


Internship proposal 2009-2010

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Oxide nano-objects of original shapes and structures



Modern technologies enable fabrication of artificial objects of original and largely unexplored properties. One of major challenges is to master the adjustment of various properties of such objects (shape, structure, stoichiometry, reactivity, etc.) by a simple control of the fabrication environment (temperature, constraints imposed by the substrate, partial pressures of different gases in the fabrication chamber, pH, etc.). The understanding of the driving microscopic mechanisms stimulates a strong demand of realistic numerical simulations. If an important number of such studies

has been dedicated to metallic and semi-conducting nano-structures, insulating oxides, while abundant in our environment (minerals, clays, oxidized metal surfaces in contact with atmosphere), have yet received much less attention.

With a direct relation to experiments in progress in our group, we propose a theoretical study of the effect of metal support on the shape and on the atomic structure of small oxide nano-objects (the effect of elastic constraints due to lattice mismatch with the metal substrate, its behavior as a function of object size, the resulting interface structure and properties), aiming the identification of experimentally accessible parameters which may enable practical fabrication of nano-objects of desired properties.

Techniques in use:

Due to large sizes and structural complexity of proposed systems the study remains well beyond the possibilities of ab initio approaches. We thus propose to use an original approach developed in our group which, while being based on a self-consistent quantum description of the electronic structure, remains very efficient numerically. On a more technical level, the stage may contain a module devoted to code optimization and/or to extension of the present model towards an efficient treatment of transition metal oxides.

Applicant skills :

Basic theoretical description of the electronic structure of solids.

Granted internship : yes (280 €/month)

C'nano IdF laboratory (France only) : yes

Possibility for a thesis : yes (type of grant : scholarship by French ministry)