ΠΑΝΕΠΙΣΤΗΜΙΟ ΚΡΗΤΗΣ
ΤΜΗΜΑ ΕΠΙΣΤΗΜΗΣ ΚΑΙ ΤΕΧΝΟΛΟΓΙΑΣ ΥΛΙΚΩΝ

ΠΡΟΣ

1) **Ολα τα μέλη ΔΕΠ του Τμήματος Επιστήμης και Τεχνολογίας Υλικών**
2) **Τους εκπροσώπους των Μεταπτυχιακών φοιτητών του Τ.Ε.ΤΥ**

3) **Την Επταμελή Εξεταστική Επιτροπή**
4) **Ολα τα μέλη της Πανεπιστημιακής Κοινότητας**

Πρόσκληση σε Δημόσια Παρουσίαση της Διδακτορικής Διατριβής του

κ. Μπαρμπαρή Γεώργιου

(Σύμφωνα με το άρθρο 12 του Ν. 2083/92)

Την Παρασκευή 5 Οκτωβρίου 2012 και ώρα 13:00 στην αίθουσα Σεμιναρίων 3ου ορόφου-Φυσικό

θα γίνει η δημόσια παρουσίαση και υποστήριξη της Διδακτορικής Διατριβής του υποψηφίου διδάκτορος του Τμήματος Επιστήμης και Τεχνολογίας Υλικών κ. **Μπαρμπαρή Γεωργίου** με θέμα:

«Environment-dependent shape and properties of gold nanoparticles: a first principles study».

ABSTRACT

In the present Thesis a computational study that links extensive quantum-mechanical calculations, based on density functional theory (DFT), to Wulff constructions in order to predict the environment-dependent equilibrium shape and properties of large gold nanoparticles is presented.
We firstly present the methodology used to obtain the equilibrium shape, including the main aspects of the density functional theory and the Wulff construction method. We continue by presenting the code developed to construct any clean or having a molecule adsorbed at a given site Au(*hkl*) surface. Then, we study the adsorption of CO and the dissociative adsorption of dimethyl disulfide (CH3S-SCH3) on every possible Au(*hkl*) with $h,k,l \leq 3$ plus the kinked Au(421) and we discuss trends on adsorption energies, bond lengths and bond angles as the surface structure changes.

We calculate the surface energy per unit area for clean surfaces and use it together with the Wulff construction method to predict the equilibrium shape of clean gold nanoparticle with diameters up to several tenths of a nanometer, inaccessible by direct atomistic simulations. We also present the codes developed to construct atomistic models of nanoparticles using the Wulff construction method and analyse the geometrical features of them. We point out a surprising agreement between Wulff construction, experiments, and atomistic simulations at small sizes. Au nanoparticles smaller than 16.3 nm in diameter have truncated octahedral shape, exposing only (111) and (100) faces. Larger nanoparticles also expose higher-index faces, mostly (332). Then we use the surface energies per unit area and the results for the adsorption energy to obtain the interface energy per unit area between Au and CO or Au and thiolates (CH3S-) at low pressure and temperature. These results are then used to obtain the equilibrium shape of CO- or thiolate-covered Au nanoparticles. In agreement with experimental data, Au nanoparticles in CO are found to be more spherical and more reactive compared to Au nanoparticles in noninteracting environments. Gold nanoparticles change their shape upon adsorption of thiolates towards shapes of higher sphericity and higher concentration of step-edge atoms. Finally, we check the stability of these nanoparticles through Molecular Dynamics simulations and we present a theoretical method providing shape-dependent spectroscopic properties of gold nanoparticles.