Postdoc position in Condensed Matter Modelling

Theoretical evaluation of the reactivity at the surface/interface of reactive materials such as metal/metal oxide structures

Location: LAAS-CNRS, Toulouse, France
Duration: 24 months

We are seeking a strongly motivated post-doctoral researcher to take in charge DFT as well as molecular dynamics (Reaxff forcefields expertise welcomed) modelling for depicting complex chemistries at metal oxide surfaces and interfaces. Position is in Toulouse (LAAS-CNRS laboratory), under the supervision of A. Estève and C. Rossi. The fellowship is funded by an ERC advanced grant and will start at the earliest convenience.

The post-doc researcher will be fully involved within a highly multi-disciplinary team (physics, chemistry and electrochemistry, experimentalists and technologists) working on the development of multifunctional & performance-tailored nanomaterials for energy applications.

The project has several scientific objectives:

(i) study the decomposition scenario of strong oxidizer such as CuO under different surface environments: in contact with clusters of metal, metal oxides and alloys. The aim is to analyze at the atomic scale, the phase and structural transformations accompanying the decomposition, as this latter plays a critical role in the oxide reactivity,
(ii) study mass transport across the different layering of materials
(iii) screening metal/metal oxide stackings, including iron oxides, boron and magnesium materials, with potential formation of ternary oxides.

In both cases, the questions raised are of great scientific and technological interest and should lead to impactful results. The applicant will work in close collaboration with researchers located in Toulouse, as well as in Germany and USA.

Required Education and Experience - A recent PhD degree (within last three years) in Materials Science, noticeably Chemistry or related disciplines is required. We seek for a strongly motivated student with strong background in computational materials sciences, with skills in manipulating Density Functional Theory codes : VASP and LAMMPS mandatory. The applicant should send a detailed CV, including a list of publications and communications and a motivation letter to aesteve@laas.fr.