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Thickness dependence of spin polarization and electronic structure of ultra-thin films of MoS_2 and related transition-metal dichalcogenides TAY-RONG CHANG, National Tsing Hua U., Taiwan, HSIN LIN, National University of Singapore, HORNG-TAY JENG, National Tsing Hua U., Taiwan, ARUN BANSIL, Northeastern U. — Thickness dependence of electronic structures of transition-metal dichalcogenides (TMDs) MX_2 (M=Mo or W; X=S, Se or Te) is investigated using first-principles calculations. When spin-orbit coupling (SOC) is included in the computations, the electronic structure of monolayer MX_2 films exhibits significant band splittings due to the breaking of spatial inversion symmetry. In particular, spin-split states appear around the valence band maximum with nearly 100% out-of-the-plane spin polarization with the spin oriented oppositely at the K and K$'$ symmetry points in the Brillouin zone. For bilayer films, the spin-polarization can be tuned by an out-of-the-plane electric field, and the spin-polarized states are weakly coupled between the layers with small k_z dispersion. We confirm a transition from an indirect to a direct band gap as the thickness is reduced to a monolayer in MoX_2, in agreement with recent experimental findings. Our study provides insight into the thickness dependence of electronic structure and the degree of spin polarization of the valence bands in ultra-thin TMD films and their viability for spintronics applications.

[1] T.-R. Chang, H. Lin, H.-T. Jeng, and A. Bansil, Sci. Rep. **4**, 6270 (2014).

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