NECEM Seminar: Interpretation of STM results with the help of numerical calculations

Dr. Xavier Bouju, CEMES-CNRS, France

14:00pm-15:00pm, 21st November 2018

Lecture Theatre 1.46, Barbara Strang Teaching Centre, Newcastle University

Refreshments available after the seminar

All welcome

Abstract

Interpretation of STM results with the help of numerical calculations

For decades, local-probe based methods like STM and AFM have demonstrated an extraordinary ability to provide images of molecules on various surfaces with atomic resolution as well as their capability to manipulate single atoms or molecules on surfaces with a high degree of precision. In parallel to these experimental developments, an important theoretical effort of image interpretation has been performed. Actually, due to many physical effects inherent in these techniques, calculations are necessary to explain experimental results, and theoretical models were proposed giving rise to several numerical codes, each of them having specific functionalities or at least having a particular range of validity. More explicitly, an important step prior to the STM calculations themselves consists in performing molecular mechanics and/or dynamics simulations. Indeed, the conformations of molecular adsorbates have to be determined inside the STM junction due to the interaction with the surface and with the probe tip in specific cases. During this seminar, I shall show the set of examples obtained by our group in Toulouse. A particular focus will be on the role of adatoms on the molecular self-assemble in the STM images. Finally, numerical experiments have been conducted to explain the mechanical behaviour of adsorbed molecules and the controlled manipulations of molecular nanocars.

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Dr. Xavier Bouju Biography

I am a CNRS research scientist working in CEMES-CNRS. My current research deals with calculations on chemical and physical properties of single molecules and molecular assemblies interacting with metallic, semiconducting, and insulating surfaces, with an emphasis on STM and AFM images calculations.

Keywords : adsorption, single molecule, self-assembly, STM, AFM, image calculations, optical force. Nanosciences. Nano-mechanics. Molecular dynamics and molecular mechanics.

Seminar Venue: Newcastle University, Barbara Strang Teaching Centre, Lecture Theatre 1.46