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Origin and design of indirect-to-direct band gap transition in group-VIB transition metal dichalcogenide films and heterostructures[1]
LIJUN ZHANG, LIPING YU, University of Colorado Boulder, JUN-WEI LUO, National Renewable Energy Laboratory, ALEX ZUNGER, University of Colorado Boulder — Group VIB transition metal dichalcogenides (TMDs) often have indirect band gaps in bulk forms but become direct at monolayer thin films. This is an effect often associated with quantum confinement as demonstrated in semiconductor nanostructures. Using first-principle calculations with van der Waals interaction included, (i) we study the indirect-to-direct transition in films of a single TMD material as a function of its thickness for a series of TMDs (MX_2, M = Cr, Mo, W; X = S, Se, Te). By systematic analysis of the obtained critical transition thickness, effective masses and energy evolution of the band edge states, we rule out the mechanism of (kinetic energy controlled) quantum confinement, in favor of an (potential energy controlled) inter-layer coupling. (ii) We explore the electronic structure of different layer stacking in the van der Waals heterostructures consisting of a few TMDs. We found in such multiple layered systems that certain stacking sequences result in a direct band gap, and thus accompanied by a remarkably different optical response. In some heterostructures, the behavior of charge separation, i.e. electron and hole in different layers, is observed. The results of our work provide new insight on engineering optoelectronic properties of TMDs.

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