Theoretical study of Hybrid Organic-Inorganic Perovskites for PV applications

Halide perovskites, in particular hybrid ones containing an organic cation, have in the last few years attracted strong interest for their potential applications as photovoltaic solar absorbers. In spite of very high efficiencies, their use is still hindered by their stability and rapid aging under illumination.

The objective of this Master Thesis is to study by means of *ab initio* calculations the stability and the electronic structure of HOIP encapsulated in graphene. The goal is to understand the ability of such protective layer to mitigate device degradation connected to the creation of halogen vacancies. The master thesis will be followed by a PhD that will address the effect of such defects in bulk devices that will be grown and characterized by experimental teams in Saclay and Grenoble.

The PhD grant and the related experiments are funded by the French National Research Agency. *Ab initio* simulations on massive parallel supercomputers, has become in the recent years, a powerful investigation tool widely used both for basic or applied research in the field of condensed matter. Two complementary codes will be used during the thesis: BigDFT (http://bigdft.org) and Quantum-Espresso (https://www.quantum-espresso.org).

The master thesis can start in February 2020 and will be located in CEA-Grenoble. The PhD is expected to start at fall 2020 and will be located in CEA-Saclay.

The successful candidate should have a solid background in Condensed Matter Physics and be highly motivated by Computational Materials Science approaches.

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