TRANSPORT THROUGH ORGANIC MOLECULES CONTAINING MAGNETIC ATOMS: EFFECTS OF SYMMETRY AND COULOMB INTERACTION

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Recent STM experimental studies on transport through CoPc and TBrPP-Co molecules adsorbed on metallic surfaces have reported several interesting results[1,2,3]: i) A high Kondo temperature as compared to those of adsorbed undressed magnetic atoms, ii) the Kondo resonance shows up either as a Kondo peak (CoPc) or as a Fano dip (TBrPP-Co), iii) the Kondo temperature depends strongly on the molecule conformation and can be manipulated experimentally, iv) in the case of TBrPP-Co two conductance peaks well below and above the Fermi level are observed, whose existence depends on molecule conformation.

In this work we discuss a simple model (Fig. 1) that, capturing the main features of the inner structure of the molecule, offers a physical interpretation for most of the main observations of those experiments[4]. In addition, it allows predicting the behavior of the system upon other symmetry or conformational changes, or when the STM tip is moved away from the Co atom (the usual point at which measurements were taken). The most relevant model parameters are the lobe-lobe hopping, the Co-tip hopping and the lobe-tip hopping.

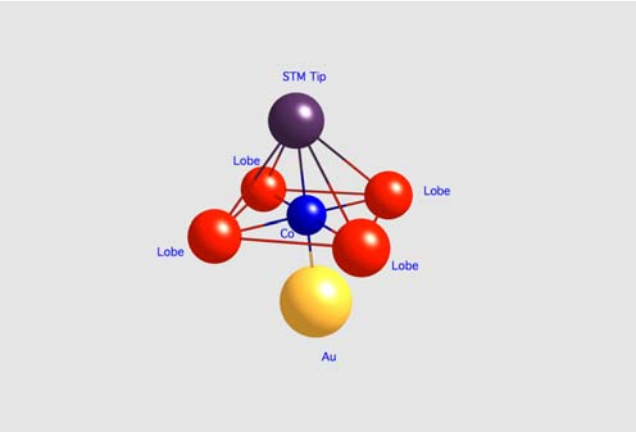

Fig. 1. Scheme of the small system used to describe the molecules here investigated. Lobes are also connected to the metal surface (through a self-energy) but this connection is not explicitlyshown for the sake of clarity.

[1]Zhao, A.; Li, Q.; Chen, L.; Xiang, H.; Wang, W.; Pan, S.; Wang, B.; Xiao, X.; Yang, J.; Hou, J.G.; Zhu, Q., *Science* **309**, 1542 (2005).

[2]Iancu, V. ; Deshpande, A.; Hla, S.-W.; *Phys. Rev. Lett.* **97**, 266603 (2006).

[3]Iancu, V.; Deshpande, A.; Hla, S.-W., *Nano Lett.* **6**, 820 (2006).

[4]J. M. Aguiar-Hualde, G. Chiappe, E. Louis, and E. V. Anda; Phys. Rev. B **76**, 155427 (2007); G. Chiappe and E. Louis; Phys. Rev. Lett. **97**, 076806 (2006)