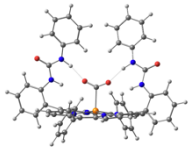

M1 /M2 Internship offer

Theoretical study of a series of CO_2 reduction catalysts

In the anthropocene era, capturing and transforming CO_2 into a higher value-added synthon is a key challenge for chemists. Iron porphyrins, combining an abundant and non-toxic metal with a highly modulable ligand, are among the most widely used and effective catalysts for electrochemical CO_2 to CO reduction. To make them technologically applicable, a reduction of their operational energy cost, i.e. the potential at which electrocatalysis is carried out, is currently being sought.

In our lab, we have developed a series of iron porphyrins decorated with various substituents that operate on a large range of potentials. We wish, through a theoretical study based on DFT, to decipher the parameters governing the activation energy of CO_2 on the metal center according to the ligand used. To this end, we will model different reaction intermediates in order to map their charge and spin densities. The fine rationalization of the observed trends will then allow us to orient the design of more efficient catalysts.

The candidate should have a good knowledge and an appetite for coordination chemistry and molecular modeling. He or she will also have to be very methodical and resourceful.

Note that the internship will take place at the Institut de Chimie Moléculaire et des Matériaux d'Orsay, but if the health context requires it, it can be held entirely or partially at a distance.

Duration of the internship 4 months minimum, beginning 1st semester 2021.

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Articles produced by our team related to the internship subject

Atropisomeric Hydrogen Bonding Control for CO_2 Binding and Enhancement of Electrocatalytic Reduction at Iron Porphyrins. P. Gotico, L. Roupnel, R. Guillot, M. Sircoglou, W. Leibl, Z. Halime, A. Aukauloo, *Angew. Chem. Int. Ed.* 2020 doi:10.1002/anie.202010859

Second-Sphere Biomimetic Multipoint Hydrogen-Bonding Patterns to Boost CO_2 Reduction of Iron Porphyrins. P. Gotico, B. Boitrel, R. Guillot, M. Sircoglou, A. Quaranta, Z. Halime, W. Leibl, A. Aukauloo, *Angew. Chem. Int. Ed*. 2019, **58**, 4504–4509.

Recent advances in metalloporphyrin-based catalyst design towards carbon dioxide reduction: from bio-inspired second coordination sphere modifications to hierarchical architectures. P. Gotico, Z. Halime, A. Aukauloo, *Dalton Trans.* 2020, *49*, 2381–2396.

These articles can be provided on request.