Proposal for a PhD research project

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Synthesis of molecular architectures on the Si(100):H surface for molecular devices

Nanosciences is a very young research domain that needs to tackle various exciting challenges. One of them involves assembling molecules on metallic or semiconducting surfaces to obtain molecular architectures which properties (including optical, electronic, magnetic or chemical) can be explored. Such molecular architecture can be used for specific purposes such as bistability, memory, molecular operator or photon sources. However, the study of a molecular architecture made of few molecules is rarely studied with the good environmental conditions. In this context, the purpose of the thesis will be to study the electronic properties of simple molecular circuits formed with few molecules whose individual electronic properties will be pre-selected among various molecular types. For this, we will use a scanning tunneling microscope working in ultrahigh vacuum and at low temperatures (9K) to allow the assembly and the analysis at the atomic scale of the molecular architecture. The molecules will be adsorbed on the passivated Si(100) surface (or Si(111)) with hydrogen. This surface is very versatile and allow to decouple electronically the adsorbates from the silicon surface (Nanolett. 9, 144 (2010)). The molecular circuit will be either contacted on metallic pads ($CoSi_2$ silicides) or via wires that can be written on the Si(100):H surface by the removal of H atoms at the atomic scale.

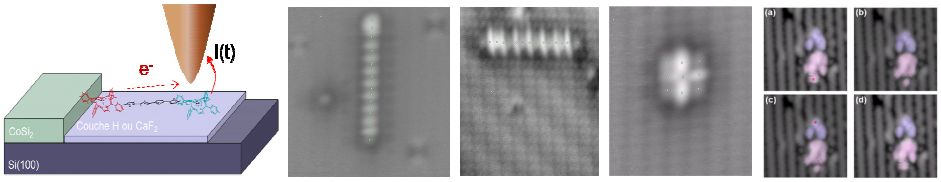

Figure: (left) Sketch of an of a molecular circuit connected to a metallic pad. (Center) example of dehydrogenated structures. (right) contacting a bi-molecular switch.

These wires are molecular orbitals that allow drawing, atom by atoms, shaped wires adapted to the connection of molecules between them via the subsurface states. By choosing the molecules redox potentials in a proper way among various molecular families (ferrocene-like, porphyrins, phthalocynins, TCNQ, pentacene), it is possible to move the molecules across the surface and fix them at a given place relatively to the wire or the metallic pad. In a second step, the aim will be to transfer one or several electrons from one side of the circuit to the other. The circuit will be activated by the STM tip as well as the analysis of the conformation change in the circuit. Several architectures can be studied with growing complexity as various geometrical conformations will be tested giving rise to specific properties of the molecular circuit.

The PhD candidate should have very good experimental skills, good knowledge in physical chemistry, molecular and solid state physics. He/she will be strongly involved in the analysis of the experimental data and the modeling of physical phenomena. Different types of simulations (DFT,TD-DFT) can be achieved at either ISMO or through external collaborations. **Visit our website for related publications** http://www.ismo.u-psud.fr/spip.php?rubrique104