Quantum modeling of nano-switches for solar energy storage

2-year Post-doctoral position
(Expected start: February 2021)

Supervisor

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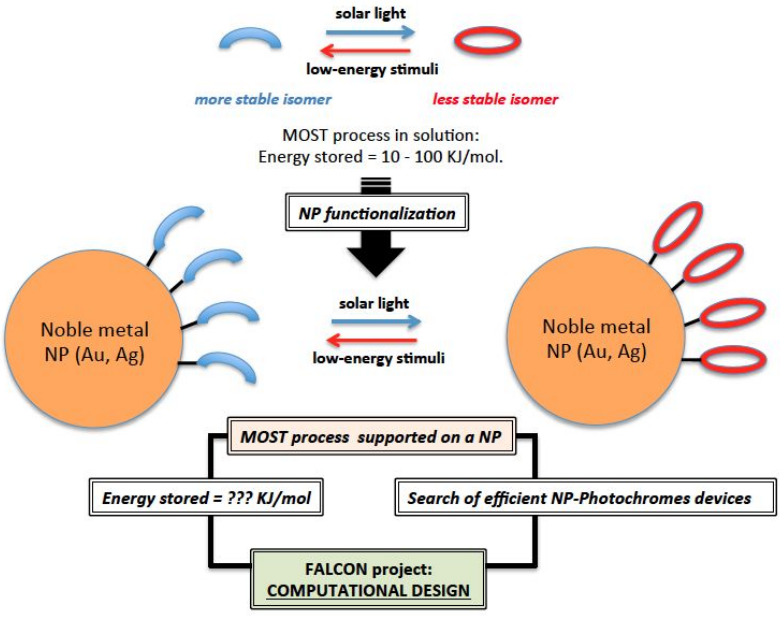
A 2-year post-doctoral position is available in the department of Inorganic Theoretical Chemistry (CTI) at the Institute of Chemical Sciences of Rennes (ISCR, University of Rennes 1) funded by the French "National Agency for Research" within the project *FALCON* (**Fa**ster and **L**ighter **C**omputational design of **O**ptical **N**ano-switches for solar energy storage).

In this material-modeling project, we aim at providing through a theoretical design a new generation of nano-objects able to convert sunlight into energy and store it in an efficient fashion. To this end we will make use of the so-called ***Molecular Solar Thermal (MOST)*** process [1] where the irradiation of an organic photochrome with solar light permits the switching to a second isomer, higher in energy (energy storage step), while the return to the most stable isomer with the help of a less energetic external stimulus induces the energy excess release as heat (energy release step). We propose here to go beyond the current state of the art of MOST process in solution and use the functionalization of metallic NanoParticles (NP) as a mean of attaining optoelectronic nanomaterial with superior solar energy storage abilities. Coating NPs with organic photochromes will indeed permit a fine control of the molecules density, a critical parameter in the energy storage mechanism, and potentially enhance the switching process of the molecule due to the effect of the Localized Surface Plasmon Resonance (LSPR) of the NP. [2]



To reach this goal, the FALCON project is dedicated to the in-silico design of NP-photochromes solar thermal fuel devices with the help of atomistic modeling. The development of a theoretical approach is crucial as it will permit an in-depth understanding of the non-trivial interactions between the two parts of the device, that are today yet to be fully rationalized with quantum chemistry models. It will also save precious time, raw material and human resources prior to the experimental device fabrication. This computational design is however by definition a challenge for fundamental

research, as one would need quantum mechanics models to describe the electronic interactions in the device up to a very large scale. The project will then take advantage of computations based on the ***Density Functional Tight-Binding (DFTB)*** model, allowing a quantum description of the system at a very low computational cost, once correctly parameterized. [3,4]
The candidate will be in charge of the construction of a DFTB protocol able to fully describe the ground state and excited states of these nano-objects, granting access to i) the description of the photochromic process of the molecules onto the NP, under the LSPR influence, ii) the quantity of energy stored during this process, and ultimately iii) the design of new devices with optimized properties. This work will be conducted in collaboration with the group of Pr. Thomas Frauenheim (Bremen University, BCCMS), recognized experts in DFTB development and applications.

The CTI team

The post-doctoral researcher will work in the Inorganic Theoretical Chemistry (CTI) team, in the Institute of Chemical Sciences of Rennes. The CTI team gathers several theoreticians (14 permanent staff members, 15 students) with complementary skills in theoretical chemistry but also physics, working with a broad set of quantum chemical tools, ranging from high precision *ab initio* wave function-based calculations to fast semi-empirical methods. The studied systems in CTI are diverse, including isolated species, bulk materials and surfaces, mainly of high experimental and societal interest. The CTI team thus provides a stimulating scientific environment, also offering regular team meetings, invited seminars as well as visitors internationally recognized. Local and national computing resources are available for the purposes of the scientific projects.

Profile of the candidate

The candidate should possess a solid background in quantum chemistry and in photophysics/photochemistry. Prior experience with DFT/TD-DFT/DFTB and/or with the description of hybrid metallic-organic systems is a plus.

Application

The position is scheduled to start around February 2021. Please send your application by e-mail, with a CV containing a description of previous research experiences, to arnaud.fihey@univ-rennes1.fr.

References:

[1] L. Dong, Y. Feng, L. Wang, W. Feng, *Chem*. Soc. Rev, **2018**, *47*, 7339-7368.
[2] H. Nishi, T. Asahi, S. Kobatake, *J. Phys. Chem. C*, **2011**, *115*, 4564-4570.
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[4] F. P. Bonafé, B. Aradi, B. Hourahine, C. R. Medrano, F. J. Hernández, T. Frauenheim, C. G. Sánchez, *J. Chem. Theory Comput*. **2020**, *16*, 4454−4469