Symmetry-induced interference effects in metalloporphyrins wires

R.Ferradás[1,2], V.M.García-Suárez[1,2,3] and J.Ferrer[1,2,3]
[1] *Departamento de Física, Universidad de Oviedo, 33007 Oviedo, Spain*
[2] *Nanomaterials and Nanotechnology Research Center, CSIC-Universidad de Oviedo, Spain*
[3] *Department of Physics, Lancaster University, Lancaster LA1 4YW, United Kingdom*

Organo-metallic molecular structures where a single metallic atom is embedded in the organic backbone are ideal systems to study the effect of strong correlations on their electronic structure. In this work we calculate the electronic and transport properties of a series of metalloporphyrin molecules sandwiched by gold electrodes using a combination of density functional theory and scattering theory. The impact of strong correlations at the central metallic atom is gauged by comparing our results obtained using conventional DFT and DFT+U approaches. The zero bias transport properties may or may not show spin-filtering behavior, depending on the nature of the d state closest to the Fermi energy. The type of d state depends on the metallic atom and gives rise to interference effects that produce different Fano features. The inclusion of the U term opens a gap between the d states and changes qualitatively the conductance and spin-filtering behavior in some of the molecules. We explain the origin of the quantum interference effects found as due to the symmetry-dependent coupling between the d states and other molecular orbitals and propose the use of these systems as nanoscale chemical sensors. We also demonstrate that an adequate treatment of strong correlations is really necessary to correctly describe the transport properties of metalloporphyrins and similar molecular magnets.

[1] D. Dolphin, *The Porphyrins Handbook*, Academic, New York (1978)
[2] M. Liao and S.Scheiner, *Electronic structure and bonding in metal porphyrins*, Journal of chemical Physics **117**, 205 (2002)
[3] J. Otsuki, *STM studies on Porphyrins,* Chemical Review **254**, 2311 (2010)
[4] V.I. Anisimov, J. Zaanen and O.K. Andersen, *Band theory and Mott insulators: Hubbard instead of Stoner I*, Physical Review B **44**, 943 (1991)
[5] A.I. Liechtenstein,V.I. Anisimov and J. Zaanen, *DFT and strong interactions: Orbital ordering in Mott-Hubbard insulators*, Physical Review B **52**, 5467 (1995)
[6] C. Tablero, *Representations of the occupation number matrix on the LDA/GGA+U method*, J. Phys.:Condensed Matter **20**, 325205
[7] M. Cococcioni and S. Gironcoli, *Linear response approach to the calculation of the effective interaction parameters in LDA+U method*, Physical Review B **71**, 035105 (2005)
[8] R.E. Sparks, V.M. García-Suárez, D.Zs. Manrique and C.J. Lambert, *Quantum interference in single molecule electronic systems*, Physical Review B **83**, 075437 (2011)