PhD Proposal 2017

School: CentraleSupélec	
Laboratory: SPMS	**http://spms-appli.ecp.fr/perso/hichem/hichem.htm**
Team: Simulation and modeling, electronic structure	**Head of the team: P. Cortona**
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Collaboration with other partner during this PhD: **In France: Yann Chalopin, EM2C, ECP**	**In China:**

Title: ***Oxide nanoparticles: advanced modeling and simulation of optical and ferroelectric properties***
Scientific field: Nanomaterial Science
Key words: molecular dynamics, Infra-red absorption, nano-oxydes, thin-films

Details for the subject:

Background, Context:
Statistical Physics. Materials sciences. Numerical Simulation.

Research subject, work plan:

The number of areas impacted by nanotechnologies has significantly expanded in recent years. Applications exist in fields such as optics, biology, electronics, mechanics and chemistry. Nanoparticles (NP) are collections of a few hundred to a few thousand atoms (1-100 nm) which is at the boundary between atomic and macroscopic scales. Their different properties ï dynamic, thermal, electrical and optical ï are different from those of the bulk material and change according to their sizes. The optical and thermal properties of metal NPs [1-3] have been widely studied whereas mechanisms carried out in insulator or semiconductor NPs remain open questions. In the case of metals, the macroscopic approach (continuous media) has often been successfully used to explain the properties of NPs. We have recently shown that in the case of an oxide (MgO), this approach is inadequate and must be supplemented by modeling at the atomic scale [4].

The **aim** is to study size effects on the dielectric, ferroelectric and optical properties of oxide NPs as a function of temperature and frequency. In particular, the dielectric properties control on one hand the heating by the absorption of radiation and on the other hand the van der Waals interaction between NPs and between one NP and a surface [5]. The results will contribute to applications in the fields of energy, memory FeRAM (Ferroelectric Random Access Memory) and medicine.

The **first part** of the subject will consider the intrinsic properties of a single NP. A previous study has shown that the IR absorption of MgO NPs, with cubic symmetry and shape, is essentially due to the surfaces [4]. It is interesting to evidence this effect on other compounds giving NPs having different symmetry and/or shapes. The aim is to highlight behaviors and generic effects that may vary depending on the size and symmetry of NPs.

The **second part** will be devoted to the study of the properties of one NP located near a surface, near another NP or even inserted into a host matrix. The aim is to highlight attenuation or enhancement effect of dielectric, IR absorption or ferroelectric properties.

The computation of the properties of these NPs will be based on the use of the technique of molecular dynamics (MD) using phenomenological potentials or *ab initio* description of the interaction forces between atoms. However, the MD method is limited to high temperatures since it is based on the equations of classical mechanics. But, the temperatures of use of the NPs are less than the Debye temperature, which requires a study of the contribution of quantum effects. These effects are particularly important for the ferroelectric properties [6] and van der Waals interactions between NPs. These contributions will be evaluated through a universal quantum thermostat (QTB: quantum thermal bath) [7-8] we have developed to take into account the quantum statistics in MD simulations.

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