Magnetic insulator proximity induced spin-polarization in graphene

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Graphene is very attractive for spintronics [1] since long spin lifetimes are expected within this material due to its intrinsic weak spin-orbit coupling and hyperfine interaction [2]. However, inducing magnetism in graphene is still jeopardizing for its applications. One way to induce magnetic states in graphene is using magnetic substrates, e.g. transition metals Co and Ni [3]. The properties of these epitaxial films have been extensively studied, however they are grown on conducting substrates which limit graphene applications for electronic devices. Alternative possibility is to use magnetic insulating material EuO as a substrate [4]. Here we addressed this problem from first principles and report promising potential for producing high spin polarization and exchange splitting values.

Our calculations were performed using Vienna Ab-Initio Simulation Package (VASP) which is based on density functional theory with generalized gradient approximation for exchange correlation and projector augmented wave based pseudopotentials [5]. All calculations have been performed to ensure the Hellman-Feynman forces acting on carbon atoms to be less than 10-3 eV/Å. Considering that Eu is a heavy element with atomic number of 63, and its outer shell ($4f^7 6s^2$) contains f electrons, GGA approach fails to describe strongly correlated localized 4f electrons of EuO giving the metallic ground state of EuO, while a clear band gap is observed in experiment [6]. Thus, we introduced Hubbard-U parameter to describe the strong intra-atomic interaction in a screened Hartree-Fock like manner, which produces correct ground state of EuO.

Using the optimized structure of graphene on EuO, we calculated the local density of states for this system [Figure 1]. Due to the existence of EuO substrate, symmetry of carbon atoms in graphene lattices are broken into six folders as shown in Figure 1(a) with different colors. For clarity, EuO substrate atoms are shown with crosses. The calculated magnetic moment of surface Eu are found a little bit enhanced giving 7.0 μB compared to the bulk values of 6.9 μB. And sublayer oxygen atoms are found to be spin polarized also with magnetic moments of about -0.11 μB. Due to very strong spin polarization of EuO substrate, magnetic properties of graphene are strongly affected. As shown in Figure 1(b), the average spin polarization in graphene layer is found to be about 12%. This value is not large, but if we shift a little bit Fermi level, the spin polarization can be strongly enhanced even up to half-metallic state. Interestingly, around -1 eV, spin up and spin down densities are zero, but the energy ranges are different which could actually be related to Dirac point's reshaping. Since these 18 carbon atoms are broken into 6 symmetry groups, their contributions to the total spin polarization are also different. For the purple one having largest magnetic moment in graphene, its spin polarization may reach up to 72%, while for the yellow one with smallest magnetic moment, its spin polarization gives just 9.6%. Also due to direct interaction between two sublattices of intrinsic graphene and interaction between graphene and EuO substrate, the spin polarization of some of carbon atoms becomes negative. Finally, the spin polarized electrons are mainly from p_z orbital [Figure 1 (c)].

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References

[1] A. Fert et al, *Mat. Sci. Eng. B,* **84** (2001) 1; S. A. Wolf et al, Science, **294** (2001) 1488.
[2] D. Huertas-Hernando et al, Eur. Phys. J. Special Topics, **148** (2007) 177.
[3] A. Varykhalov et al, Phys. Rev. Lett., **101** (2008) 157601; O. Rader et al, Phys. Rev. Lett., **102** (2009) 057602.
[4] H. Haugen et al, Phys. Rev. B, **77** (2008) 115406.
[5] G. Kresse and J. Hafner, Phys. Rev. B, **47** (1993) 558; P. E. Blöchl, Phys. Rev. B **50** (1994) 17953; G. Kresse and J. Joubert, *ibid.* **59** (1999) 1758.
[6] N. J. C. Ingle et al, Phys. Rev. B., **77** (2008) 121202; A Mauger et al, Phys. Reports, **141** (1986) 51.

