

Responsable :
Martine Logé
☎ 01 69 08 51 67

SEMINAIRE



Service de Recherches de Métallurgie Physique

DEN/DANS/DMN

Bibliothèque du SRMP – Bâtiment 520 – Pièce 109

***First-principles simulations of surfaces
and materials under pressure :
Applications of SIESTA method to some experimental problems***

Eduardo Machado-Charry

Laboratory of Electronic Structure of Materials
Institut de Ciència de Materials de Barcelona-CSIC,
Campus UAB, 08193 Barcelona, Spain

In the first part of this seminar, we will give a summary of results obtained by us in the last years in the fields of surfaces and III-VI compounds under pressure. Our Density Functional Theory (DFT) calculations have been carried out based in the SIESTA method and the corresponding code. One of the goals of this research has been to collaborate with experimental groups in order to achieve with the help of *ab-initio* calculations a better comprehension of some relevant systems.

Thus, in the field of surface science we highlight these topics:

- Study of the reactivity of transition metal barrier layers. An effort to get insights and in the poor adhesion problem in deposition of Cu films by CVD process using organometallic precursors.
- The structural determination of deposited C₆₀ monolayers on Ge surfaces.

In the field of III-VI materials under pressure we will show:

- The study of structural and electronic properties of the group of III-VI semiconducting compounds under hydrostatic pressure.
- The study of electronic structure of cubic GaS.

We will focus the second part of the seminar in the analysis of Charge Density Waves (CDW) STM Images Blue Bronze (Rb_{0.3}MoO₃) and Niobium triselenide (NbSe₃) quasi-one-dimensional compounds.

Recently, high resolution images by ultra-high vacuum Scanning Tunneling Microscopy (STM) of the (CDW) phase has been obtained on these compounds. The interpretation of these images has brought some questions, as for example, the role played by some superficial atoms in the features observed.

We will present our simulations carried out on these systems, considering both the phases before the transition and the modulated structures. These have provided a clear understanding of the nature of the experimentally observed STM images, and solve some questions in the interpretation of these images.

Mardi 9 Octobre 2007 à 10h30

N.B : *Les visiteurs de nationalité étrangère hors Union Européenne sont priés de bien vouloir avertir impérativement 3 semaines à l'avance - les visiteurs de l'Union Européenne 1 ou 2 jours avant le séminaire*
- *le Secrétariat du Service de leur entrée sur le Centre :*
Tel : 01 69 08 66 64 - Fax : 01 69 08 68 67

Commissariat à l'énergie atomique
SAC/DEN/DANS/DMN/SRMP/Bat 520
91191 Gif-sur-Yvette Cedex - France
☎ Tel : 01.69.08.66.64 - ☎ Fax : 01.69.08.68.67