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Possible Structural Phase Transitions in Transition Metal Dichalcogenides ENGIN DURGUN, UNAM - Bilkent University, HASAN SAHIN, FRANCOIS PEETERS, University of Antwerp — Most of the the transition metal dichalcogenides (TMD) have graphene-like hexagonal crystal structure which are composed of metal atom layers (M) sandwiched between layers of chalcogen atoms (X) and these structures have MX_2 stoichiometry. Chalcogen layers can be stacked on top of each other in two different forms: H phase made of trigonal prismatic holes for metal atoms and T phase that consists staggered chalcogen layers forming octahedral holes for metals. Among the TMDs that have been reported to be stable, individual layers of MoS_2, $MoSe_2$, WS_2 and WSe_2 have 1H structure in their ground state while dichalcogens of Ti, V and Ta prefer the 1T phase. In our study we investigate the physical mechanisms underlying for the possible phase transitions in TMDs. Our calculations based on first-principles techniques reveal that in addition to H and T phases various distorted H and T phases can be also stabilized by point defects. These new phases have entirely different electronic properties.

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