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# Scanning Tunneling microscopy and Local Electric field

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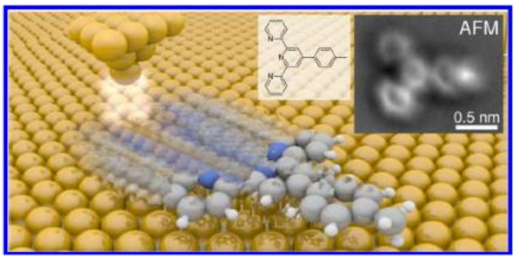
| **Period** | 6 months beginning not later than:<br>☐ January ☐ February ☑ **March** ☐ April ☐ May ☐ June ☐ July ☐ September 2021 |
| **Internship supervisor(s)** | name: Dr. Xavier BOUJU<br>e-mail: xavier.bouju@cemes.fr<br>group: Nanosciences group |
| **Location** | CEMES-CNRS,<br>29 rue Jeanne-Marvig<br>31000 TOULOUSE - FRANCE |
| This research master's degree research project could be followed by a PhD | ☐ YES ☑ **NO** |

The scanning tunneling microscope (STM) provides remarkable images of surfaces, with or without adsorbates, at the atomic scale. The STM probe also offers the possibility of manipulating individual atoms or molecules. Understanding the underlying physical mechanisms, that is, the interactions between the STM tip and the sample, has resulted in various manipulation methods. One implies the electric field inside the STM junction [1] due to a bias voltage between the probe and the substrate. Diffusion or desorption of molecules on surfaces can be induced by this local electric field.

This electric field under the STM tip has a spatial extent determined by the size of the tip apex (typically a few tens of nanometers in diameter). Depending on the polarization voltage and the tip-to-surface distance, the electric field strength can be adjusted. More precisely, there are two mechanisms to explain the forces induced by the electric field. First, diffusion is triggered by the interaction between the inhomogeneous electric field near the tip apex and a local dipole moment induced in the adsorbate. This is the so-called induction force, which is a function of the multipolar polarizability of the adsorbate. The force is always attractive and has the direction of the electric field gradient (independent of the sign of the polarization voltage). The second mechanism involves charged atoms or molecules or molecular adsorbates having a static dipole moment. Here, charge transfer between the substrate and the adsorbate can cause such a dipole or if the molecular adsorbate exhibits a permanent dipole. We will consider the latter case with molecules specifically designed for the second edition of the NanoCar Race in 2021. Depending on the polarity of the electric field and its gradient, the force is either repulsive or attractive towards the tip.

The calculation of the field requires special attention because of the reduced geometry of the junction. Likewise, confinement effects are at work for the van der Waals-type interaction forces between the tip and the adsorbed molecule. The purpose of this internship will be to tackle this problem from theoretical and numerical aspects. The internship can therefore be developed in two stages. First of all, the student will be familiarized with existing calculation tools in the form of STM image simulations. Then, and this will constitute the heart of the internship, the confinement effects of the electric field and of the van der Waals forces will be carried out by the development of an adapted analytical method (in the form of field propagators) before code implementation to study the controlled manipulation of adsorbates by enhanced field effect.

The candidate will be able to acquire skills in computer numerical simulation and in surface physics during this internship.



From [2]. Displacement under an electric field, generated by an STM tip, of a molecule that participated in the 2017 NanoCar Race[3]. Inset, image of the molecule obtained by atomic force microscopy.

References:
[1] *Recent advances in submolecular resolution with scanning probe microscopy*, L. Gross, Nature Chemistry **3**, 273 (2011).
[2] *Design and Characterization of an Electrically Powered Single Molecule on Gold*, R. Pawlak *et al.*, ACS Nano **11**, 9830 (2017).
[3] http://nanocar-race.cnrs.fr/ and for 2021 https://www.memo-project.eu/flatCMS/index.php/Nanocar-Race-II

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| **Keywords, areas of expertise** | Surface science – STM – Manipulation – Calculation – Simulation — Electric field |
| **Required skills for the internship** | Fortran — Condensed matter physics |