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Development of porphyrins-based molecular catalysts toward hybrid photocathodes for solar energy conversion

Storing renewable energy in chemical bonds, particularly through hydrogen (H_2) production or the reduction of carbon dioxide (CO_2) into fuels like methanol and ethanol, is a promising strategy for addressing current energy and environmental challenges.[1] Significant efforts to develop efficient catalytic systems for these transformations are increasingly focused on molecular catalysts. These catalysts' well-defined structures allow for precise control and analysis of the structure-reactivity relationship.[2,3] Successive iterations of ligand design enable us to identify and rectify the weaknesses of previous generations of catalysts, leading to progressively more efficient versions.[4, 5] However, to achieve large-scale photo-electrolyzers for H_2 production or CO_2 reduction, it is essential to modify these molecular catalysts for integration into the design of hybrid photocathodes.

This PhD project, which is part of the PEPR LUMA SYNFLUX-LUMICALS (https://www.pepr-luma.fr/projet/synflux-lumicals/) program involving 19 laboratories, aims to develop molecular catalysts for CO_2 reduction and H_2 evolution. These catalysts will then be modified for grafting onto hybrid photocathodes. The PhD research project will include organic synthesis related to the preparation and functionalization of porphyrins. Catalysts derived from these modified porphyrins will then be incorporated onto photocathodes and studied in photo-electro-catalytic reactions for H_2 evolution and CO_2 reduction.

The candidate should have a strong background in organic synthesis and a willingness to learn new techniques related to photo- and electro-catalysis.

The PhD will be co-supervised by Dr. Philipp Gotico from CEA Saclay.

Interested applicants should send their CV (with contact information of two referees), and motivation letter (with brief summary of past research experiences) to zakaria.halime@universite-paris-saclay.fr and philipp.gotico@cea.fr.

References :

1) H. B. Gray, *Nat Chem* **2009**, *1*, 7.
2) P. Gotico, Z. Halime and A. Aukauloo, *Dalton Trans* **2020**, *49*, 2381-2396
3) V. Artero and M. Fontecave, *Coord Chem Rev* **2005**, *249*, 1518-1535.
4) P. Gotico, *et al. Angew Chem Int Ed* **2019**, 58, 4504-4509.
5) P. Gotico, *et al. Angew Chem Int Ed* **2020**, 59, 22451-22455.