

Intitulé du Sujet de Thèse : Development of Synthetic Model Complexes for Electrocatalytic Nitrite Reduction to Ammonia

Laboratoire : Institut des Sciences Moléculaires de Marseille ([iSm2](#))

Equipe : [BiosCienc](#)

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Descriptif du projet

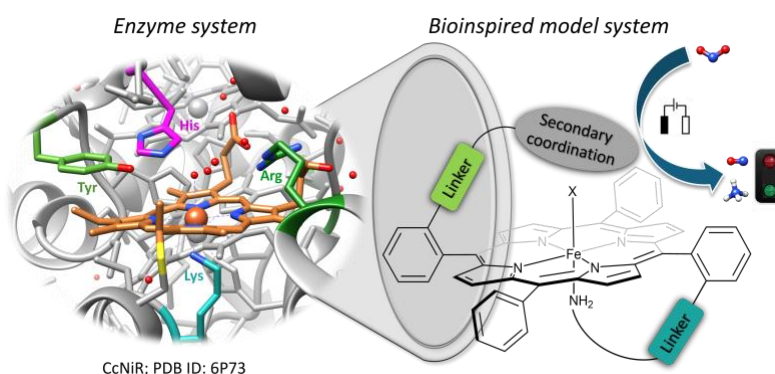
In the quest for sustainable chemical transformations, NO_x mitigation has become a critical challenge, similar to CO₂ conversion, with ammonia synthesis as a key objective. Excessive nitrogen fertilizer use causes environmental issues through both nitrification and denitrification, leading to nitrate leaching, which causes eutrophication, and N₂O (a potent greenhouse gas) emissions. A catalytic system is needed to reduce nitrite to ammonia without releasing intermediates. Nature employs two heme-based enzymes for nitrite-to-ammonia conversion: multi-c-heme nitrite reductases (C_nNiR) with penta- or octa-heme structures, and siroheme-containing nitrite reductases (CSNiR) with a [Fe₄-S₄] cluster linked to siroheme. Key residues in the proximal and distal-sites

(lysine, histidine, tyrosine, and arginine) are proposed to play a key role in nitrite binding and reduction process.^[1] This thesis aims to develop synthetic analogues mimicking the active site environment of C_nNiR and explore the *electrocatalytic reduction of nitrite to produce ammonia, avoiding the release of NO*.

Objectives of the project: This thesis project will focus on three deliverables: i) synthesis of functional mimic of C_nNiR active site; ii) electrocatalytic nitrite reduction studies on the molecular catalysts; iii) mechanistic elucidation through identifying the reactive intermediates either by *in-situ* spectroelectrochemistry or by trapping the intermediates at low temperature and performing *ex-situ* characterization.

Profile: Candidates should have background in synthesis of organic molecules and inorganic complexes and characterize with NMR, UV-Vis, and IR spectroscopy. A basic understanding of electrochemistry would be a plus. The candidates must have at least 12 out of 20 in a M2 chemistry specialization (or equivalent).

How to apply: Send a detailed CV (with contact details of 2 referees), a cover letter and transcripts of grades from M1 and current M2 year to: thierry.tron@univ-amu.fr and amanullah.sk@univ-amu.fr. A hearing (in person) before the Institute Council and Doctoral School Council will be part of the recruitment process.



Références Bibliographiques

[1] Luisa B. Maia, José J. G. Moura*, *Chem. Rev.* **2014**, *114*, 5273–5357