

Abstract Submitted
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Energetics and Electronic Structure of Transition Metal Adatoms and Clusters on Graphene¹ CHRISTOPHER PORTER, DAVID STROUD, Ohio State University — Using density functional theory (DFT), we calculate both the atomic arrangement and electronic structure of transition metal (TM) adatoms, and clusters of adatoms, on graphene. We use a periodic arrangement of unit cells which typically include about 64 C atoms. For Fe on graphene, we have found that the stable position of the adatom is above the center of a hexagon of C and that most of the relaxation in the graphene occurs in the six C atoms closest to the adatom. We use DFT to map out a potential energy surface for Fe adatoms on graphene at any point in the unit cell, allowing an estimate of the energy barrier for an adatom to hop from one energy minimum to another. We also calculate the lowest energy configurations of pairs and larger clusters of TM adatoms on graphene. Finally, we have calculated the electronic structure and density of states associated with the adatoms and clusters on graphene, and have extended these calculations to spin- dependent properties, using a spin density functional approach. These results should be relevant to electronic and spin transport properties of graphene, both of which are expected to be strongly influenced by TM adatom impurities.

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