

## **Postdoc Atomistic methodology to treat Solid-Liquid interfaces for water splitting application by Density Functional Theory**

2-years postdoctoral position offered at the Foton Institute-OHM - INSA Rennes (France) founded by Brittany Region as part of the specific program: Sustainable Attractiveness Strategy (SAD). Immediate start is possible with competitive salary with qualification, ability, and experience.

### **Supervisors:**

**Pr. Laurent Pedesseau**

**Pr. Charles Cornet**

**Keywords :** theoretical physics, density functional theory, water splitting, semiconductor, materials science.

### **Project description**

The present SAD project has several objectives: i) To provide a physicochemical understanding at the atomic scale of solar photoelectrochemical (PEC) devices, ii) To study complex multilayer stacks approximating the devices experimentally developed, and in particular focusing on the description of solid surfaces and solid/liquid interfaces between semiconductors (III-V on silicon, and hybrid Perovskites) and the electrolyte, and iii) To provide a fundamental description of the physical processes induced by addition of catalysts (metals or 2D materials) which are used to extract the charges in these devices.

### **Profile of the candidate**

Candidates should have a master degree and PhD in materials science or solid state physics or physics, preferably including documented qualifications in the areas of semiconductor, liquid, or glass. The candidate should have experience on interacting with experimentalists. The ideal profile would combine an existing background on materials science, liquid or material/liquid interaction by using DFT codes (ABINIT, SIESTA, VASP), high performance computing, and also a great sense of autonomy. Molecular dynamics is required on microcanonical (NVE), canonical (NVT) or isobaric-isothermal (NPT) ensembles. Good communication skills in English are required.

### **Foton Institute - INSA Rennes (CNRS, UMR6082)**

The Foton institute is a research laboratory managed by the National Center for Scientific Research (CNRS), the Rennes University and INSA Rennes. The specificity of Foton is to gather around common research programs three groups and three facilities spanning multiple fields from photonics to green energy generation and conversion, including photovoltaics and hydrogen production which are European, national and regional priorities. General information's about FOTON: <http://foton.cnrs.fr/v2016/?lang=en>.



The postdoctoral associate will mainly work within the theory group in Rennes (around 15 staff, PhD students and postdocs) involving the Foton Institute and the Rennes Chemical Sciences Institute in tight collaboration with experimentalists on the topic of water splitting or materials for energy. The group is involved in European Union projects, national projects (ANRs or PEPR), and regional projects.

### **High Performance Computing**

Access to National (CINES, TGCC) supercomputing facilities will be provided under the GENCI proposal. The candidate will also have access to local facilities and will be requested to update the DFT codes.

### **Applying**

To apply and for any further information, please contact  
Pr. Laurent Pedesseau ( [job-ref-i9ijwb9lon@emploi.beetween.com](mailto:job-ref-i9ijwb9lon@emploi.beetween.com) ).

A successful application must contain the following elements:

- Cover letter
- Detailed *curriculum vitae*
- Copy of Ph.D. or equivalent
- Experience after the Ph.D.
- Publication list
- Two letters of recommendation or two references

All qualified candidates are invited to apply.