First principles calculation of magnetism in Fe atom adsorption on graphene nanoribbon

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Graphene nanoribbon (GNR) are made of carbon atoms and are expected to be applied in a wide variety of fields due to the properties of graphene, such as electrical conductivity and its two-dimensional structure, as well as its ability to significantly change properties depending on the edge configuration. Although graphene is inherently nonmagnetic, theoretical studies have shown that adsorbed Fe atoms can enhance its properties. Among these, spintronics applications utilizing electron spin are expected to emerge. In this study, we focused on GNRs and Fe atoms and evaluated the effect of coverage (the fraction of Fe atoms occupying H sites) on the stability of the structure. The influence of Fe was also evaluated by varying the width of GNRs for the most stable coverage ratio.

We performed our calculations using spin-polarized density functional theory (DFT) with the VASP package. The energy cutoff was set to 550 eV. A 15×1×1 k-point sampling grid was used, along with a convergence threshold of 1×10^{-7}.

According to our calculations, with increasing surface Fe coverage, the graphene surface becomes activated, reaching a peak at a specific coverage. Calculations show that the graphene surface becomes more active with increasing surface Fe coverage, reaching a peak at a specific coverage.

It is also found that the magnetic moment and adsorption energy tend to decrease as the ribbon width is increased.

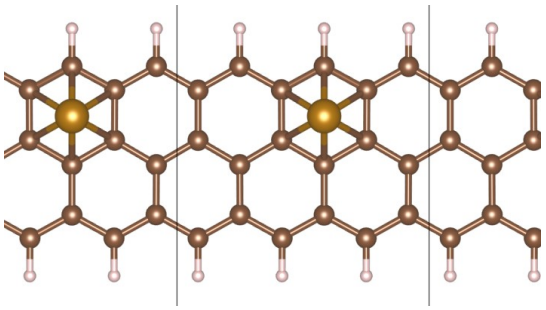

Fig. 1. An example of a GNR model.

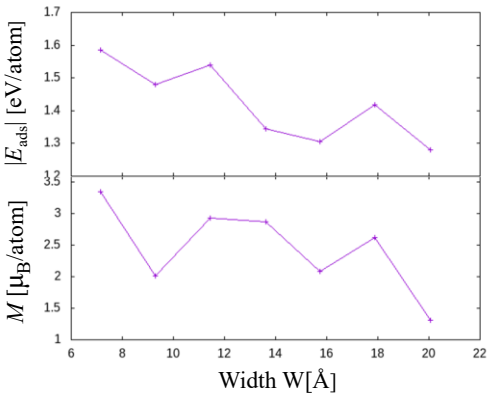

Fig. 2. The relationship between ribbon width, adsorption energy, and magnetic moment of GNR.

References

1. Yuan Ping Feng, Lei Shen, et al, *Computational Molecular Science*, **2017**,1313-1391