RECRUITMENT OF A 'CHARGE DE RECHERCHE' AT THE CNRS – 2019 CAMPAIGN

Laboratory: Institut de Chimie Moléculaire et des Matériaux d'Orsay (ICMMO)
Team: Synthèse, Propriétés et Modélisation des Matériaux (SP2M)

Theme: Numerical simulations of heterogeneous systems based on oxides: functional oxides, multilayers, defects, surface reactivity, metal/oxide interfaces, oxidation. Development of realistic semi-empirical atomic models.

Detailed profile: Oxides are the most abundant natural materials and are becoming increasingly important in modern technologies, such as electronics, spintronics, energy and environment. This is due to the fact that oxides may be insulating, semiconductors, conductors, or magnetic, leading to a wide diversity of their electronic properties (superconductivity, ferroelectricity, thermoelectricity, giant magnetoresistance...). Oxides are rarely used as bulk materials but rather in the form of multilayers, thin layers, nanoparticles or dopant, which allows modifying the electronic, thermal or mechanical properties of the material as a whole. One particular field relates to oxidation, a phenomenon to which any material in contact with the atmosphere is subjected, and its corollaries which are corrosion and surface reactivity of the materials with oxygen or any other oxidant.
Numerical simulations of heterogeneous systems require considering a large number of atoms (a few hundreds of thousands) and treating the kinetic aspects. Therefore, these are still out of reach of purely ab initio calculations, although the latter are essential in the development of semi-empirical potentials needed to perform such simulations. These potentials must be realistic enough to take into account the specificity of the oxides, namely the iono-covalent nature of the metal (or non-metal)-oxygen bond. This nature is linked to the charge transfer between the anion and the cation, which varies according to cases. For example, in the case of a metal/oxide interface, the charge of the metal passes continuously through the interface from a finite value in the oxide to zero in the metal. The purely ionic empirical models still widely used in the scientific community are essentially ineffective in describing this situation.
At ICMMO, we develop a more adapted model based on a variable charge algorithm in which the metal (or non-metal)-oxygen bond is described by the second-moment of the electronic density of states as expressed in the Tight-Binding scheme, namely the SMTB-Q model. Thus, in an approximate manner, the electronic structure of the oxide is correctly described (band structure, gap). This model has made it possible to study the structure and the energetics of many different oxides, in the bulk as well as for surfaces and interfaces, and it is in constant evolution to deal with more and more complex situations: multi-cations, dislocations, nano-oxides, phase diagram calculations ... For example, collaborations are in progress with IRSN Cadarache and CEA Saclay for the study of defects and fission products in UO_2 and MOX fuels (UO_2/PuO_2), as well as with Centrale-Lyon for the study of dislocations in Al_2O_3. As proof of the success of this model, it has recently been implemented in the international molecular dynamics code LAMMPS, which should increase its diffusion, its use and its developments in the coming years. We aim to make it one of the flagship models in the design of new materials. The second objective is to increase the links with the oxide-related experimental activities developed within the ICMMO/SP2M team (high entropy oxides, perovskites, pyrochlores, oxychalcogenides, thin oxide/oxide or metal/oxide films and some of their associated structural, chemical or physical properties). The recruitment of a researcher on this promising and rapidly growing topic is therefore essential to reinforce and maintain at a high level this expertise within the Institute, and more broadly at the CNRS.

Qualifications: Earned doctorate in Physics, Chemistry or related discipline, at least two years of post-doctoral research experience, and a body of work that includes strong peer-reviewed journal article publications. Applicants must also have:

- Experience in using and possibly developing quantum chemical methodologies and atomistic (Molecular Dynamics and/or Monte Carlo) models.
- Good theoretical background in the physical chemistry of oxides and heterogeneous systems based on oxides.

- Proficiency in one scientific programming language (Fortran, python, C++, etc.) and ability to translate theoretical concepts into algorithms.
- Expertise in semi-empirical methods and/or DFT calculations.

Requirements:
Cover Letter/Letter of Application
Curriculum Vitae
List of References
Research Statement (should be a maximum of three-page summary of research activities that would be undertaken at ICMMO/SP2M)

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The CNRS is strongly committed to promoting equality and diversity, including for gender in the French scientific community. We particularly welcome applications from women for this post. For further information: http://www.cnrs.fr/mpdf/IMG/pdf/english_version_-_fiche_mission.pdf