

Postdoctoral position: theory and simulation to advance the metal halide perovskite technology

A full-time postdoctoral research associate position is available in the department of [theoretical inorganic chemistry](#) at Institut des Sciences Chimiques de Rennes ([ISCR, France](#)) for a talented and ambitious researcher. The position is funded through the **H2020 Innovation Action** under the **PEROCUBE** proposal on *High-Performance Large Area Organic Perovskite devices for lighting, energy and pervasive communications*.

The postdoctoral fellow will be involved in the task dedicated to the optimization of perovskite materials and device heterostructures based on theoretical studies, mainly periodic density functional theory (DFT) calculations. This implies a close collaboration between [CNRS](#) and partners developing the perovskite materials and device architecture, namely Oxford and Patras Universities.^[1] He/She will benefit from the expertise developed in Rennes on metal halide perovskites by chemists and physicists from ISCR and FOTON Institutes.^[2] Local and national computing means will be made available for the purposes of the relevant project.

Starting date: 1 April 2020

Duration: 12 month (Contract renewal possible up to a total of 23 months)

Supervisor: KATAN Claudine (<https://publons.com/researcher/1389063/katan-claudine/>)

Salary: between 2617 and 3730 € gross monthly (depending on past experience)

Required level of education: PhD

A PhD Degree in Physics, Materials Science, Chemistry or related disciplines is required. We are looking for a candidate with a strong background in quantum theories, in particular DFT and its extensions applied to solids. Complementary skills in material science, such as mastering concepts and tools of solid-state physics, simulation code development and/or expertise using Python or MATLAB are desirable. The candidate shall be able to demonstrate his/her expertise in the above-mentioned fields through publications in high quality, peer reviewed journals. A good command of English, both spoken and written, is mandatory for efficient interaction with members of the PEROCUBE consortium. Autonomy and communication skills are also expected to participate in our project and benefit from the existing rewarding working atmosphere.

The applicant should use <https://emploi.cnrs.fr/> job portal to submit his/her application; **applications sent by e-mail will be considered ineligible**. The file shall contain detailed CV, including a list of publications and communications, a motivation letter as well as contact information of two scientists for possible request of recommendation letters. The selection will start immediately and will continue until the position is filled.

[1] Koutselas, I. *et al.* Some Unconventional Organic–Inorganic Hybrid Low-Dimensional Semiconductors and Related Light-Emitting Devices. **J. Phys. Chem. C** 115, 8475 (2011); Tan, Z.-K. *et al.* Bright light-emitting diodes based on organometal halide perovskite. **Nat. Nanotechnol.** 9, 687 (2014); Snaith, H. J. Present status and future prospects of perovskite photovoltaics. **Nat. Mater.** 17, 372–376 (2018).

[2] Katan, C. *et al.* Quantum and dielectric Confinement Effects in Lower-Dimensional Hybrid Perovskite Semiconductors, **Chem. Rev.** 119, 3140 (2019).

