

Post-doctoral fellowship:

Ab initio modelling of doped maghemite

Subject:

In the framework of OPTYMAL (Operando and in-situ specTroscopies for renewable energy MaterialS) ANR, we plan to combine different experimental spectroscopies with *ab initio* calculations in order to improve the molecular understanding of materials interfaces. Among materials of interest, one can mention iron oxides, well-known for solar energy conversion. During the OPTYMAL project, SPEC group from CEA Saclay will synthesize maghemite ($\gamma\text{-Fe}_2\text{O}_3$) either pure or Ni-doped by epitaxial growth on a platinum substrate. These samples will be analyzed by several spectroscopic techniques.

In consistency with these experiments, the aim of this post-doc will be to theoretically investigate the epitaxial growth of Ni-doped maghemite on platinum, by comparison with pure maghemite. After a first part dedicated to structural and electronical analysis of the materials, the influence of the environment, more particularly the presence of water will be considered.

Skills:

The candidate must have a good background in solid-state chemistry and quantum chemistry. A good knowledge of oxide modelling would be an advantage. Knowledge of VASP is required.

Application:

Interested candidates must send a CV, a list of publications and recommendation letters to:
Dr. Céline DUPONT celine.dupont@u-bourgogne.fr (+33) (0)3.80.39.61.57

Period: 12 months

Salary: based on experience

Location: Laboratoire Interdisciplinaire Carnot de Bourgogne (ICB) in Dijon (FRANCE), in close collaboration with CEA (Saclay) and SOLEIL Synchrotron, in the framework of ANR OPTYMAL