MASTER 2 INTERNSHIP PROJECT

Institut des Sciences Chimiques de Rennes - Theoretical Inorganic Chemistry group

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Impact of surface grafting on Single Molecule Magnets properties: a theoretical (DFTB) study

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Single Molecule Magnets (SMM) allow to carry a magnetic information at the molecular level that can be switched, typically upon heat.[1] For a use in nanoscaled solid-state devices, SMMs have to be immobilized, for instance on a metallic substrate. In fact, SMMs adsorbed on surfaces as magnetic building blocks represent a hot topic of research in the area of molecular magnetism. However, understanding the properties of such complexes and fragile molecules once deposited is extremely challenging, as atomistic structures are not readily available. In this regard, theoretical studies, as reliable tool to reproduce and predict the structure and the magnetic ground state of SMMs in the bulk phase and adsorbed on a surface, are considered very appealing. More specifically, one efficient family of SMM that will be modeled in this project is built on four Fe(IV) atoms arranged as depicted in Figure 1. Indeed, Experimental works already showed that a network of such molecules on a gold (111) surface is expected to retain its intrinsic magnetic behavior.[2]

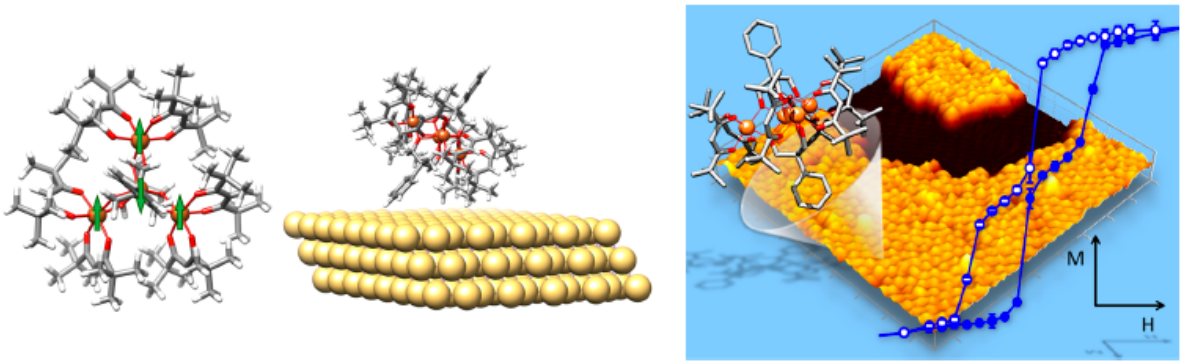

***Figure 1**: Representation of the isolated Fe-based SMM, of the grafted molecule on Au(111), and experimental characterizations.*[2]

Despite some recent theoretical efforts to model the whole surface/SMM systems,[2] this type of quantum calculation remains challenging and costly in term of computational resources. In this context, the student will assess the accuracy of faster calculation schemes, especially the so-called « Tight-Binding DFT » method (DFTB) for the description of such nanosized system. After validation, DFTB will permit to consider for example a dynamical approach to search for the conformational possibilities in the grafting process of the molecule, and to obtain rapidly the corresponding magnetic behavior of the device (within minutes to a few hours) that will be compared to experimental data. Such DFTB methods are fast because they are parameterized, depending on the nature of the atoms in the system. Previously published parameters for Fe, Au and organic atoms[3,4] will be first tested and new parameters will be potentially developed to reach a better description of the targeted properties.

1- *Chem. Rev.*, **2013**, *113*, 5110-5148.
2- *Nano Lett.*, **2015**, *15*, 535-541.
3- *J. Chem. Theory Comput.*, **2007**, *3*, 1349-1367.
4- *J. Comput. Chem.* , **2015**, *36*, 2075-2087.