

Abstract Submitted
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Understanding Electronic, Optical and Thermal Properties of Transition Metal Chalcogenides (TMCs) CAN ATACA, RAJAMANI RAGHUNATHAN, Massachusetts Institute of Technology, SEFAATTIN TONGAY, University of California, Berkeley, JUNQIAO WU, Lawrence Berkeley National Laboratory, JEFFREY C. GROSSMAN, Massachusetts Institute of Technology — The fundamental properties of a material depend on their atomic structure, nature of bonding and elemental/chemical composition. Confinement of electrons in 2 dimensional planar structures leads to realization of several intriguing properties that are not seen in the bulk 3-dimensional counterparts. In this work, we explore the properties of single and few layer MX (M:Transition metal, X: chalcogen atom) both theoretically and experimentally. Using state of art density functional theory (DFT) we carried out a stability analysis through phonon and electronic, magnetic and elastic structure calculations where M=Cu, and X=S, Se, Te. The stacking of transition metal chalcogenide (TMC) monolayers is of the type MX-M₂X₂ instead of the usual X-M-X stacking found in TMDs. The differences in geometric structure result in many different stable monolayer forms with different electronic and magnetic properties. Depending on the number of layers, MX structures can be found in 2, 3, 4 and 6 MX layer stable configurations. These dimensionality effects predicted by DFT such as energy band structures and Raman active modes are confirmed by experiments. Various different monolayers of MX possess a number of properties that make them highly promising materials for future nanoscale applications.

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