**EDF R&D PhD Position**

**Atomic modeling of the materials for photovoltaic applications ageing**

**under different conditions.**

EDF R&D, and partners of IPVF (Institut Photovoltaïque d'Ile de France, www.ipvf.fr ), are intended for research and development of new materials and devices used for different PV channels to ruptures of performance and cost. One of the proposed technologies is based on devices called "tandem" combining different compounds to improve the overall efficiency of the cells. The electrical properties of materials used in these devices are strongly influenced by the operational conditions. Indeed, these parameters (difficult to characterize experimentally) are the source of many metastabilities (disturbance of the stability of crystalline phases, variation of the band gap, occurrence of electronic level "parasite" in the band gap, etc.) that can strongly degrade the efficiency and durability of solar cells. Understanding the materials ageing is thus necessary for their optimization and improvement for photovoltaic.

This PhD will mainly focus on the study of the physical and chemical properties of the perovskites. These materials are of the most promising for photovoltaic applications but they stay sensitive to their conditions of uses and syntheses (temperatue, UV, presence of water and oxygen, etc …). The proposed PhD paims to develop a « simple » theoretical multi-scale approach, from first-principles to molecular dynamics or Monte-Carlo, to deepen this knowledge and try to link the nanoscopic and microscopic properties of materials.

Depending on the candidate, the different proposed themes are : *i)* stability of the materials under different factors (UV, temperature, $H_2O$, …) ; *ii)* stability of the 2D/3D compounds ; *iii)* effects of the grain boundaries and passivating films, and, *iv)* influence of the atomic substitutions on the various properties of peroskites.

For each point, the structural, electronic and spectroscopic (vibrational and electronic) properties of the various configurations of the material will be studied and compared with various experimental results.

The PhD will take place in the team "Modeling and characterization" at IPVF at Palaiseau (91, near Paris).

The candidates must have skills and interests in the structural and electronic properties of condensed matter, computer modeling and simulation. They should send us a CV, a cover letter, and the contact information of referring persons.

Contact : Philippe Baranek, EDF R&D, EDF Lab Chatou, 78400 Chatou Cedex.

email : philippe.baranek@edf.fr