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 12-months Postdoctoral position, that could be extended up to 36 months 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 November 2019

Supervisors:
- Laurent PEDESSEAU: https://cv.archives-ouvertes.fr/laurent-pedesseau
- 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). DROP-IT 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 tasks of the Postdoctoral fellow are two-fold:

i) Screening lead-free perovskite materials from the simplest halide perovskites $A(I)B(II)X_3$ to related compounds $A_aB_bX_{(a+3b)}$. A preliminary literature survey will be performed at the beginning of the project. Special attention will be paid to predicted absorption coefficient, electronic band gap, effective masses and structural stability. A first report is expected at M12 and a final one at M30.

ii) Studying the interfaces between the chosen perovskite materials and the charge transport layers. A preliminary literature survey will be developed in collaboration with experimentalists to select the charge transport layers for inkjet printing. A first report is expected at M18 and a final one at M36.

Qualifications

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, insulator, or material. The candidate should have experience on writing reports and interacting with experimentalists. The ideal profile would combine an existing background on perovskite materials, materials screening using DFT codes (ABINIT, SIESTA, VASP), high performance computing and management of local workstations, and also a great sense of autonomy. Good communication skills in English are required.

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

Your application should include:
- Cover letter
- Detailed CV
- Copy of Ph.D. or equivalent
- Grade transcripts of M.Sc. degree
- List of publications, if applicable
- Contact details of two references

All qualified candidates are invited to apply.