby shift and unit cells of NaCl and Au in a diamond-anvil cell: new constraints on pressure scales to 20 GPa</p> <p>5:15pm - 5:30pm Christoph Otzen: Lamellar amorphization in quartz and its relation to the formation of a rosielite-structured high-pressure phase of silica</p> <p>5:30pm - 5:45pm Yunhua Fu: Analysis of hydrogen concentration in anorthite from angrite by developed micro-NMR technique</p> <p>5:45pm - 6:00pm Taku Tsuchiya: Effects of light elements on the water partitioning between liquid metal and molten silicate under high pressure and temperature</p>
	Lammermuir	<p>Facility Development 1 (Session Chair: Sakura Pascarelli)</p> <p>4:30pm - 5:00pm Olivier Mathon: Static and dynamic high-pressure opportunities at ESRF XAS beamlines BM23 and ID24</p> <p>5:00pm - 5:30pm Ioannis Tzifas: Novel High-Pressure Irradiation Platform at GSI: Investigation of structural modifications under extreme conditions</p> <p>5:30pm - 5:45pm Jesse Smith: Overview of beamline 16-ID-B of the High Pressure Collaborative Access Team at the Advanced Photon Source</p> <p>5:45pm - 6:00pm Nenad Velisavljevic: Overview of High-Pressure Collaborative Access Team (HPCAT) facility at the Advanced Photon Source at Argonne National Laboratory</p> <p>6:00pm - 6:15pm Helen Walker: Developments in measuring collective excitations using inelastic Neutron Scattering under pressures up to 8kbar</p> <p>6:15pm - 6:30pm Yusheng Zhao: Integrated Neutron Diffractometer at Extreme Conditions (INDEC) at China Spallation Neutron Source (CSNS)</p>

	Moffat	<p>Nanoscale Systems (Session Chair: John Proctor)</p> <p>4:30 pm - 5:00 pm Zhidan Zeng: Preservation of high-pressure materials in nanostructured diamond capsules</p> <p>5:00 pm - 5:15 pm Alexander Soldatov: Response of a few-layer graphene to high shear stress</p> <p>5:15 pm - 5:30 pm Beatrice D'Alò: High-pressure photoluminescence study of monolayer TMDs: an extensive investigation of the role of defects induced by sample/substrate interaction</p> <p>5:30 pm - 5:45 pm Riccardo Galafassi: Investigation of environment and substrate roles on high pressure tuning of graphene properties</p> <p>5:45 pm - 6:00 pm Camino Martín-Sánchez: Monitoring gold nanoparticles at high pressure through in situ small-angle x-ray scattering</p> <p>6:00 pm - 6:15 pm Christopher Schröck: Swift heavy ion irradiation of bismuth nanowire networks pressurized in diamond anvil cells</p> <p>6:15 pm - 6:30 pm Marina Teresa Candela: Cubic $(Eu_{1-x}Y_x)_2O_3$ nanophosphors under compression: a joint structural and spectroscopic study</p>
6pm to 8pm	Organiser's Room	AIRAPT Committee Meeting
6:30pm to 8pm	Lennox	Cocktail Reception