ENS DE LYON

Post-doctoral fellowhship:

Ab initio modelling of semiconductor/co-catalyst interface for water splitting application.

Supervisors:

Tangui Le Bahers tangui.le_bahers@ens-lyon.fr Tel: +334 72 72 88 46

Philippe Sautet philippe.sautet@ens-lyon.fr Tel: +334 72 72 81 55

Period: From 01/04/2016 to 31/03/2017 (possibility of an additional year of fellowship)

Location: The Chemistry Laboratory of ENS Lyon, Lyon, France

Subject:

Since the discovery of the ability of TiO_2 to dissociate water into O_2 and H_2 upon irradiation, an impressive amount of work has been devoted to the development of photocatalysts. The most important targeted reaction is probably the photo-dissociation of water (water splitting) generating H_2 and O_2. As H_2 is considered as a promising fuel candidate to replace hydrocarbons fuels in the future, the photosynthesis of this molecule from water is of major importance.

The aim of the project is to continue the work of the group dedicated to the design and the *in silico* characterization of semiconductors for water splitting application.[1–5] Beyond the semiconductor, the post-doc will have to start the modelling of the full catalyst including the interface between the semiconductor and the co-catalyst and the reaction of water splitting at the surface of the co-catalyst. The modelling will be based on theoretical chemistry (DFT) but also can involve macroscopic modelling of the electronic structure of the system using the semiconductor equations (Poisson equation, charge diffusion…). All this work will be done in collaboration will the group of Pr. Takanabe (KAUST, Saudi Arabia), which will perform the experimental counter part of this work.

Skills:

The candidate must have a good training in chemical physics especially in solid-state chemistry and physics. Knowledge in theoretical chemistry will also be important. Due to the multidisciplinary aspect of the project, the candidate must be motivated by working in a team with different expertises. From a practical view point, knowledge in Gaussian, VASP and CRYSTAL codes will be appreciated.

References:

(1) Bhunia, M. K.; Melissen, S.; Parida, M. R.; Sarawade, P.; Basset, J.-M.; Anjum, D. H.; Mohammed, O. F.; Sautet, P.; Le Bahers, T.; Takanabe, K. Dendritic Tip-on Polytriazine-Based Carbon Nitride Photocatalyst with High Hydrogen Evolution Activity. *Chem. Mater.* **2015**. DOI: 10.1021/acs.chemmater.5b02974

(2) Melissen, S. T. A. G.; Labat, F.; Sautet, P.; Le Bahers, T. Electronic Properties of PbX3CH3NH3 (X = Cl, Br, I) Compounds for Photovoltaic and Photocatalytic Applications. *Phys. Chem. Chem. Phys.* **2015**, *17*, 2199–2209.

(3) Melissen, S.; Le Bahers, T.; Steinmann, S.; Sautet, P. The Relationship Between Carbon Nitride Structure a Nd Exciton Binding Energies: A DFT Perspective. *J. Phys. Chem. C* **2015**, *119*, 25188–25196.

(4) Le Bahers, T.; Rérat, M.; Sautet, P. Semiconductors Used in Photovoltaic and Photocatalytic Devices: Assessing Fundamental Properties from DFT. *J. Phys. Chem. C* **2014**, *118*, 5997–6008.

(5) Kandiel, T. A.; Anjum, D. H.; Sautet, P.; Le Bahers, T.; Takanabe, K. Electronic Structure and Photocatalytic Activity of Wurtzite Cu–Ga–S Nanocrystals and Their Zn Substitution. *J. Mater. Chem. A* **2015**, *3* (16), 8896–8904.