For a fully funded PhD position at CEA-Saclay, France, we look for candidates with:

- *Strong motivation, fuelled by interest in research*
- *A master degree and a solid background in physics and chemistry of solids*
- *Skills in numerical simulations*

Contact: Guido Roma (guido.roma@cea.fr), supervisor

Collaborations: Jacky Even (Photon, Rennes), CEA INES (tandem cell preparation)

Simulation of interfaces to improve the stability and performance of perovskite solar cell

Hybrid halogenated perovskite solar cells are rapidly emerging as third generation photovoltaic devices with low cost and high efficiency. Although remarkable improvements to the problematic stability of the perovskite materials have been reported, the best strategy to increase the device lifetime without degrading the photovoltaic performances is still not established. One of these strategies consists in performing surface treatments that tend to reduce the concentration of intrinsic defects detrimental to device performance and/or stability. The success of this strategy stands on the influence of the surface treatment (or the choice of hole/electron transporting layer) on the final structure of the interface on which we are focusing, and of the defect concentrations in its vicinity. In the framework of tandem solar cells, the role of the numerous interfaces becomes even more important, not only from the electrical point view, but also from the optical one.

In this PhD project we intend to study the influence of some additional foreign atoms on the structure and dielectric properties at the interface between the perovskite and one of the charge transporting layers, relying on quantum mechanical, so called ab initio, calculations at the atomic scale. From such detailed study of the electronic and dielectric properties of perovskite surfaces doped with various impurities, and possibly of the kinetics of the latter, we aim to understand why and how surface treatments are effective and how they affect the optoelectronic properties of the devices.

Web reference :
https://instn.cea.fr/en/these/simulation-of-interfaces-to-improve-the-stability-and-performance-of-perovskite-solar-cell/

Applications, to be submitted before end of May, should include :

- Curriculum Vitae with publication list
- Motivation letter
- Degree certificates and academic transcripts
- Recommendation letters and contact details of referees

For a fully funded PhD position at CEA-Saclay, France, we look for candidates with:

- *Strong motivation, fuelled by interest in research*
- *A master degree and a solid background in physics and chemistry of solids*
- *Skills in numerical simulations*

Contact: Guido Roma (guido.roma@cea.fr), supervisor

Collaborations : ENSAM, Paris (X. Colin), University of Bologna (D. Fabiani)

Towards the prediction of dielectric properties of irradiated polymers and other inhomogeneous materials

Electric cables are important elements in the security of nuclear power plants. Their integrity, in particular their capability of keeping their functional property (power supply or signal transmission), must be ensured during the whole lifetime of the power plant. The weakest component of the cables are the polymers providing electric insulation.

Predicting the dielectric properties of a polymer under irradiation is a particularly hard task, first because the polymer is, by itself, a multicomponent composite material with a complex microstructure, second, because irradiation modifies its chemical composition with time, by triggering various reactions, depending on the environment.

The goal of this PhD project is to develop a multiscale approach able to to predict static and dynamical dielectric properties of polymers used as electric cables insulators, especially when undergoing irradiation, starting from elementary atomic scale properties, using first principles calculations based on quantum mechanics.

Such an approach aims to be applicable also in other technological domains, for example for the development of new advanced dielectric materials for non-conventional microelectronics using organic components, or for supercapacitors, which are devices for energy storage.

Web reference :

https://instn.cea.fr/en/these/towards-the-simulation-of-dielectric-properties-of-irradiated-polymers-and-other-inhomogeneous-materials/

Applications, to be submitted before end of May, should include :

- Curriculum Vitae with publication list
- Motivation letter
- Degree certificates and academic transcripts
- Recommendation letters and contact details of referees