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Electronic properties of few-layer MoS2 under an external electrical field JOSE EDUARDO PADILHA, HARTWIN PEELAERS, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, University of California Santa Barbara — MoS_2 is a two-dimensional (2D) layered material with a band gap in the 1-2 eV range, depending on the number of layers, and with promising applications in nanoelectronics. Field-effect transistors based on MoS_2 have been fabricated, displaying room-temperature electron mobility of $200 cm^2 V^{-1} s^{-1}$ and high on/off ratios on the order of 10^8. In these devices, the effect of the electric field across the MoS_2 layers is important for device operation, so understanding these effects will aid in improving device performance. Here we use first-principles calculations to determine the electronic properties of MoS_2 layers as a function of an electric field applied perpendicular to the layers, representing the effect of gate electrodes. In the absence of an external field, the valence and conduction bands of multilayer MoS_2 are degenerate. However, an applied external field generates a gradient potential inside the material, breaking the symmetry between the layers, lifting the degeneracies, and modifying the band gap. We will discuss the evolution of the band gap and the various minima in the conduction band as a function of the field intensity and the number of layers. Work supported by FAPESP and by NSF-IMI.

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