Laboratoire de Physique des Interactions Ioniques et Moléculaires - UMR 7345

# Electronic structure calculations for energy-producing systems: Hydrogen-metal interaction in fusion science and hybrid organic-inorganic heterostructures for solar cells applications

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A PhD fellowship is available at Aix-Marseille University in the Laboratory *Physique des Interactions Ioniques et Moléculaires* (PIIM). The subject is twofold: the first part focuses on fusion science, the second lies in the field of photovoltaic cells.

The appointed candidate will be integrated in a team with long-standing expertise in the fields of theoretical and experimental material science. We are looking for a candidate with a background in theoretical solid-state chemistry or physics and in quantum mechanics. The knowledge of DFT would be appreciated.

Skills and expertise developed at PIIM in the field of plasma-material interaction related to nuclear fusion devices. ITER - *International Thermonuclear Experimental Reactor* - is built in Cadarache close to Marseille; it is designed to demonstrate the feasibility of controlled nuclear fusion for the production of clean and sustainable energy. However, several issues remain open. In particular, interactions between the hydrogen plasma and the tungsten surface degrade the fusion vessel, increasing the risk of hazard and may prevent fusion from occuring. In accord, the first purpose of this PhD thesis is to investigate the interaction of hydrogen with tungsten by means of electronic structure calculations within the Density Functional Theory (DFT). Since DFT simulates systems at zero temperature, the overall model will be improved by a statistical approach in order to yield temperature-dependent data directly comparable with experimental measurements [1].

The second part is exploratory and will be focused in the field of Hybrid Organic-Inorganic Perovskites (HOIP) [2]. The crystal structure of perovskite is typically made of $ABX_3$ units. Three-dimensional HOIPs with relatively small organic cations have been suggested as a novel class of low-cost solution-processable materials for high efficiency hybrid photovoltaic cells. Moreover, their controllable band gap enhances the versatility of their applications. In order to control the band gap and tune it according for suitable applications, we propose to model the electronic and structural properties using quantum mechanical methodologies in the framework of Density Functional Theory (DFT) and beyond DFT.

[1] N. Fernandez, Y. Ferro*, and D. Kato, Acta Mater. 94 (2015) 307-3018
[2] Kojima, A.; Teshima, K.; Shirai, Y.; Miyasaka, T. Organometal Halide Perovskites as Visible-Light Sensitizers for Photo-voltaic Cells. J. Am. Chem. Soc. 2009, 131, 6050 – 6051

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