Excitonic Insulator Phases in 2D Transition Metal Dichalcogenides: The Case of Monolayer WTe_2 as an Excitonic Spin Density Wave

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Two-dimensional transition metal dichalcogenides (TMD) monolayers are in the spotlight as candidates for the long-sought 'excitonic insulator' (EI) phase [1], where electrons and holes bound by Coulomb attraction—excitons—spontaneously form at equilibrium and break the pristine symmetry of the crystal through Bose-Einstein condensation. We have previously shown [2-4] how strong exciton binding can exist even in TMDs with very small band gap, as screening is quenched owing to the reduced dimensionality, thus exceeding the band gap and leading to instability.

Within this vibrant research field, here we focus especially on the case of WTe_2. We have recently demonstrated that the two-dimensional bulk of monolayer WTe_2 contains excitons that spontaneously form at equilibrium [2]. The natural paradigm to interpret its ground state is the formation of the EI phase. Since lowest-energy excitons have finite momentum, one expects the EI to break the periodicity of the crystal, but no charge order has been observed at low temperature [2,5]. Our theoretical description, based on a full microscopic theory that builds on the ab-initio treatment of excitons [2-4,6], indicates that the strong spin-orbit interaction of WTe_2 largely enhances the splitting between spin singlet and triplet excitons, thus stabilizing the spin order and leading to the EI as spin density wave. We further discuss the consistency of the computed band structure, photoemission spectra, and chemical potential of the EI with available experimental data. Finally, we propose paths to unveil the macroscopic quantum coherence possibly hidden in the ground state.

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References

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