

Postdoctoral Position

Mapping onto empirical tight-binding Hamiltonians starting from Density Functional Theory calculations on multilayered halide perovskites

The FOTON Institute – INSA Rennes is offering a 1-year Postdoctoral position, that could be extended up to 2-years within the M-Eranet European project PHANTASTIC “PHysics- and dAta-driven multiscale modelling design of layered lead halide perovskiTe mATerials for Stable phoTovoltaICs”. PHANTASTIC aims at a predictive materials and device engineering approach of mixed lead halide perovskite solar cells. FOTON Institute – INSA Rennes is in charge of a part of a simulation task of the project. This task will focus on the mapping onto empirical tight-binding Hamiltonians starting from Density Functional Theory.

Starting date: immediate start possible

Supervisors:

- Jacky EVEN: <https://cv.archives-ouvertes.fr/jacky-even>
- Laurent PEDESSEAU: <https://cv.archives-ouvertes.fr/laurent-pedesseau>
- Simon THEBAUD

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 PHANTASTIC consortium (5 European partners). PHANTASTIC aims at a predictive materials and device engineering approach of mixed lead halide perovskite solar cells.

The main task of the Postdoctoral fellow is to expand a 3D perovskite empirical tight-binding model to 2D perovskites of variable thickness (quasi 2D perovskite) including electroactive organic cations.

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 empirical tight-binding model coding, on halide perovskite materials, electronic band structure 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>.

<https://cv.archives-ouvertes.fr/jacky-even>

High Performance Computing

Access to National (CINES, TGCC, IDRIS) supercomputing facilities will be provided under the GENCI proposal. The candidate will also have access to local facilities and will be requested to perform the coding of TB models and use classical DFT codes used by the group (SIESTA, VASP, QE, ABINIT).

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:

Jacky.even@insa-rennes.fr and simon.thebaud@insa-rennes.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.