Figures

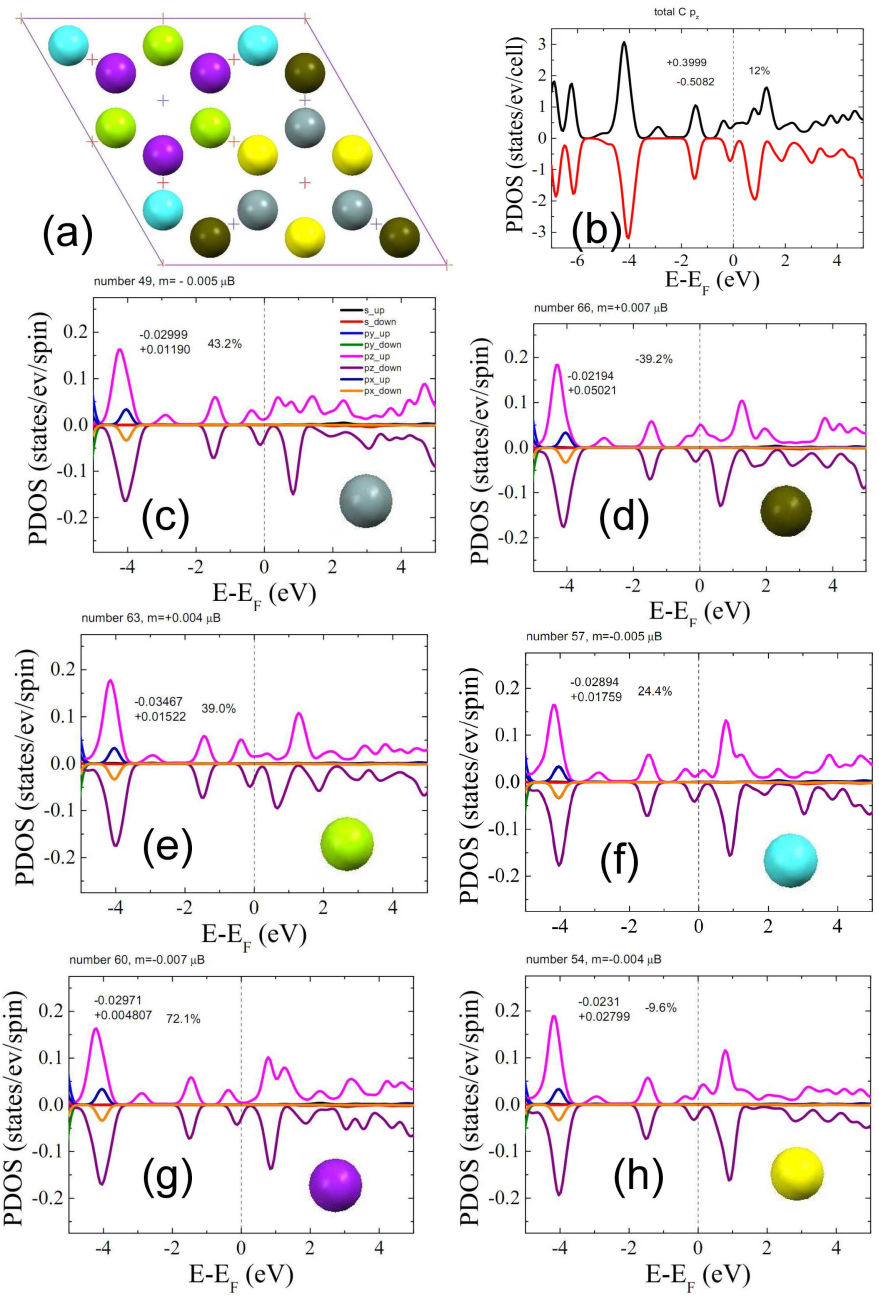

Fig.1. (a) the six lattices of graphene on EuO represented with different colors, (b) total density of states for graphene layer and the average spin-polarization, (b)-(h) local density of states for each lattice of carbon atom in graphene, respectively.