THEORY OF MOLECULE/METAL SPINTERFACES

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Electronic spin effects have open promising perspectives in the field of information data storage [1]. Indeed, injection, transport, control and detection of spin polarized currents give access to new components based on this additional spin degrees of freedom. The progress in this topic is due to the description of the spin polarized transport properties. In particular, hybrid systems like metal/organics represent an important class of such materials. Giant magnetoresistance junctions, tunnel junctions [2] or magnetotransport through a unique molecule [3] are major advances. This research has also underlined the fundamental role of molecular arrangement near the metal substrate. The understanding of of the physics is only partial due to the lack of a theoretical frame to describe the relations between growth and electronic transport. In this project, the aim is to describe the interactions between a unique metalphthalocyanine molecule (MPc) and a ferromagnetic metallic substrate like Co or Fe, or a paramagnetic substrate like gold or copper, and where M= Mn or Co. We will focus especially on, (1) the role played by van der Waals interaction, (2) tunnel microscopy image modelisation (STM) for the characterization of these hybrid systems, and more particularly on (3) the determination of surface states energies between the highest occupied and the lowest unoccupied molecular Orbitals of the molecule. This project is based on ab initio methods to describe both short and long range electron-electron interactions. Indeed, the determination of the molecule/substrate geometry must take into account the molecule-substrate interaction, leading to physi- or chimisorption regarding the strength of the interaction, and the molecule-molecule interaction, of van der Waals (VdW) type, which is also weak as in the case of physisorption. The complexity of the VdW force is the reason of a poor knowledge of the interaction between a single molecule and a substrate, leading to a poor understanding of the interface structure. For this reason, it is essential to know the effect of such interaction over the distance between the single molecule and the surface, as well as its orientation, and more precisely, the influence of the metallic atom in the phthalocyanine on the electronic structure of the molecule and the substrate [4].

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