

# Density functional calculation for various adatom adsorptions on graphene for using graphene as substrate of nanomaterial

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The graphene itself is very interesting material to be investigated both experimentally and theoretically. Nowadays, excellent experiments for graphene sheets become possible. However, the graphene is very interesting also for substrates of nanostructure because of its two dimensionality. In order to promote such investigations, the adsorption of atoms and molecules on graphene should be studied, but such studies have not been done so much.

In recent theoretical study[1,2,3,4], the adsorption sites and adsorption energies for some atomic species have been reported. The aim of this investigation is understanding of the general mechanism of the adatom adsorption on a graphene sheet. In this work, we investigate computationally adsorption energies, adsorption sites and migration barrier energies on graphene sheet for a lot of atomic species including transition metals, noble metals, nitrogen and oxygen, from atomic number 1 to 83, using the DFT calculation. We used VASP[5,6,7,8] which was first-principle calculation code of the high precision using the PAW method. The calculations are done for adatom at three site having symmetry, H(hexagonal),B (bridge) and T (on-top) on 3 x 3 super cell. The spin-polarization is included in the calculation. The both magnetic and non-magnetic calculations are done.

We discuss stability of the adatom in the graphene by analysis from the electronic structure. The calculated results show that adsorption at the H-site mainly for simple and transition metal elements. The non-metallic element showed the tendency to be adsorbed at the B-site. As shown in fig.1, some atomic species have chemisorption adsorption. Many metallic adatoms show ferromagnetic behavior at least for single adsorption on graphene. As shown in figure 2 for Mn on graphene, we found in our DFT calculation that some transition metal atoms adsorb in vertical alignment with spin polarization. Such structure can be applied to some nano-scale magnetic devices. Moreover, magnetic behavior of adatoms on graphene is also reported along the atomic elements table. In figure 3, we show the calculation for nitrogen as an example of non-metal elements.

The result of this work will be helpful for the choice of material for electrode on graphene or growth of graphene on substrates. This work is supported by JST-CREST project.

## References

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Figure 1. Calculated wave function image of a typical orbital for the adsorption of chromium adatom on graphene using non-magnetic DFT calculation. The picture shows us the strong hybridization of chromium orbital and carbon orbitals of graphene.

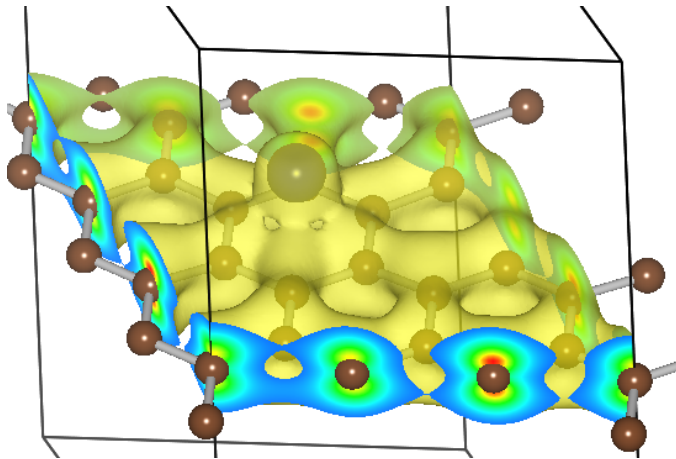


Figure 2 The adsorption structure of transition metal atoms on graphene with vertical alignment. The figure is the example of spin density map for two Mn atoms on graphene obtained by using the density functional calculation. The calculation shows magnetic polarization for the two Mn atoms.

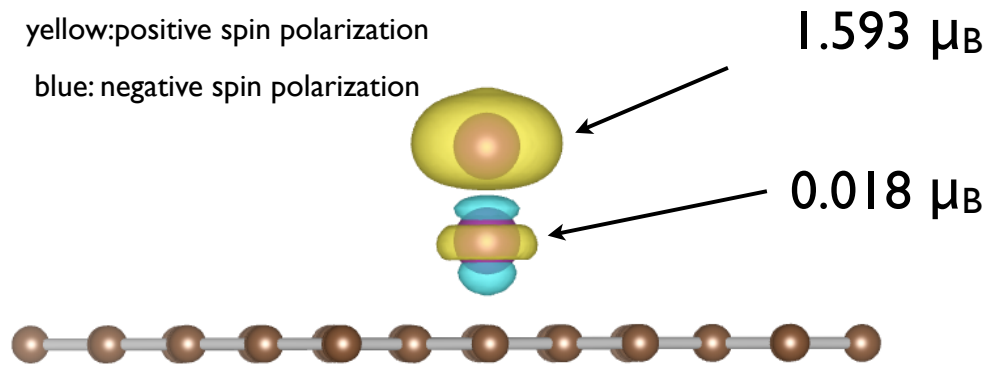


Figure 3

The calculated local density of states for nitrogen adatom at the most stable site on graphene. The result shows us the magnetic polarization of nitrogen on graphite.

