11th International Conference
on Advanced Materials

Rio de Janeiro Brazil
September 20 - 25

ICAM2009

DFT study of magnetic coupling in Cu(II) and Ni(II) complexes with nitronyl nitroxide radical

A. S. Alves[(1)(2)*] and P. Venezuela[(2)]

(1) Departamento de Física - Universidade Estadual de Feira de Santana
(2) Instituto de Física - Universidade Federal Fluminense
* asa@if.uff.br.

Abstract – A theoretical investigation on magnetic coupling in Cu(II) and Ni(II) complexes using density functional theory is presented. The results confirm the experimental analysis, showing a weak ferromagnetic interaction between the metal ions and the coordinated NITmPy radical with a coupling constant of 8.06 cm^{-1} and 3.82 cm^{-1} respectively. The spin polarization mechanism explains the coupling in both cases.

In this work, we report the results of the study of magnetic coupling in Cu(II) and Ni(II) complexes with nitronyl nitroxide radical. The basic mechanism for understanding the magnetic behavior of the systems is the spin polarization. The formula of the investigated compound is $[M(NITm\text{-}Py)_2(N_3)_2(DMSO)_2]$[M=Cu(II), Ni(II), NITmPy=2-(3'-pyridyl)-4,4,5,5-tetramethylimidazoline-1-oxyl-3-oxide]. Our calculations are based in the pseudopotential scheme and the density functional theory within the generalized gradient approximation (GGA) for the correlation and exchange functional, using the PWscf(Plane-Wave Self-Consistent Field) code. Within this methodology we are able to calculate, with good accuracy, a lot of physical quantities of interest as such, local magnetic dipoles, magnetic coupling and charge transfers. The experimental analysis shows a weak ferromagnetic interaction between the metal ions (Cu, Ni) and the NITmPy radical, and the magnetic coupling constant is 7.43 cm^{-1} and 3.41 cm^{-1} respectively. The theoretical results confirm this weak ferromagnetic interaction. We found the values 8.06 cm^{-1} and 3.82 cm^{-1} for Cu(II) and Ni(II) complexes. In table I, we show the spin population on nitronyl nitroxide radical (O3-N7-C21-N8-O8) and metal ion for complexes 1 and 2.

Table 1: Spin population on nitronyl nitroxide radical and metal ion for complexes 1 and 2

Complex 1		Complex 2	
Cu	0.41	Ni	1.35
N7	0.26	N7	0.25
N8	0.26	N8	0.25
C21	-0.11	C21	-0.11
O3	0.31	O3	0.28
O4	0.29	O4	0.30

References

[1] O. Kahn, Molecular Magnetism, VCH, New York, 1993.
[2] S. Baroni, A. Dal Corso, S. De Gironcoli, P. Giannozi, C. Cavazzoni, G. Ballabio, S. Scandolo, G. Chiarotti, P. Focher, A. Pasquarello, K. Laasonen, A. Trave, R. Car, N. Mazari, A. Kokalj, http://www.pwscf.org.
[3] Yun-He, Xiao-Ni Qu, Hai-Bin Song, Li-Cuan Li, Zong-Hui Jiang, Dai-Zheng Liao, Polyhedron 26, 741-747, 2007.
[4] Cheng-Bu Liu, You-Min Sun, Bin Zheng, Ruo-Xi Wang, Chemical Physics Letters 411, 416-422, 2005.