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van der Waals interactions in MoS_2 and MoO_3[1] HARTWIN PEELAERS, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, California 93106-5050 — Molybdenum disulfide (MoS_2) is a layered material that attracted a lot of attention recently for use in electronic devices, such as field-effect transistors, as it has high electron mobilities and high on/off ratios. MoO_3 is a layered n-type semiconductor that shows good properties for energy applications. The layers in both materials are weakly bound by van der Waals interactions. A good theoretical description of these interactions is thus required. In this talk I will discuss different approaches to include van der Waals interactions in density-functional theory (DFT), focusing on MoS_2 and MoO_3. In particular, a combination of hybrid functionals, which correct for the DFT band gap problem, and explicit inclusion of van der Waals interactions, to correct for the long range interactions, shows a lot of promise. The validity of this approach will be demonstrated by comparing the structural parameters of MoS_2 under hydrostatic pressure with experimental data.

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