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The stability, energetics, and magnetic states of Co adsorption on graphene[1] YUDISTIRA VIRGUS, WIRAWAN PURWANTO, HENRY KRAKAUER, SHIWEI ZHANG, College of William and Mary — The adsorption of transition metal adatoms on graphene has attracted significant research interest due to their possible use to induce magnetism on graphene for spintronic applications. Single Co atoms on graphene have been extensively studied both theoretically and experimentally. In our previous work, we used auxiliary-field quantum Monte Carlo (AFQMC) and a size-correction embedding scheme to calculate the binding energy of Co/graphene for the six-fold hollow site.[2] Recent experimental results show that single Co atoms can be adsorbed on graphene at both the hollow and the top sites.[3] We use AFQMC to investigate Co/graphene for the three high-symmetry adsorption sites; six-fold hollow site, two-fold bridge site, and top site. Highly accurate binding energy curves for the three sites are obtained. The stabilities of the different magnetic states and adsorption sites will be examined and discussed in relation to the experimental observations.

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