MAGNETIC PROPERTIES OF TRANSITION METALS (3D) ADD ON GRAPHENE: A DENSITY FUNCTIONAL STUDY

Mahdi Sargolzaei[1,2] **and Farideh Gudarzi**[1]

[1] *Department of Physics, Iran University of Science and Technology, Narmak 16345, Tehran, Iran.*

[2] *Computational Physical Science Laboratory, Department of Nano-Science, Institute for Research in Fundamental Sciences (IPM), Tehran, Iran.*

E-mail: sargolzaei@iust.ac.ir

Magnetic properties of 3d transition metals (TM) in contact with its substrate have been extensively studied for both fundamental and technological applications in nanomagnetic devices. A high magnetic anisotropy energy (MAE) is needed to have long-term magnetic data storage. In this work we used a single hexagonal carbon ring and a sheet of graphene as two different substrates for TM individual atom. A full-potential local-orbital scheme, FPLO, was employed for density functional theory (DFT) calculations [1]. All calculations have been done in a full-relativistic regime, in which the explicit form of the spin-orbit coupling have been take into account. It has been found out that the transition metal atoms are located on the most symmetric axis perpendicular to the plane of the graphene. We estimated the position of the TM atoms, with respect to the plain of the graphene. The spin and orbital magnetic moments of TM atoms have been calculated for different quantization axes of the considered system. In order to obtain an upperlimit estimation for orbital magnetic moment, an orbital polarization correction (OPC) was added to the local spin density approximation energy functional in the framework of DFT [2,3]. We calculated MAE as the difference energy between the perpendicular and parallel quantization axes. We found out that Cr and Co atoms have largest MAE compare to the other 3d transition metals.

References

[1] K. Koepernik and H. Eschrig, Phys. Rev. B (59) 1743 (1999); http://www.FPLO.de.
[2] M.S.S. Brooks, Physica B (130) 6 (1985).
[3] Eschrig, M. Sargolzaei, K. Koepernik and M. Richter, Europhys. Lett. (72) 611 (2005).