Research Doctorate (Ph.D.) in Chemical Sciences
32nd Cycle – Academic Year 2016/2017

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Project Information

1 - Title

Ab initio modeling of solar energy conversion processes at hybrid organic-inorganic interfaces

2 - Key words

1. Computational Chemistry
2. Density Functional Theory
3. Dye sensitized solar cells
4. Photoelectrochemical processes
5. Heterogeneous functional materials

3 - Abstract

The project addresses the development of a new computational tool purposely tailored to model heterogeneous functional materials. Target applications are solar energy conversion devices such as dye-sensitized solar cells (DSC). These devices are based on hybrid organic-inorganic photoelectrodes, made of molecular dyes and semiconductor nanoparticles in electrolyte solution. The energy conversion process results from complex steps that are regulated by energy, charge and mass transport at the nanoscale.

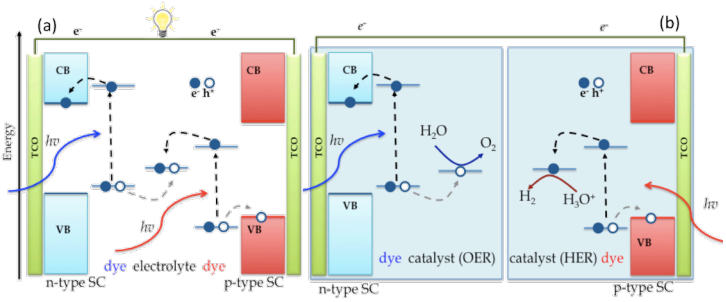

Figure 1. Scheme of the components and the processes in dye sensitized solar cells (DSC): (a) photovoltaic tandem cell and (b) photo-electrocatalytic cell for oxygen evolution reaction (OER) at the photoanode and hyrdogen evolution reaction (HER) at the photocathode.

The complexity of DSC constituent materials and the electronic nature of the undergoing processes highlight the limits of state-of-the-art *ab initio* methods. In particular, current standard approaches are not able to cast all DSC features within a unique model. This limitation will be addressed by further development of a recently proposed embedding scheme combining density functional theory and correlated wave-function methods. The key innovation lies in the inclusion of mutual QM polarization among all the DSC constituents and interfaces. DSC photocathodes will provide a suitable and challenging playground for benchmark and applications.