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Substrate Effects on Adsorbate-induced Magnetism in Graphene

PRATIBHA DEV, Naval Research Lab, THOMAS REINECKE, Naval Research Laboratory, Washington, D.C. — Using density functional theory, we show that substrates play an important role in the properties of layered systems such as graphene. In particular, we focus on the effects of a copper substrate on magnetic properties associated with functionalized graphene. Local magnetic moments are created in freestanding graphene by decorating it with an unequal number of fluorine (hydrogen) adatoms in the two sublattices. However, when the functionalized graphene is placed on copper, the local moments completely disappear. We attribute this to several interconnected effects – doping by the substrate, increased distortion relative to the freestanding case and broadening of the defect states. We show that the interactions with the substrate and the formation of local magnetic moments can be modified by using multiple layers of graphene. This work also shows the importance of including the effects of the immediate environment in determining the properties of functionalized, layered structures such as graphene.

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