Graphene: Reversible Spin Manipulator of Molecular Magnet

S. Ghosh,[1] S. Bhandary,[2] H. Herper,[3] H. Wende,[3] O. Eriksson,[2] and B. Sanyal[2]

[1] *School of Applied and Engineering Physics, Cornell University, Ithaca, NY 14853, USA.*
[2] *Department of Physics and Astronomy, Uppsala University, 75120 Uppsala, Sweden.*
[3] *Faculty of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE), University of Duisburg-Essen, 47048 Duisburg, Germany.*

One of the primary objectives in molecular nanospintronics is to manipulate the spin states of organic molecules with a d-electron center by suitable external means. Fe-porphyrin (FeP) molecule is one of the potential candidate, where it is possible to tune the magnetic coupling between Fe at the center of FeP with a ferromagnetic substrate [1]. On the other hand, graphene has made an enormous sensation in the scientific community due to its exotic multidisciplinary features [2, 3]. During the synthesis of graphene a number of defects may arise, specially in sp^2 bonded carbon the divacancy defect can easily be introduced in a graphene lattice [4]. These divacancy defect sites are excellent trapping centers for atom and molecules when dispersed on the graphene lattice [5].

Utilizing the novel properties of FeP and graphene, we demonstrate by first principles density functional calculations, as well as second order perturbation theory, that a strain induced change of the spin state, from $S = 1 \rightarrow S = 2$, takes place for FeP molecule deposited at a divacancy site in a graphene lattice. The process is reversible in the sense that the application of tensile or compressive strains in the graphene lattice can stabilize FeP in different spin states, each with a unique saturation moment and easy axis orientation. The effect is brought about by a change in Fe-N bond length in FeP, which influences the molecular level diagram as well as the interaction between the C atoms of the graphene layer and the molecular orbitals of FeP [6].

[1] H. Wende *et al.*, Nature Mater. **6**, 516 (2007).

[2] K. S. Novoselov *et al.*, Science **306**, 666 (2004).

[3] A. K. Geim and K. S. Novoselov, Nature Mater. **6**, 183 (2007).

[4] M. H. Gass *et al.*, Nature Nanotech. **3**, 676 (2008).

[5] B. Sanyal *et al.*, Phys. Rev. B **79**, 113409 (2009).

[6] S. Bhandary *et. al.*, Phys. Rev. Lett. **107**, 257202 (2011).

Contact: sg827@cornell.edu