Contribution Poster

First-principles investigation of titanium and titanium dioxide adsorption on graphene

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Graphene with its uncommon electronic properties provides an open playground for chemical modification of its surface. The study of adsorption of metals and insulators is essential for further application in electronic device construction and to understand the impact of electrical contacts on the electronic properties of graphene.

We have performed ab initio ground state calculations for titanium and titanium dioxide decorated graphene. This includes the investigation of adsorption of a single titanium and titanium dioxide molecule, a covalently bonded titanium monolayer also as a weakly physisorbed monolayer of titanium dioxide crystal. Ground state structures were calculated with corresponding binding energies, electronic structure and an investigation of charge transfer by multiple charge population analysis approaches was performed.

The work was motivated by the recent experimental observation of adsorption of titanium on graphene which uncovers substantial n-type doping and reduction of graphene's mobility by charged impurity scattering and subsequent recovering of graphene properties to the almost intrinsic values by exposing samples to oxygen [1].

References

[1] K.M. McCreary, K.Pi, and R.K.Kawakami, Applied Physics Letters **98**, 192101 (2011), “Metallic and insulating adsorbates on graphene“