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Many-body study of cobalt adatoms adsorbed on graphene[1] YUDISTIRA VIRGUS, WIRAWAN PURWANTO , HENRY KRAKAUER , SHIWEI ZHANG, College of William and Mary — Interest in the adsorption of transition metal adatoms on graphene has grown rapidly. The interaction between magnetic adatoms and graphene may have applications in designing spintronics devices. Several theoretical and experimental 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 and with an empirical Hubbard on-site repulsion U (LDA+U). We use auxiliary-field quantum Monte Carlo (AFQMC), in combination with DFT and quantum chemistry methods, to examine the effects of electron correlation in Co–graphene systems, without adjustable parameters. Binding energy curves for Co–graphene and model structures will be presented, and their implications on the electronic and structural properties will be discussed.

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