Title: Tuning and understanding Quantum phases in 2D materials - Quantum2D

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Project coordinator: F. Mauri (University of Rome La Sapienza)

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Project objectives. Recent advances in field-effect doping and material exfoliation have made it possible to tune the density of the 2D electron gas in atomically-thin layers of transition-metal dichalcogenides (TMDs). The proximity within the same system of different electronic phases, such as superconductivity (SC) and charge density waves (CDW), holds an enormous potential for the realization of new devices, while the reduced dimensionality brings novel opportunities for their optimization and control. Layered TMDs are an ideal playground for analyzing the interplay between competing SC and CDW in tunable 2D systems. Depending on their chemical composition and structural configuration, they may display metallic, semimetallic and semiconducting behaviors. Controllable, large-scale, and uniform atomic layers of diverse TMDs are nowadays feasible; moreover, their band structure can be tuned by mechanical strain, the Fermi level by gating and the spin-orbit interaction by changing the transition metal. Nonetheless, a comprehensive understanding of SC, CDW and of their mutual interaction in ultrathin TMDs is still lacking, while the experimental information on field-effect doping and spectroscopic responses both in the normal and broken-symmetry phases is still limited.

The project aims at combining the most advanced theoretical and experimental tools available in our team in order to assess the still open questions in the field: How is the band structure modified under doping/strain? How does this influence the SC and CDW phases? What is the role of electron-electron and spin-orbit interaction? The predictive power of ab-initio methods and field-theory approaches will be tested by tuning the electronic phases via electrochemical gating and mechanical strain in samples optimized for transport and spectroscopic investigation. The closed feedback loops between theory and experiments will provide a comprehensive description of electronic and structural ordering in ultrathin TMDs, paving the way for the optimization of the physical properties of tunable 2D materials.



Ion-gated field-effect device realized at Polytechnic of Turin on a MoS₂ flake, with contacts for four-probe magnetotransport measurements and the gate electrode.



Schematic phase diagram of electron-doped semiconducting TMD, as MoS_2 , including SC and CDW phases and the boundary between electrostatic doping and ion intercalation.