Many-Body Study of Cobalt Adatoms Adsorbed on Graphene

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Since its discovery, graphene has been the subject of intense efforts to adapt it for a variety of promising applications. One proposal is to adsorb transition metal atoms to provide localized magnetic moments for use in spintronic devices. Several theoretical [1–3] and experimental [4] studies have examined Co adatoms on graphene. Calculations of Co/graphene systems have largely been done at the density functional theory (DFT) level with local or semi-local functionals, or with an empirical Hubbard on-site repulsion U (LDA+U). However, there has been controversy regarding the bonding nature of Co/graphene systems as these results have shown significant variations with how the correlation effects are treated. We use auxiliary-field quantum Monte Carlo (AFQMC) [5–6] to calculate the binding energy of Co/benzene systems. An embedding size-correction scheme is employed to efficiently calculate the binding energy of Co/graphene system as a function of Co absorption height.

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