Post-doctoral fellowship:

Ab initio modelling of ferroelectrics compounds for water photoelectrolysis

Subject:
Solar light is intermittent and supply is not synchronized with demand. One way to store solar energy is to use photo-electrolysis of water where hydrogen is produced directly from photons and water. But this reaction, which can be decomposed in three steps (photon absorption, migration of photogenerated carriers and surface reaction) requires efficient photocatalysts. In our project, we propose to use the electric field present in ferroelectric compounds to improve the performance of photoanodes.
More precisely, in consistency with experiments, epitaxial films of $BaTiO_3$ will be studied on different substrates, with periodic DFT calculations. Doping will be first considered as a possible way of improving photoelectrochemical efficiency. Influence of chemical nature of dopants and levels of doping will be investigated both to reproduce the experimental results to provide deeper analyses, and also prior to experiments to help in the design of new experimental devices

Skills:
The candidate must have a good background in solid-state chemistry. A good knowledge of oxide modelling would be an advantage. Knowledge of VASP is required and some notions of USPEX will be appreciated.

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)3.80.39.59.23

Period: 18 months
Salary: the gross salary is ca. 2000 € / month
Location: Laboratoire Interdisciplinaire Carnot de Bourgogne (ICB) in Dijon (FRANCE), in close collaboration with CEA (Saclay) and SOLEIL Synchrotron, in the framework of ANR PHOTO-POT