PhD position Computational Physics, between Strasbourg University, France and Karlsruhe Institute of Technology (KIT), Germany

Strasbourg University and KIT invite applications for a **PhD position in Condensed Matter theory about the physics of molecules on metallic surfaces.** The PhD student will work in the group of Prof. Mebarek Alouani at the Institute of Physics and Chemistry of Materials of Strasbourg (IPCMS), France (http://www-ipcms.u-strasbg.fr), with a collaboration with Prof. Wolfgang Wenzel, at KIT, Germany (http://www.kit.de/english). Both institutes are renowned for their research on electronic structure of materials and multiscale modeling, and in particular, in magnetism and spintronics. The two institutes are part of the EUCOR European Campus and are located about 60 km from each other.

The theoretical work will focus on (1) the description of the interaction of a single molecule or a bundle of molecules with a metallic ferromagnetic or paramagnetic substrate by treating correctly the van der Waals interaction, (2) the spin polarized transport properties on **scanning tunneling microscope (**STM) mode in order to characterize these hybrid systems and make a direct contact with experiment. The work will then be extended to compute the quantum transport using non-equilibrium Green's function and the Landauer formalism. This generalization will allow us to determine STM images beyond the well know s-wave tip Tersoff-Hamann (TH) approximation, where the intensity of the current is proportional to the local density of states of the system [1]. The difficulty of computing the STM images beyond the TH approximation is that one has to move the tip over the molecule and compute the current at each step. This is where the experience of the KIT group of Prof. Wolfgang Wenzel will come to the rescue. His group has developed a world-class numerical code to compute accurately the conductance and have used it to understand multilevel atomic-scale transistors based on metallic quantum point contacts and switchable atomic quantum transistors [2-4].
This PhD project will use therefore the experience and complementarity of the two groups to focus particularly on spin crossover complexes such as $Fe(Phen)_2(NCS)_2$, where the transition of Fe^{2+} between low spin and high spin states can be triggered by light, temperature, electric field [5,6]. Our previous studies on non-magnetic surfaces will be extended to magnetic surfaces like Co(001), which is a model system before the integration of these systems into spintronics devices. We will also address the presently open question whether the magnetic polarization at the interface from a magnetic substrate can only stabilize a high spin ground state. As an extension of our previous work related to $Fe(Phen)_2(NCS)_2$/Cu [6,7], we will explore theoretically 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. The second hybrid system is constituted of porphyrin moieties functionalized with photochromic groups. In the latter situation, new diarylethenes (DAE)-based porphyrins are synthesized, and their switching behavior in the solid and in solution has been established. The next step

will be the deposition in UHV by our experimental partners on a copper or cobalt surfaces, via the photochromic units. The electronic/magnetic coupling between the porphyrin moieties and the substrate will be optically triggered via the DAE behavior to switch the molecule. The theoretical work will address the geometry of adsorption of the molecule for different conformations of the DAE units, the intensity of the magnetic coupling between the ferromagnetic substrate and the molecule when the porphyrin unit is substituted by a M^{2+} ion like Mn. We will determine the change of the electronic and optical spectra due to the interaction with the metallic surface.

References

[1] J. Tersofff and D. R. Hamann, Theory and application for the scanning tunneling microscope, Phys. Rev. Lett. 50, 1998 (1983) and Phys. Rev. B 31, 805 (1985).
[2] F.Q. Xie et al., Independently Switchable Atomic Quantum Transistors by Reversible Contact Reconstruction. Nano Letters 8, 4493 (2008).
[3] F.Q Xie et al., Multilevel Atomic-Scale Transistors Based on Metallic Quantum Point Contacts, Advanced Materials 22, 2033 (2010).
[4] Branchi et al. Self-Assembled Metal-Terpyridine Wires for Robust Large Area Molecular Devices, Adv. Materials (in press).
[5] T. Miyamachi, et al., Spin Crossover-induced Robust Memristance across a Single Molecule, Nature Communication 3, 938 (2012).
[6] S. Gueddida and M. Alouani, Phys. Rev. B 87,144413 (2013).
[7] S. Gueddida et al., Exchange Coupling of Spin-Crossover Molecules to Ferromagnetic Co Islands, Phys. Chem. Lett. 7, 900 (2016).

Qualifications

Applications are welcomed from candidates with M.Sc. degree (or equivalent) in physics with a strong background in solid state physics, quantum mechanics, statistical physics and computational solid state physics. Computer and programing/scripting skills are highly desirable. The interested candidate should be strongly self-motivated, to show a keen interest in science and fundamental research, and be willing to work at both IPCMS and KIT (about 60 km from Strasbourg).

Appointment

The time of appointment is limited to the equivalent of three years of full time research training. You further will actively participate in the PhD training activities, and complete 60 ECTS credits required for a PhD courses at Strasbourg University. Starting time is fall/winter 2017 (by agreement). The take home salary for PhD students is about 1300 euros/month, and the travel to KIT will be fully paid by the French-German University.

Application

Please send a letter of motivation, together with your CV, Bachelor and Master transcripts and a letter of recommendation to Prof. Mébarek Alouani (email: mea@ipcms.unstra.fr). Your application must be received before September 1st, 2017.