Abstract Submitted
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Ab Initio **Many-body Study of Cobalt Adatoms Adsorbed on Graphene**[1] YUDISTIRA VIRGUS, WIRAWAN PURWANTO, HENRY KRAKAUER, SHIWEI ZHANG, College of William and Mary — Research interest in the adsorption of transition metal adatoms on graphene has grown rapidly because of their promising use in spintronics. Single Co atoms on graphene have been extensively studied recently, and possible Kondo effects have been considered. However, these calculations show significantly varying results on the bonding nature of Co/graphene system. We use auxiliary-field quantum Monte Carlo (AFQMC) and a size-correction embedding scheme to accurately calculate the binding energy of Co/graphene.[2] We find that as a function of the distance h between the Co atom and the six-fold hollow site, there are two states that provide binding and exhibit a double-well feature with nearly equal binding energy of 0.4 eV at $h = 1.51$ and $h = 1.65$ Å, corresponding to low-spin ^{2}Co ($3d^9 4s^0$) and high-spin ^{4}Co ($3d^8 4s^1$), respectively. Binding of Co on bilayer graphene is also investigated.

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[2]Y. Virgus, W. Purwanto, H. Krakauer, and S. Zhang, arXiv:1210.6973.

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