Theory of Spin Crossover Molecules on Metal Surfaces: From Surface Science to Quantum Information

DIRECTEUR DE THESE : MEBAREK ALOUANI
INSTITUT DE PHYSIQUE ET CHIMIE DES MATERIAUX DE STRASBOURG
TEL : 03 88 10 70 06 ; E-MAIL : MEA@IPCMS.UNISTRA.FR

The manipulation of the electron spin degrees of freedom has opened new avenues in the way the computer information is stored and novel electronic devices with low energy consumption [1]. Organic molecules with low-spin high spin-spin transition will certainly play a crucial role in the development of this exciting field of research and are the subject of this theoretical PhD project. This research will focus essentially on (1) the description of the interaction of a single spin crossover molecule or a bundle of molecules with a metallic ferromagnetic or paramagnetic substrate by treating correctly the electronic correlation within the dynamical meanfield theory [2] and the van der Waals interaction, (2) the physics of spin polarized transport on STM mode in order to characterize these hybrid systems and make a direct contact with experiment [3]. The project will use ab initio methods together with the description of the van der Wall dispersive forces to describe both long and short-range interactions of molecular systems on metallic surfaces. The work will then be extended to quantum transport using non-equilibrium Green's function and the Landauer formalism [4]. We can then determine STM images beyond the s-wave tip Tersoff-Hamann approximation, where the intensity of the current is proportional to the local density of states of the system [5].

This PhD project will focus particularly on spin crossover complexes such as $Fe(Phen)_2(NCS)_2$, (Fephen) where the transition of Fe^{2+} between low-spin and high-spin states can be triggered by light, temperature, electric field. Our previous studies [6] will be extended to magnetic surfaces. We will explore the possibility to improve or restore bi-stable behavior when an ultrathin dielectric layer, such as nitride or Al_2O_3, covers the magnetic substrate and the effect of the substitution of H by electronegative Cl or NH2 ligands on the energy barrier of the spin transition.

References:

[1] S. A. Wolf *et al.*, "Spintronics : A Spin-Based Electronics Vision for the Future", **Science 294**, 1488 (2001).

[2] A. Georges et al., Rev Mod. Phys. **68**, 13 (1996).

[3] T. Miyamachi, et *al.*, Nature Communication **3**, 938 (2012).

[4] A. R. Rocha *et al.*, Nature Materials **4**, 335 (2005).

[5] J. Tersofff and D. R. Hamann, PRL **50**, 1998 (1983) and Phys. Rev. B **31**, 805 (1985).

[6] S. Gueddida and M. Alouani, PRB **87**, 144413 (2013); PRB **93**, 184433 (2016).