EDF R&D PhD Position

Multiscale approach to improve our understanding of light- and temperature-induced performance degradation of silicon solar cells.

EDF R&D and partners of the IPVF (Institut Photovoltaïque d'Ile de France, <u>www.ipvf.fr</u>) are aiming at research and development of new materials and devices used for different photovoltaic (PV) channels leading to performance and cost breakthroughs. 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 meta-stabilities (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 life-time of solar cells. Understanding the materials ageing is thus crucial for the optimization and improvement for photovoltaic devices.

The selected PhD student will mainly focus on the study of the different mechanisms of the Light- and elevated-Temperature-Induced Degradation (LeTID) of the Passivated Emitter and Rear Cell (PERC) modules. This technology is on the market since 2013 and has an outstanding efficiency of 24%, but may show a fast performance ageing appearing after few years of exploitation. There is a « consensus » around the fact that hydrogen could play a precursor role in this behavior. The proposed PhD subject aims to develop a « simple » theoretical multi-scale approach, from first-principles to molecular dynamics or Monte-Carlo simulations, to deepen the existing knowledge and to link the nanoscopic and microscopic characteristics of LeTID with a specific focus on the role of hydrogen (depending on its origin), of the extrinsic or intrinsic defects, and of the interfaces.

The different topics addressed in this PhD work are: *i*) stability of the materials under different factors (temperature, H_2O , O_2 , ...); *ii*) effects of the grain boundaries and passivating films, and, *iii*) influence of the electric field on the stability of the studied systems.

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

The PhD study will take place in the team "Modeling and characterization" at the IPVF in cosupervision with the LPICM (Ecole Polytechnique) at Palaiseau (Paris, area).

The candidates must have skills and interests in the structural and electronic properties of condensed matter, computer modeling and simulation with good fundamentals in physico-chemistry of solid materials. If interested, you should send us a CV, a cover/motivation letter, and the contact information of referring persons.

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