l'Ingénierie au service des défis sociétaux

PhD Fellowship in Chemistry for Solar Energy Conversion

Laboratory : [*L2CM-UMR7053*] (Université de Lorraine)
Thesis supervisor (Université de Lorraine, France, L2CM) : Dr Philippe C. GROS
Thesis supervisor (Université of Ferra, Italie): Pr Stefano Caramori
Thesis scholarship: French doctoral contract funded by Lorraine Université excellence (LUE)

Earth abundant metal-based new generation solar cells

Keywords: Solar cells, Ligands, Photoactive complexes, Spectroscopy, Quantum simulations

The aim of the project is the development of abundant metal-based light-responsive complexes and their use in DSSCs (Dye-sensitized Solar Cells). Several noble metal complexes (Ru, Ir, Pt) have long been considered as lead compounds due to their ideal photophysical and geometrical properties with power conversion efficiency (PCE) values in the 9-11 % range. Despite these ideal photophysical properties, ruthenium is a scarce metal, toxic and expensive and limits the real-world industrial development of the cells. In consequence, the main goal of our project is the replacement of such expensive metals by cheap and environmentally benign metals in the search for developing low-cost efficient devices, and resource-preserving industrial processes.

The L2CM has recently contributed to the field by investigating different approaches to tune the electronic properties of abundant organoferrous complexes (ANR PhotIron). By combination of chemical synthesis and quantum simulations, the parameters influencing the excited state lifetime of organo-ferrous dyes and their interfacial behaviour after chemisorption on semiconductor have been pointed out. [1,2] The L2CM and the University of Ferrara in Italy (S. Caramori) are currently leaders in the field of iron-sensitized DSSC cells with a record efficiency of 2% very recently obtained. [3,4]

In spite of these promising results, the efficiency of the Fe-sensitized DSSCs is still to be improved. In this regard, dye-TiO_2 interfacial TD-DFT computations have already shed light on the reasons for such limited performance. Therefore, current synthetic efforts are targeted to overcome these specific aspects with the aim to make organoferrous complexes a genuinely alternative to their ruthenium counterparts.

References:

[1] Pastore, M.; Duchanois, T.; Liu, L.; Monari, A.; Assfeld, X.; Haacke, S. & Gros, P. C. Phys. Chem. Chem. Phys. **2016**, 18, 28069-28081 (10.1039/C6CP05535D)
[2] Reddy Marri, A.; Marchini, E.; Diez Cabanes, V.; Argazzi, R.; Pastore, M.; Caramori, S.; Gros, P.C. *J. Mater. Chem. A*, **2021**, 9, 3540-3554. (10.1039/D0TA10841C).
[3] Reddy Marri, A.; Marchini, E.; Diez Cabanes, V.; Argazzi, R.; Pastore, M.; Caramori, S.; Gros, P.C. *Chem. Sci.*, **2023**, *14*, 4288 – 4301 (10.1039/D2SC05971A).
[4] Pastore, M.; Caramori, S.; Gros, P.C. *Acc. Chem. Res.* **2024** (10.1021/acs.accounts.3c00613)

Profile:

The candidate should have an excellent background in **organic/organometallic synthesis** and related characterization techniques (e.g. UV-Vis, fluorescence). **An experience in an international environment as well as a good English level will be appreciated**. The candidate must be open-minded and willing to work in a multidisciplinary and international environment.

To apply, please send by email to philippe.gros@univ-lorraine.fr :

1. A detailed Curriculum Vitae
2. A copy of your master's degree with a breakdown of the marks
4. A motivation letter
5. A letter of recommendation from the Master's research supervisor

Deadline for application: **[May 1st 2024]**
Starting time: October 1st 2024