



PhD fellowship offer

Deoxygenation of N–O and S–O Bonds – a Molecular Electrocatalytic Approach

Financial Support: Agence National de la Recherche

Starting – Duration : October 2023 – 36 months

Gross salary : 2044 €/month

Location: Département de Chimie Moléculaire UMR CNRS 5250

301 rue de la Chimie, 38000 Grenoble, France

Contact : Cyrille Costentin cyrille.costentin@univ-grenoble-alpes.fr

Working environment : The EMPRe team (<https://dcm.univ-grenoble-alpes.fr/node/9/emp-re-team>) conducts research in the field of molecular electrochemistry and redox photochemistry toward the understanding of bond activation triggered by electron transfer. Students in the EMPRe team are trained in synthesis of ligands and transition metal complexes. Then, they apply methods of molecular electrochemistry and spectroelectrochemistry, to study mechanisms of electro/photo-catalytic processes.

Project description : The project is part of the funded DeNOSOr research ANR project, a collaborative research consortium between three teams (EMPRe-DCM Grenoble, NIMBE CEA-Saclay and JOLIOT CEA-Institut Joliot). The DeNOSOr project aims at tackling an important topic, the deoxygenation of nitrogen and sulfur oxides. This is a central issue that needs unlocking to close the nitrogen and sulfur cycles, which are at the moment open due to human activities. Building on results recently gathered by the host team on N₂O reduction,^{1,2,3,4} the PhD student will investigate the electrochemical deoxygenation of N–O based compounds catalysed by molecular complexes. Low-valent transition metal complexes, able to accumulate a large electronic density on the metallic centers, will be targeted. The catalytic activity will be tested first on pyridine *N*-oxide, before moving on to more challenging heterocyclic *N*-oxides, then to amine *N*-oxides. A thorough investigation of the mechanism will be done using the tools of molecular electrochemistry (cyclic voltammetry, spectroelectrochemistry, electrolysis) mastered by the host team.⁵ Then the PhD student will tackle the deoxygenation of sulfoxides and sulfones, starting with sulfoxides R₂SO. This step presents yet another exciting challenge, due to the lower reduction potentials of the substrates compared to the *N*-oxide derivatives.

Keywords : N-O and S-O bonds activation, molecular catalysis, electrochemistry

Profile: The candidate should hold a M.Sc. degree or equivalent in chemistry or physical-chemistry with interest for organometallic synthesis, molecular electrochemistry, catalysis and mechanistic studies.

Application: Complete application in a single pdf file (detailed CV, one-page cover letter, one page summary of Master thesis, University marks) should be sent to:

cyrille.costentin@univ-grenoble-alpes.fr

¹ Deeba, R; Molton, F.; Chardon-Noblat, S; Costentin, C. *ACS Catal*, **2021**, *11*, 6099.

² Deeba, R; Chardon-Noblat, S; Costentin, C. *Chem. Sci.* **2021**, *12*, 12726.

³ Deeba, R; Chardon-Noblat, S; Costentin, C. *ChemElectroChem*, **2021**, *8*, 3740.

⁴ Deeba, R; Chardon-Noblat, S; Costentin, C. *submitted*

⁵ Savéant, J-M; Costentin, C. *Elements of Molecular and Biomolecular Electrochemistry*, 2nd. Ed.; Wiley, 2019.