

Spin and Valley Control in Transition Metal Dichalcogenides

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Layered transition metal dichalcogenides (TMDCs) constitute a large materials class characterized by a crystal structure in which stacks of covalently bonded, atomically thin sheets are held together by weak van der Waals interactions. The class of materials is diverse, from the standpoint of its electronic properties, with band structures ranging from insulating to metallic. In the “two-dimensional” limit of a single atomically thin sheet, many of the fundamental properties of the bulk crystal persist. However, at the same time, important differences arise; these are the result of several factors, among which quantum confinement and reduced symmetry are important. Also, substrate interactions can be crucial for a single layer (SL) in a realistic device architecture.

In group-VI semiconducting TMDCs such as MoS₂ and WS₂, there are important differences between the band structures of the bulk and the SL, for the reasons described above, and these differences have dramatic implications for the materials’ optical properties. While the bulk crystals are indirect-bandgap semiconductors, the bandgap in the SL is direct, with the conduction band minimum and the valence band maximum occurring at the K and K’ points (the K and K’ “valleys”) of the two-dimensional hexagonal Brillouin zone. The fact that these materials possess direct bandgaps makes them particularly interesting for “post-Si” technologies, and it means that they interact strongly with light. The particular symmetries of the SL imply that the K and K’ points are inequivalent to one another: they are both spin-split, with the splitting at K being opposite to that at K’. The fact that electrons can occupy either of these two inequivalent valleys can be understood in terms of a valley pseudospin degree of freedom. Importantly, optical selection rules allow valley-specific excitation of free electron-hole pairs using circularly polarized light. Thus, one can envision “valleytronic” devices based on the manipulation of valley occupancy, in contrast with traditional electronic devices based on manipulation of electronic charge.

In this talk, I will discuss spin and valley physics in two-dimensional semiconducting TMDCs. I will give an introduction to the angle-resolved photoemission spectroscopy (ARPES) technique, and I will discuss how we use ARPES as a tool to understand the electronic structure of these materials.