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Characterization of Thin Film Materials using SCAN MetaGGA, an Accurate Nonempirical Density Functional IOANA-GIANINA BUDA, CHRISTOPHER LANE, BERNARDO BARBIELLINI, Northeastern University, ADRIENN RUZSINSZKY, JIANWEI SUN, JOHN P. PERDEW, Temple University, ARUN BANSIL, Northeastern University — The exact ground-state properties of a material can be derived from the single-particle Kohn-Sham equations within the framework of the Density Functional Theory (DFT), provided the exact exchange-correlation potential is known. The simplest approximation is the local density approximation (LDA), but it usually leads to overbinding in molecules and solids. On the other hand, the generalized gradient approximation (GGA) introduces corrections that expand and soften bonds. The newly developed nonempirical SCAN (strongly-constrained and appropriately-normed) MetaGGA [Phys. Rev. Lett. 115, 036402] has been shown to be comparable in efficiency to LDA and GGA, and to significantly improve LDA and the Perdew-Burke-Ernzerhof version of the GGA for ground-state properties such as equilibrium geometry and lattice constants for a number of standard datasets for molecules and solids. Here we discuss the performance of SCAN MetaGGA for thin films and monolayers and demonstrate improvements of predicted ground-state properties. Examples include graphene, phosphorene and MoS_2.

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