

## PhD proposal

### Electrochemical interfaces for N<sub>2</sub> reduction into green ammonia

**Laboratoire :** Institut Parisien de Chimie Moléculaire (IPCM) - UMR 8232- Sorbonne Université

<https://ipcm.fr/en/en-home/>

eMOCA group : <https://ipcm.fr/en/category/research/emoca-group/>

**Key Words:** electrochemistry – molecular catalysis – operando spectroscopy – N<sub>2</sub> reduction

**Context:** Nitrogen reduction into ammonia (NH<sub>3</sub>) emerges as a pivotal player in the future energy landscape due to its capacity for direct energy generation and its potential to decompose into dihydrogen. Furthermore, ammonia plays a crucial role in world food production as a key component in fertilizer formulations. However, for NH<sub>3</sub> to fulfil its role as a green energy carrier and main source for fertilizers, its industrial production must circumvent the consumption of H<sub>2</sub> and the generation of CO<sub>2</sub>. Presently, most of the ammonia production hinges on the Haber-Bosch process, corresponding to the catalytic direct reaction of nitrogen with hydrogen which is energy-intensive, economically burdensome, and environmentally problematic. An alternative approach involves the direct electrochemical N<sub>2</sub> reduction (eNRR) to produce NH<sub>3</sub>. However, there is currently no straightforward method for developing an efficient eNRR catalyst. Therefore, achieving a fundamental understanding of the electrocatalysis of ammonia formation at the atomic scale is crucial, yet it remains a significant experimental challenge as the tiny active zone close to the electrode is often concealed by the bulk of the electrolyte making it inaccessible to experimental characterization techniques.

Based *on our expertise and recent work on the electrochemical splitting of N<sub>2</sub> with molecular catalysts*,<sup>1</sup> the present PhD project proposes to better *understand how electrocatalysts interact with the reactant(s), the electrode and electrolyte under operating conditions*. We will design molecular interfaces at conductive (carbon, gold) surfaces, positioning the catalyst centre at different distances from the electrode and in different orientations. We will focus on molecular macrocyclic complexes of transition metals (Co, Fe).

**This project includes** (1) synthesis of catalyst, (2) modification of carbon and gold electrodes, (3) characterization by UV-vis absorption, IR, XPS, NMR, elementary analyses and electrochemistry of these new materials, (4) study of the electrochemical behaviour and mechanisms of the modified carbon and gold electrodes under nitrogen species (N<sub>2</sub>, nitrogen oxides) in various electrolyte pH conditions. Analysis of the reaction products (in the gas and liquid phase) with various analytical techniques (NMR, GC, GC-MS, labelled studies under <sup>15</sup>N<sub>2</sub>) will be carried out.

**Working environment:** Understanding how small molecule (CO<sub>2</sub>, O<sub>2</sub>, N<sub>2</sub>) can be activated using metal complexes is at the heart of the scientific efforts developed in the eMOCA group,<sup>2</sup> internationally recognized in the field of molecular electrochemistry and catalysis. All necessary equipment and expertise are available in the eMOCA team (synthesis, electrochemistry set-up, GC, GC-MS, LC-MS, UV-Vis, IR spectroscopies, DEMS, high performance NMR spectroscopy, etc.). Close collaboration with a group of theoretical chemists (ICGM, CNRS - Université de Montpellier) will lead to a comprehensive view of the catalytic mechanisms and to the design of optimized catalytic systems.

**Candidate profile:** MSc degree in chemistry or physical chemistry. Focus on electrochemistry and/or surface chemistry and interest in mechanistic understanding is mandatory. Self-motivation and ability to achieve goals independently as well as to contribute effectively to the group. The candidate should be highly motivated, hardworking, able to work as part of a team. No French level required while good proficiency in English (B1) is mandatory.

**To apply,** please submit:

- a cover letter
- a detailed CV
- academic transcripts (Bachelor + Master 1 and first semester Master 2)
- contact information of at least two references (name + e-mail + phone number)

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**Funding:** Contract from ANR. Starting October 1<sup>st</sup> 2026.

Gross salary: ~2200 €/month.

**Location:** Institut Parisien de Chimie Moléculaire (IPCM), Equipe eMOCA - Couloir 32-42 4ieme étage – Sorbonne Université, Campus Jussieu, 4 place Jussieu, 75252 Paris Cedex 05.

## References

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