PhD 2020-CSC

Charge transfer at the nanoscale with STM

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Keywords: scanning tunneling microscope, molecule, surface, silicon, STM/AFM, charge transfer

Context:
Charge transfer processes are at the heart of our daily life as they are covering various fields such as biology (photosynthesis), chemistry (catalysis), electronics (OLED, solar cells), or even energy (photovoltaic cell, energy storage). While all these processes usually involve mesoscopic descriptions, the origin of charge transfer phenomena occurs at the nanoscale. It is therefore particularly judicious to access information at the right scale to provide further understanding and describe new aspects of these processes (adiabatic transfers, coherent/resonant tunnel, superexchange, etc ...). Ultra-low temperature tunneling microscopy is an ideal tool for this type of study. Recently, we demonstrated that relevant information on charge transfer dynamics can be derived in a single molecular switch or molecular dyade [PCCP 2017, 19, 28982, Nanoscale, 2018, 10, 17603].

Internship contour and requested skills: The PhD will start in 2020. After a training period, the candidate will participate to experiments. The work of this thesis aims, in a first part, to study charge transfer in non-covalent molecular homo or heterodimers composed of metalloporphyrins in order to explore a wide range of charge transfer processes. The second part will focus on the study of charge transfer with in-situ covalently bonded heterodimers in order to understand the influence of the symmetry and the role of a certain type of molecular orbitals. A third part will treat the case where charge transfer occurs in non-covalent trimers. Here, the central molecule will acts as a molecular bridge and these devices will allow to study amplification phenomena via eg. superexchange processes. The experiments will use a scanning tunneling microscope operating under ultra-high vacuum and low temperature (9 K). The dynamics of the charge transfer will be studied by the analysis of the molecular structure during conformational change and via light luminescence analysis.

Student Profile: The student should have serious knowledges in fundamental physics and physical-chemistry in order to be able to apprehend the molecular properties and structures used as well as the interactions of molecules with the surface. The student’s profile should be mainly oriented to the realization of experimental work. Basic knowledges on tunneling microscopy are essential. Notions about numerical simulations in quantum chemistry would be appreciated. Autonomy, rigor, motivation, dynamism and a good sense of organization will be essential skills to run these research. This PhD will be involved in the daily use of various techniques starting from ultra-high vacuum and cryogenic STM/AFM, with also signal processing and optics providing a complete set of expertise in these domains after the doctorate.

1H. Labidi, H.P. Pinto, J. Leszczynski, D. Riedel, Exploiting a single intramolecular conformational switching Ni-TPP molecule to probe charge transfer dynamics at the nanoscale on bare Si(100)-2x1, Phys. Chem. Chem. Phys., 2017, 19, 28982–28992.
2P. Ramos, M. Mankarious, M. Pavanello, D. Riedel Probing charge transfer dynamics in a single iron tetraphenylporphyrin dyad adsorbed on an insulating surface Nanoscale 2018, 10, 17603-17616.