Transport Properties of Iron-Porphyrin / Graphene Junction

M. I. Trioni, E. del Castillo, S. Achilli, F. Cargnoni

CNR, National Research Council of Italy, ISTM and Chemistry Department, University of Milan,
via Golgi 19, 20133 Milano, Italy
m.trioni@istm.cnr.it

Abstract

Spintronics is one of the possible applications of graphene-based materials [1]. To this end, a robust spin polarization in the graphene layers is required. This can be achieved via functionalization with magnetic transition metals, adsorbates, or organic molecules. It has been demonstrated that a Fe atom incorporated in the graphene network replacing a carbon-carbon dimer and bound to substitutional N atoms forms an almost-planar stable structure with notable magnetic properties [2].
In this work we study by first principles a Fe-Porphyrin molecule (FeP) embedded in the graphene nanoribbon junction connected with two semi-infinite graphene regions using the density functional theory (DFT) as implemented in the SIESTA package [3]. The analysis of the spectral properties shows a rearrangement of the orbital occupancy with respect to the isolated FeP molecule, while the magnetic moment remains unchanged ($2\mu_B$). The Fe $3d_{xz}$ and $3d_{yz}$ orbitals of both spin components hybridize with the carbon π bands. The other *d* states, due to their different parity, remain unperturbed.
We also investigate the interaction of a carbon monoxide and O_2 molecule with the Fe atom (see Figure). CO adsorbs with the carbon atom facing the metal center while O_2 prefers a tilted configuration. The interaction is strong enough to be stable at room temperature, amounting to about 2 eV and 1 eV for CO and O_2, respectively. The adsorption of CO modifies the occupancy of the Fe 3*d* states and totally quenches the magnetic behavior of the system. Differently, the adsorption of O_2 molecule leaves the system in a magnetic configuration.
We explore the effects of molecular adsorption on the electronic transport properties calculating the transmission coefficient T(E) and the electric current in both cases. The calculations were performed using the TranSIESTA code [4], which combines the non-equilibrium Green's function (NEGF) technique with DFT. At zero bias the T(E) of the FeP junction does not significantly differ from that of pure graphene, except for a small perturbation at 0.1 eV below E_F in the minority component due to the hybridized $3d_{xz}$ Fe state, which for higher voltages becomes more evident. Consequently, the currents of the two spin components are different giving a polarization of 5%. When the CO molecule is adsorbed the magnetic character of the system vanishes and the current becomes unpolarized. Finally the adsorption of O_2 molecule increases for a little contents the spin polarization of the current.
This suggests the possibility of using the current measurement in order to detect the adsorption of CO or O_2 molecule: both the disappearance or increasing of spin polarization or also the variation of the total current are evidences of the presence of gas.

References

[1] O.V. Yazyev, M.I. Katsnelson, Phys. Rev. Lett., **100** (2008) 047209.
[2] A.T. Lee, J. Kang, S. Wei, K,J. Chang, and Y. Kim, Phys. Rev. B, **86** (2012) 165403.
[3] J.M. Soler, E. Artacho, J.D. Gale, A. García, J. Junquera, P. Ordejón, and D. Sánchez-Portal, J. Phys.: Condens. Matter, **14** (2002) 2745.
[4] M. Brandbyge, J.-L. Mozos, P. Ordejón, J. Taylor, and K. Stokbro, Phys. Rev. B, **65** (2002) 165401.

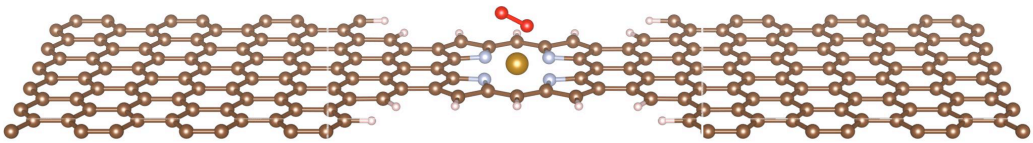

Figure: Fe-Porphyrin molecule (FeP) embedded in the graphene nanoribbon junction connected with two semi-infinite graphene regions. The adsorption of O_2 molecule is also shown.