Semi-empirical tight-binding modelling of multilayered halide perovskite

2-years postdoctoral position (1-year reconducible)
offered at the Foton Institute in Rennes, France.
Immediate start is possible with competitive salary at the European level commensurate with qualification, ability, and experience.

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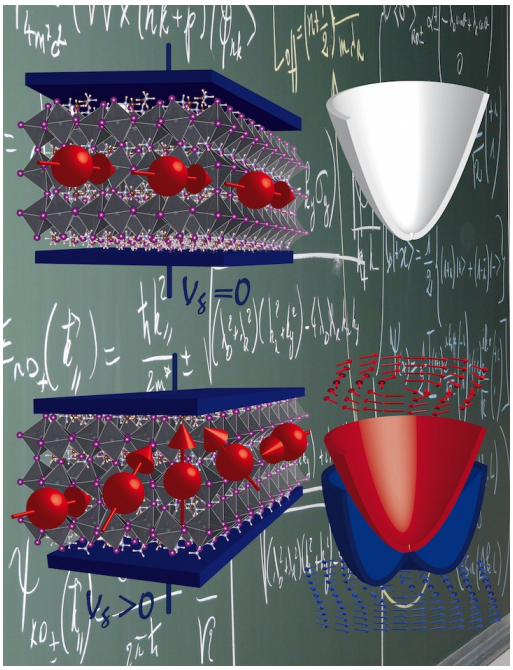
Keywords : theoretical physics, numerical simulations, tight-binding models, density functional theory, k.p methods, electron-phonon coupling, excitons, photovoltaics, perovskites.

The theory group at the Foton Institute has developed since 2010 a world-class expertise in understanding the physics of perovskite materials as well as modeling and simulating their optoelectronic properties. This work, done in tight collaboration with experimental laboratories in Europe and the US, has yielded multiple publications in high-impact journals such as Nature and Science.

Perovskite semiconductors have become paramount for photovoltaic applications and optoloelectronics more generally, especially in the form of multilayer stackings. The 2-years postdoctoral position (1-year reconducible) is fully funded by 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. The Foton Institute – INSA Rennes is in charge of a simulation task within the project. This task will focus on the modeling of multilayered perovskites by semi-empirical tight-binding hamiltonians supported by density functional theory calculations, with potential use beyond solar cells to exciton-lattice pump-probe dynamics [1] and single-photon emission [2].

[1] Zhang, H., Li, W., Essman, J. et al. *Ultrafast relaxation of lattice distortion in two-dimensional perovskites.* Nat. Phys. (2023)
[2] Tamarat, P., Hou, L., Trebbia, JB. et al. *The dark exciton ground state promotes photon-pair emission in individual perovskite nanocrystals.* Nat Commun 11, 6001 (2020).

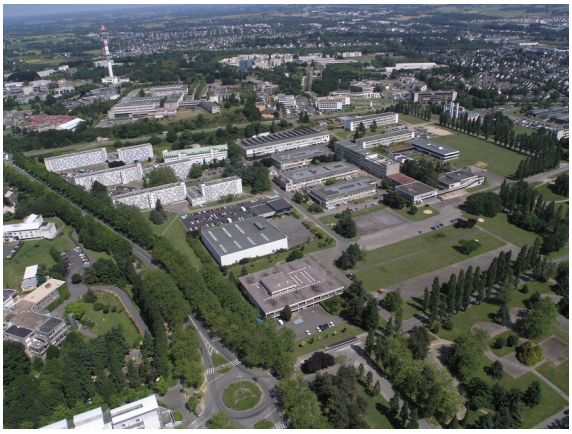
Profile of the candidate

The successful candidate must have a PhD in condensed matter physics, materials science or related fields. The ideal profile would combine a strong background on empirical tight-binding model coding, halide perovskite materials, crystallography, electronic band structure calculations using DFT codes, high performance computing and management of local workstations.

The ability to work in autonomy, prior experience writing progress reports, and a marked interest in interacting and collaborating with experimentalists are a plus. Spoken and written proficiency in english is required.

The Foton Institute (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, and for which perovskites materials are a topic of intense research activities worldwide.

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 on the topic of perovskite materials. The group is involved in three European Union projects (Dropit/Perocube/Polloc), a M-ERA.NET project (Phantastic), and in a consortium of american universities and laboratories (Rice University in Houston, Northwestern University in Chicago, Los Alamos National Laboratory in Los Alamos).

Applying

To apply and for any further information, please contact
Pr. Jacky Even (jacky.even@insa-rennes.fr) and Pr. Simon Thébaud (simon.thebaud@insa-rennes.fr).

A successful application must contain the following elements :

- Cover letter
- Detailed *curriculum vitae*
- Publication list
- Two letters of recommandation or two references

Other opportunities in the group

The theory group in Rennes has two other openings :

- A 3-year PhD position offered at the Rennes Chemical Sciences Institute from Sept-Oct 2023 to Sept-Oct 2026, contact George Volonakis (yorgos.volonakis@univ-rennes1.fr).
- A 3-year PhD position at the Foton Institute from Sept-Oct 2023 to Sept-Oct 2026, contact Simon Thébaud (simon.thebaud@insa-rennes.fr).