Post-doc position on simulation of halide perovskites at CEA-Saclay, France

Term and Location: A one-year postdoctoral position at Section de Recherche de Métallurgie Physique (SRMP), CEA-Saclay (Université Paris-Saclay), under the supervision of Guido Roma. The position is funded by Project Minotaure/PEPR TASE and is expected to start beginning 2025. Funding for an optional second year is actively searched.

Context: Halide perovskites are a very active field of research for their applications in photovoltaics (PV), light emitting devices, X-ray detectors, and more. The role of interfaces in the devices, especially in enhancing carrier extraction in solar cells, is crucial. Atomic scale modelling of bulk and surfaces of these materials is challenging, because of their softness, associated with anharmonic behaviour and local atomic disorder (polymorphism), spin-orbit coupling and polar distortions. In spite of recent advances in describing polymorphism and anharmonic lattice dynamics in the bulk, studies of surface and interface properties are recent and still rare.

Description and duties: The work will focus on building predictive models of interfaces between perovskites light absorbers and electron/holes transport layers (ETL/HTL) based on Density Functional Theory. Existing and new HTL/ETL materials will be investigated with a special focus on understanding passivation mechanisms, defects at the interface, their stability and kinetics. Development of machine learning potential is envisaged.

Required Skills: The applicant should hold a PhD degree in physics or chemistry or related field, have a strong background in solid state physics and chemistry. She/he should have demostrated experience in using Density Functional Theory-based techniques, ab initio molecular dynamics or post-dft many body electronic structure methods (beyond DFT), simulation of electronic and/or vibrational spectra. Further experience in machine learning approaches is appreciated.

Organization skills, being able to work independently and in team work (e.g., with PhD students working on close subjects), and to collaborate with experimentalists, are required. The candidate is expected to present results at national/international meetings and in publications in high profile peer-reviewed journals, for which excellent oral and written communications skills are required.

Collaborations: with other partners of the Minotaure project and, in particular, University of Rennes (J. Even) and CEA/INES, Chambery (S. Berson).

How to apply: Applications, should include a CV, at least two reference contacts, estimated availability, and a one page descriptive summary of past accomplishments and future research interests, possibly in a single PDF document. Applications should be sent to `guido.roma@cea.fr` and will be considered until the position is filled.