Absorption of iron oxide nano clusters (Fe_4O_6) on graphene surface: A density functional study

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Abstract

Nanocluster iron oxides in the form of clusters and nanoparticles find a number of applications owing to their unique magnetic, biochemical and catalytic properties. These include applications in catalysis, biomedical uses like magnetic hyperthermia in cancer treatment, targeted drug release, magnetic resonance imaging and immunoassays as well as magnetic data storage.[1–6] In this study, the number of iron oxide nano-clusters optimized energy. The electronic properties of clusters and interaction with graphene surface were studied. The functional PBE of density functional theory are used. Relative stability, features of electronic and magnetic properties were investigated.
The results show that the three nano clusters (Fe_4O_6) are stable and relatively strong interaction with graphene have led to significant changes in the band structure. Their interaction energy has been reported. Our results show significant chemical interactions between the clusters and graphene.

References

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Figures

(a)Structure of optimized models for stable adsorption of Fe_4O_6 cluster on the graphene, and their band strctuer plot. Bonds are in Å