

Novel structural and electronic phases of 2D transition metal dichalcogenides

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Layered transition metal dichalcogenides (TMDs) of chemical composition MX_2 (M = transition metal; X = S, Se, or Te) represent a broad family of materials with diverse electronic properties, including metals, insulators, as well as more complex states such as the charge-density-wave (CDW) and superconducting phases. More recently, the possibility of realizing single- and few-layer TMDs has brought the two-dimensional (2D) forms of these materials into the spotlight of prospective application in electronics, optoelectronics and beyond [1]. In my talk, I will review the “periodic table” of TMDs attempting to reveal systematic trends and develop chemical intuition across this family of 2D materials. Using a Wannier function approach, I will address the relevance of the crystal and ligand fields in determining the relative stability of 1T and 1H polymorphs as a function of the filling of the d-shell in 2D TMDs [2]. Then, I will present a unified picture of lattice instabilities in metallic TMDs that describes both the CDW phases and the strong-coupling scenario resulting in the formation of metal-metal bonds (as e.g. in the dimerized 1T' phases) [3]. In the rest of my talk, I will focus on topological and magnetic phases of TMDs. The 1T'-phase of Mo and W TMDs that have recently been shown to host the topologically non-trivial quantum spin Hall (QSH) insulator phase. The robustness of the QSH phase as well as the topological edge states [4] and interface states at the well-ordered 1T'-1H lateral heterojunctions will be discussed in conjunction with recent experiments on 1T'-WSe₂ [5]. I will also cover our recent discovery of magnetic ordering and magnetoresistive switching in metallic few-layer and insulating single-layer PtSe₂ [6,7].

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