

## PhD research proposal

### Electrocatalytic and photocatalytic reduction of carbon dioxide by Cu-based molecular complexes

**Place:** Laboratoire CEMCA, UMR CNRS 6521, University of Brest (UBO), France

**Dates:** 1<sup>st</sup> Oct. 2021 – 30<sup>th</sup> Sept. 2024

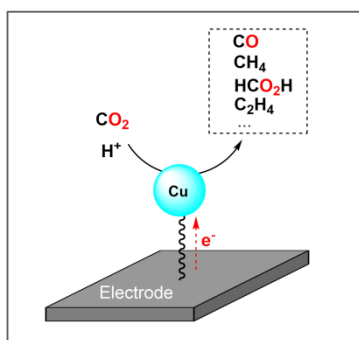
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#### Context

The electrochemical conversion of CO<sub>2</sub> into useful carbon feedstocks such as carbon monoxide, methanol, methane, ethylene, ethanol... using renewable energy represents one challenging approach to tackle problems of the global energy crisis and carbon emission. Electro- and photocatalytic reduction of carbon dioxide by molecular complexes involving Co, Fe and Ni metals has been particularly investigated for the last 10 years.<sup>1,2</sup> In contrast, Cu-based mono and dinuclear complexes have only recently drawn more attention. Although these systems display remarkable electrocatalytic and photocatalytic performances in aqueous and non-aqueous conditions, there is still some debate on the nature of the real active species for the catalytic reaction. In particular, the *in-situ* and reversible generation of Cu clusters has been recently suggested as being the key strategy to develop stable, selective and efficient catalysts.<sup>3,4</sup>

#### PhD project



The aim of the PhD project is to develop new Cu mono and dinuclear complexes for the electrocatalytic and photocatalytic reduction of CO<sub>2</sub>. For this purpose, different strategies will be foreseen. Mono- and dinuclear complexes bearing cyclic and acyclic nitrogen ligands will be developed. Their electrocatalytic properties for CO<sub>2</sub> reduction will be investigated in homogenous and heterogeneous phases. Photocatalytic reactions under CO<sub>2</sub> will be performed with standard set-ups. Products of the catalytic reactions will be analyzed by *in-situ* (IR spectroelectrochemistry) and *ex-situ* (NMR and IR spectroscopies, GC) methods available in the team. The project will also focus on the mechanistic studies

through the characterization of transient species.

#### Working environment

The doctoral student will develop his/her work mainly in CEMCA in Brest, but will also be required to carry out occasional missions within partner laboratories for particular analyses.

#### Candidate profile (skills)

This project is at the interface of electrochemistry, inorganic chemistry and material science. We are seeking for a motivated candidate with MSc degree or equivalent in chemical or physical sciences. Knowledge in inorganic synthesis, electrochemistry, surface modification would be highly appreciated. - No French level required if good proficiency in English (B1): Possibility to work/write the dissertation in both. To apply please submit the following in one pdf file:

- A cover letter
- A detailed CV,
- An academic transcript (Bachelor + Master 1 and first semester Master 2)
- Contact information of at least two references (name +e-mail + phone number)

### Bibliography

1. Franco, F., Rettenmaier, C., Jeon, H. S. & Roldan Cuenya, B. Transition metal-based catalysts for the electrochemical CO<sub>2</sub> reduction: from atoms and molecules to nanostructured materials. *Chem. Soc. Rev.* **49**, 6884-6946, doi:10.1039/d0cs00835d (2020).
2. Dalle, K. E. *et al.* Electro- and Solar-Driven Fuel Synthesis with First Row Transition Metal Complexes. *Chem. Rev.* **119**, 2752-2875, doi:10.1021/acs.chemrev.8b00392 (2019).
3. Weng, Z. *et al.* Active sites of copper-complex catalytic materials for electrochemical carbon dioxide reduction. *Nat. Commun.* **9**, 415, doi:10.1038/s41467-018-02819-7 (2018).
4. Balamurugan, M. *et al.* Electrocatalytic Reduction of CO<sub>2</sub> to Ethylene by Molecular Cu-Complex Immobilized on Graphitized Mesoporous Carbon. *Small* **16**, e2000955, doi:10.1002/sml.202000955 (2020).