

## Postdoctoral Position

### Screening of lead-free perovskites and their interfaces with charge transport layers by Density Functional Theory

The FOTON Institute – INSA Rennes is offering a 1-year Postdoctoral position, that could be extended up to 2-years within the H2020 European project DROP-IT “DRop-on demand flexible Optoelectronics & Photovoltaics by means of Lead-Free halide perovskITes”. FOTON Institute – INSA Rennes is in charge of the simulation task of the project. This task will focus on the exploration of new lead-free materials and their interfaces with charge transport layers by Density Functional Theory.

**Starting date:** 1 January 2021

#### Supervisors:

- Laurent PEDESSEAU: <https://cv.archives-ouvertes.fr/laurent-pedesseau>
- George VOLONAKIS: <https://scholar.google.com/citations?user=Viti3pwAAAAJ&hl=en>
- Jacky EVEN: <https://cv.archives-ouvertes.fr/jacky-even>

**Research team:** Simulation group, at FOTON Institute - INSA Rennes

**Keywords:** Materials science, Condensed matter physics, Density Functional Theory

#### Project description:

FOTON Institute - INSA Rennes is part of the DROP-IT consortium (8 European partners). FOTON Institute – INSA and the Institute of Chemical Sciences Rennes (ISCR) at the University of Rennes 1, are part of a joint perovskite simulation group in Rennes. The DROP-IT project aims at combining optoelectronics and photonics in a single flexible drop-on demand inkjet technology platform by means of exploiting the enormous potential of lead-free perovskite materials.

The main task of the Postdoctoral fellow is the investigation of the surfaces and interfaces between chosen lead-free perovskite materials and a selection of charge transport layers. A preliminary literature survey will be developed in collaboration with experimentalists to select the charge transport layers that are compatible with inkjet printing.

## Qualifications

Candidates should have a master degree and PhD in materials science, solid state physics or related fields. The candidate should have experience on writing progress reports, interacting and collaborating with experimentalists. The ideal profile would combine a strong background on halide perovskite (lead or lead-free) materials, computational material screening methods, surface and interface calculations using

DFT codes, high performance computing and management of local workstations, and also a great sense of autonomy. Good communication skills in English are required (written and spoken).

### **About the FOTON Institute (CNRS, UMR6082)**

The FOTON Institute conducts research in the area of photonics for information technology, advanced concepts of photovoltaics, sensors and microwave applications, etc. The targeted technological applications, including many societal challenges, concern optical high-speed telecommunications, optical connections intra and inter chips, the Internet of Things, the autonomous systems, gas detection, medical diagnosis, terahertz metrology, and the development of high-efficiency PV cells on low-cost substrates. The simulation team is involved in all stages of the research effort from fundamental questions up to optoelectronic device simulations. The successful candidate will carry out his research in Rennes.

General information's about FOTON: <http://foton.cnrs.fr/v2016/?lang=en>.

### **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.

### **Competitive salary**

A competitive salary at the European level commensurate with qualification, ability, and experience.

### **Application procedure**

Please submit your application at your earliest convenience by e-mail to: [laurent.pedesseau@insa-rennes.fr](mailto:laurent.pedesseau@insa-rennes.fr) and [yorgos.volonakis@univ-rennes1.fr](mailto:yorgos.volonakis@univ-rennes1.fr)  
The position will remain open until filled.

Your application should include:

- Cover letter
- Detailed CV
- List of publications
- Contact details of two references

All qualified candidates are invited to apply.