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PhD Project: Development of New Catalysts to Explore the Effect of the Second Coordination Sphere on Catalytic CO_2 Reduction

The conversion of carbon dioxide (CO_2) into high-value-added fuels and chemical products through electrocatalysis or photocatalysis represents an innovative and forward-looking approach for the valorization of this molecule while facilitating the large-scale integration of intermittent renewable energy sources. By leveraging these advanced technologies, it becomes possible to transform CO_2, a major contributor to global warming, into valuable resources, thereby supporting the establishment of a circular carbon economy. This approach holds great promise for reducing CO_2 accumulation in the atmosphere while developing sustainable alternatives to fossil fuels and petrochemical-based precursors.[1]

As part of the collaborative ANR *MultiSCOR* research project, which brings together three research laboratories, this PhD thesis focuses on the design, synthesis, and study of new metalloporphyrin-based catalysts incorporating specific functionalities in the second coordination sphere. Inspired by natural enzymes, this strategy aims to develop more efficient and selective catalysts for CO_2 reduction. Our previous work on metalloporphyrin functionalization has led to significant improvements in their catalytic performance and has provided a deeper understanding of the underlying reaction mechanisms.[2-4] These advancements now offer the opportunity to further rationalize the design of these catalysts and explore new strategies to optimize their efficiency.

The PhD project will involve an important part of organic synthesis applied to the preparation and functionalization of modified porphyrins. These catalysts will then be evaluated in (electro-/photo-)catalytic CO_2 reduction. A strong focus will be placed on optimizing reaction conditions and conducting an in-depth study of the mechanisms to refine catalyst design strategies. The ideal candidate should have a strong background in organic synthesis and a keen interest in acquiring new skills in the fields of electro- and photo-catalysis. Additional expertise in coordination chemistry and catalysis would be highly appreciated.

This PhD will be conducted at the *Institut de Chimie Moléculaire et des Matériaux d'Orsay* (*ICMMO*), under the supervision of Dr. Zakaria Halime, and the co-supervision of Dr. Philipp Gotico (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.

Références :

1) T. P. Senftle, E. A. Carter, *Acc. Chem. Res.* **2017**, *50*, 472-475.
2) P. Gotico, B. Boitrel, R. Guillot, M. Sircoglou, A. Quaranta, Z. Halime, W. Leibl, A. Aukauloo, *Angew Chem Int Ed* **2019**, 58, 4504-4509.
3) P. Gotico, L. Roupnel, R. Guillot, M. Sircoglou, W. Leibl, Z. Halime, A. Aukauloo, *Angew Chem Int Ed* **2020**, 59, 22451-22455.
4) A. Smith, P. Gotico, R. Guillot, S. Le Gac, W. Leibl, A. Aukauloo, B. Boitrel, M. Sircoglou, Z. Halime, *Advanced Science* **2025**, *12*, e2500482.