Phase Engineering in 2D Transition Metal Dichalcogenides

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Two-dimensional transition metal dichalcogenides (2D TMDs) — whose generalized formula is MX_2, where M is a transition metal of groups 4–7 and X is a chalcogen — exhibit versatile chemistry and consist of a family of over 40 compounds that range from complex metals to semiconductors to insulator. Complex metal TMDs assume the 1T phase where the transition metal atom coordination is octahedral. The 2H phase is stable in semiconducting TMDs where the coordination of metal atoms is trigonal prismatic. Unlike mechanical exfoliation and chemical vapor deposition, chemical exfoliation of semiconducting layered TMDs yields monolayered nanosheets with heterogeneous atomic structure consisting of metallic (1T) and semiconducting (2H) phases (Figure 1). Metal (1T phase) to semiconductor (2H phase) transition can be achieved via mild annealing of exfoliated materials. Semiconductor to metal transitions can be achieved via chemistry. The 1T phase in *semiconducting* TMDs has scarcely been studied but it deserves urgent attention as it exhibits promise as a hydrogen evolution catalyst and as contact electrode in electronic devices. We will describe these phase transitions in semiconducting TMDs and provide examples of how we have learned to exploit them for enhanced catalytic and electronic performance.

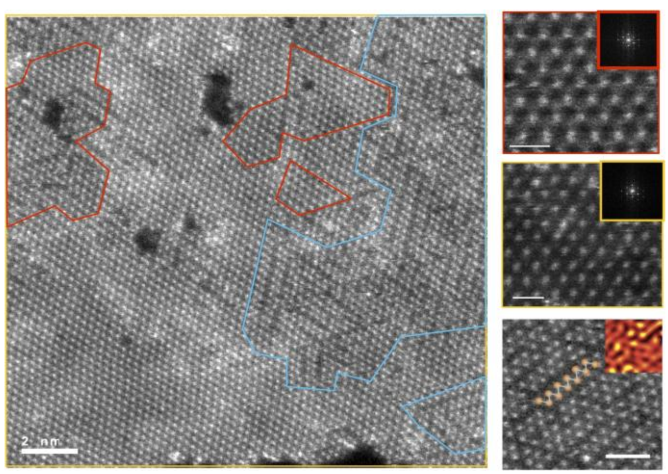

Figure 1: STEM image of single layer MoS_2 showing the richness of phases in chemically exfoliated nanosheets. 2H (red) and 1T phases (yellow) along with the strained 1T phase (blue) are shown. The corresponding atomic resolution image and diffraction patterns for 2H (top right) and 1T (middle right) phases are shown. The bottom right image also shows strain map of the distorted 1T phase.