

Chemical Bonding of Transition-metal Co₁₃ Clusters with Graphene

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Abstract

We carried out density functional calculation to study Co₁₃ clusters on graphene [1]. We deposit several free isomers in different disposition respect to hexagonal lattice nodes, studying even the hcp 2d isomer recently obtained as the most stable one [2]. Surprisingly, Co₁₃ clusters bonded to graphene prefer icosahedron-like structures where the low lying isomer is much distorted, because it is linked with more bonds than in previous works [3].

For any isomer the most stable position binds to graphene by the Co atoms that can lose electrons. We find that the charge transfers between graphene and clusters are small enough to conclude that the Co-graphene binding is not ionic-like but chemical. Besides, the same order of stability among the different isomers on doped graphene is well kept. These findings could also be of interest for magnetic clusters on graphenic nanostructures such as ribbons and nanotubes.

References

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Figures

