METAL-MOLECULE INTERACTION FOR NANOELECTRONICS BY ATOMIC-SCALE DYNAMICAL SIMULATIONS

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The realization of metal-molecule nano-junctions for future electronic devices relies on our understanding of the nature of the fundamental interaction of the target molecules to be used and the underlying metallic surface. A lot of efforts have targeted so far planar metal-organic molecules, specifically phtalocyanine. Instead, in this project we propose to focus on three-dimensional “double-decker” molecular building block, namely ferrocene. On the theoretical side, our computational efforts (see Phys. Rev. Lett. **107**, 216801 (2011), provided a first evidence for a successful deposition of ferrocene on a clean Cu(111) surface. The PhD candidate is expected to work in the field of atomic-scale simulations focusing on the project proposed here, aiming at pursuing computer experiments in which different metal atoms (Cu, Co, Au, Fe, etc.) will be deposited on top of ferrocene molecules placed on the Cu(111) surface, thus leading to the realization of the complete junction metal-molecule-metal and by extending our simulations to a full monolayer of double-decker molecules. This can provide understanding of the peculiar delocalized interface states near the metal Fermi level, which are considered a key ingredient for tailoring charge injection. Since it is unclear how such interface states respond to a subsequent deposition of single metal atoms and electron excitations, the present project is prone to provide the still missing knowledge and to serve as a guideline to experiments and practical applications.

The candidate will work within first-principles molecular dynamics approaches, combined with free energy sampling techniques, based on the density functional theory (DFT) and exploiting either the free energy functional (FEMD) formalism, or the Born-Oppenheimer one. Both these approaches are available in our computer codes (CPMD, CP2k), for which we are co-developers. Given the generality of the theory behind, an initial period of intensive training will be provided to a newcomer student in order to make the applicant familiar with these complex algorithms and to provide her/him the background needed to the targets proposed here.

The simulations required by this project can be classified as massively parallel computer applications for which high performance computing (HPC) platforms are available at national centers (CINES, IDRIS) and at. local resources at our institute thanks to the HPC of the Pôle Matériaux et Nanoscience d’Alsace (PMNA).

The computational research group includes the thesis director mentioned above, Dr. Carlo MASSOBRIO (DCMI), Dr. Christine TUGENE (IPCMS-Informatique) and PhD students already working in realted fields. The candidate will be warmly invited to interact with proficiency with all the members of the research group.