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Chemi- and Physisorption Together from a Semilocal Density Functional: Graphene on Ni (111) JIANWEI SUN, BING XIAO, ADRIENN RUZSINSZKY, JOHN PERDEW, Tulane University, JOHN PERDEW TEAM — Conventional semilocal approximations of density functional theory at the level of local spin density approximation (LSDA) and generalized gradient approximations (GGA) are thought to lack the ability to describe weak interactions. This is well illustrated by the system of a graphene adsorbed on a Ni (111) surface, in which the graphene can adsorb on the Ni (111) surface chemically or physically at different distances. LSDA, the standard Perdew-Burke-Ernzerhof (PBE) GGA, and its variant designed for solids, PBEsol, miss the physisorption. We show improved descriptions for weak interactions from a newly-developed semilocal meta-GGA (MGGA)—that performs equally well for molecules, surfaces, and solids—by demonstrating its ability to capture both the chemisorption and the physisorption.

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