Effects of strain on band structure and effective masses in MoS$_2$

HARTWIN PEELAERS, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106-5050 — Molybdenum disulfide (MoS$_2$) is a layered semiconductor that shows great promise for devices such as field-effect transistors. It has an important advantage compared to graphene, namely that it has a band gap. However, a lot of crucial information about the band structure and electronic properties of this material is still lacking, hampering interpretation of experiments and preventing accurate device modeling. Here we use hybrid density functional theory to calculate key materials parameters such as band gaps and effective masses, as well as to investigate effects of strain. We show how strain allows engineering the nature (direct vs. indirect) and size of the band gap and the magnitude of effective masses. In addition, insight into the fundamental physics is provided by considering the transition between the bulk and the monolayer as a function of tensile uniaxial stress.

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