Postdoctoral fellow: Mechanistic investigation of H2 production with molecular electrocatalysts

18 months postdoctoral position is open for a highly motivated candidate in The Department of Molecular Chemistry, in Grenoble.

Laboratorie	The Department of Molecular Chemistry, DCM, is a joint research unit (UMR). It is organized around six thematic research teams comprising sixty CNRS researchers and UGA professors/researchers. These teams are supported by the scientific platforms of the Grenoble Institute of Molecular Chemistry. https://dcm.univ-grenoble-alpes.fr/
Team	The candidate will join the CIRE and Sith teams to develop this project with Carole Duboc and Anne Milet. https://dcm.univ-grenoble-alpes.fr/research/chimie-inorganique-redox https://dcm.univ-grenoble-alpes.fr/research/spectrometrie-interactions-chimie-theorique
Context and scientific objectives	Identifying alternatives for the production of “green H2” is imperative to replace current unsustainable industrial processes. One strategy involves substituting noble-based metals with 3d metals. Building upon promising results achieved by the teams in the development of efficient bio-inspired electrocatalysts for H2 production (HER), this project aims to advance HER activity through a comprehensive mechanistic investigation. The acquired knowledge will provide valuable insights for designing highly performant catalysts for other crucial reduction processes involving multi-electron multi-proton processes, such as CO2 or N2 reduction.
Project name	In-depth mechanistic investigation of hydrogen production under both homogeneous and heterogeneous conditions with bio-inspired electrocatalysts
Project description	This project will focus on investigating the HER performance of molecular hetero/homodinuclear MM’ complexes (M = Ni, Fe, Cu, Co, Mn, and M’ = Fe, Mn) under both homogeneous (organic solvents) and heterogeneous (aqueous solutions) conditions. The elucidation of the mechanism, particularly through the generation and identification of catalytic intermediates using complementary experimental techniques (spectroscopic and spectrometric techniques combined with electrochemical methods) and theoretical modeling, will be conducted not only in solution but also at the electrode surface (after immobilization of the molecular catalysts). Understanding degradation pathways, especially at the electrode surface, will also be a focal point for the rational design of the next generation of HER catalysts or the optimization of the experimental catalytic conditions.
Mission	The candidate will develop a project combining experiments (electrochemistry, spectroscopy, handling reactive species) and quantum chemistry. The teams' proximity in geographical location will facilitate the candidate in combining both the experimental and theoretical aspects of the project.

Responsibilities	• Investigation of the performance of the complexes under homogeneous conditions • Investigation of the catalytic mechanisms, especially based on the generation and characterization of intermediates • Theoretical calculations to support the experimental data in the mechanistic elucidation, and propose catalytic cycles • Immobilization of the complexes on carbon-based materials & characterization of the corresponding modified electrodes • Evaluation of their HER performance of the modified electrodes • Investigation of the mechanism at the electrode surface • Theoretical calculations to assist in the identification of intermediates and to predict catalytic cycles for the immobilized complexes
Expected results	Performance evaluation and understanding of the catalytic mechanism of the HER activity of bio-inspired molecular catalysts in organic solvents (under homogeneous conditions) and in aqueous solutions (under heterogeneous conditions after their immobilization on an electrode surface).
Skills	• Experience in physical and analytical chemistry (electrochemistry, spectroscopic techniques, manipulation of reactive species, operando techniques) and an experience in quantum chemistry will be considered a positive point. • Soft skills: autonomy, rigor, and ability to communicate and work as part of a team.
Experience	From 2 to 5 years, beginners accepted
Applications Close	15/04/2024
How To Apply	Send the application including CV, cover letter and at least one letter of recommendation to the project leader: carole.duboc@univ-grenoble-alpes.f
Funding	Labex Arcane: https://arcane.univ-grenoble-alpes.fr

ARCANE bio-driven chemistry

UGA Université Grenoble Alpes

dcm département de chimie moléculaire

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