

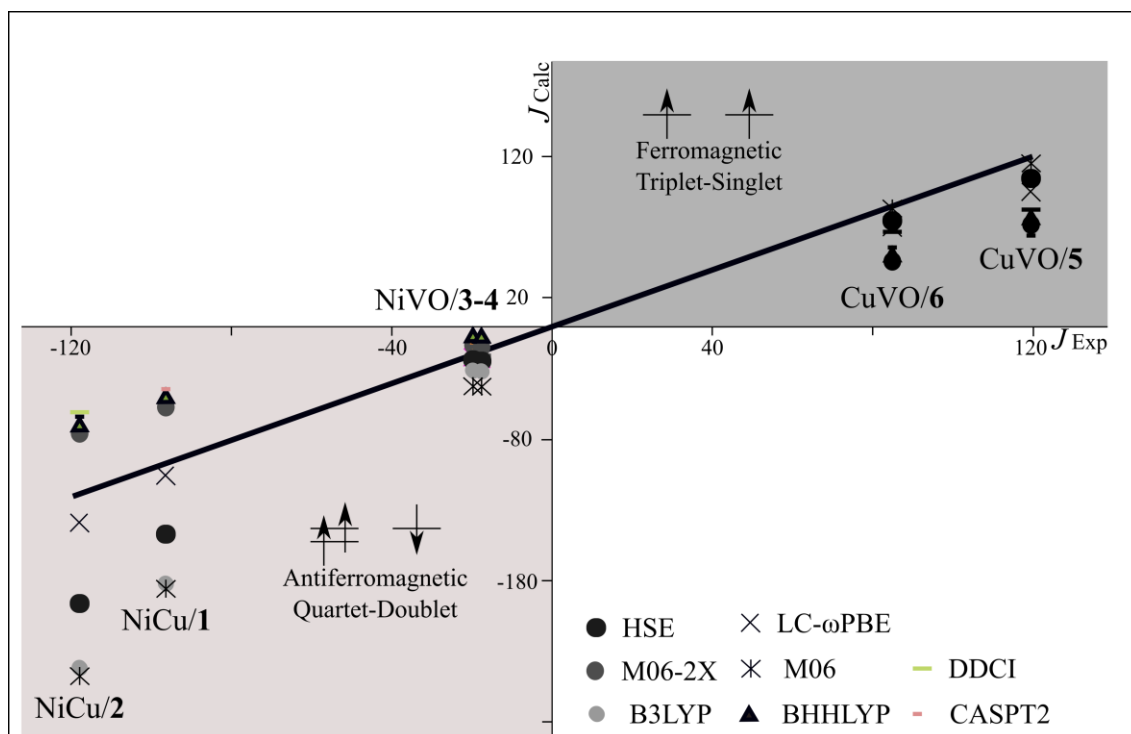
MAGNETIC COUPLING IN HETERODINUCLEAR COMPLEXES

D. Reta Mañeru^{*,1,2} R. Costa,^{2,3} R. Valero,⁴ I. de P. R. Moreira,^{1,2} F. Illas^{1,2}

¹Departament de Química Física & ²Institut de Química Teòrica i Computacional (IQTCUB). ³Departament de Química Orgànica, Universitat de Barcelona, C/Martí i Franquès 1, 08028 Barcelona, Spain. ⁴Center for Superfunctional Materials, Department of Chemistry, School of Natural Science, Ulsan National Institute of Science and Technology (UNIST), UNIST-gil 50, Ulsan 689-798, Korea

*e-mail: dreta@ub.edu

A family of heterodinuclear magnetic complexes displaying different spin moment in each magnetic center ($S_a=1/2; S_b=1/2$ and $S_a=1; S_b=1/2$) was used to study the performance of a series of wave function and density functional theory based methods for predicting magnetic coupling constants. It is found that for the first case in which the two magnetic centres bear the same spin moment, the accuracy is similar to other simple cases involving homodinuclear complexes,^[1] the main limitation being a sufficient inclusion of dynamical correlation effects. However, for the second case, special care is needed when using broken symmetry approach to describe the magnetic interaction. The existence of a local triplet in one of the magnetic centres makes impossible to univocally define a spin projector to reconstruct the pure spin doublet state from broken symmetry solutions. Despite this, an appropriate mapping procedure is derived guided by the expectation value of the total spin operator. Moreover, present results also show that current implementation of spin flip techniques leads to unphysical results



- 1) Moreira, I. de P. R.; Illas, F. A Unified View of the Theoretical Description of Magnetic Coupling in Molecular Chemistry and Solid State Physics. *Phys. Chem. Chem. Phys.* **2006**, *8*, 1645–1659.