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A density functional theory investigation of select transition metal dichalcogenides RODRICK KUATE DEFO, Physics Department, Harvard University, GEORGIOS TRITSARIS, SEAS, Harvard University, SHIANG FANG, EFTHIMIOS KAXIRAS, Physics Department, Harvard University — As a result of the extensive work done on graphene, leading to advances in sample preparation, optical detection, and transfer and manipulation of 2D materials, there has been a resurgence of interest in layered materials from which single sheets can be extracted, such as molybdenum disulfide. Particularly intriguing is the fact that layered MoS_2 transitions from an indirect band gap in the bulk to a direct band gap in the monolayer opening up the possibility of optoelectronic applications. These results have been verified using density functional theory and, further, dependence of the band gap on lattice strain has been investigated. This dependence is crucial in understanding emergent properties of compounds consisting of MoS_2 layered with other materials where there is a lattice mismatch. $MoSe_2$, MoSSe, WS_2, WSe_2 and WSSe have also been studied. Finally, dielectric functions have also been obtained for these compounds to explore the effect particularly of the asymmetric atom configurations on polarization of the material.

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