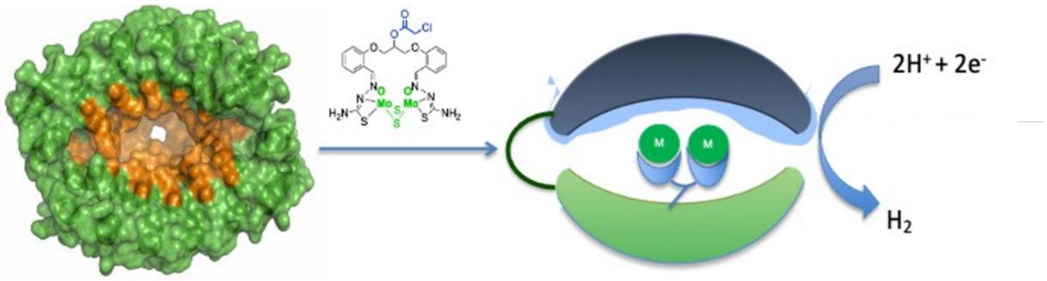
Offre de doctorat : Université Paris-Saclay / Institut Lavoisier de Versailles

Development of artificial enzymes for the reduction of protons to hydrogen

Keywords: Inorganic molecular chemistry, bioinorganic chemistry, electrocatalysis, NMR spectroscopy, electrochemistry

One of the most important challenges facing our society is to replace current fuels with new, abundant and renewable energy sources. Among these new sources, hydrogen appears to be a very interesting alternative, and the development of catalysts for hydrogen production is a major research challenge. Original molecular complexes based on non-noble metals such as iron or molybdenum, or polyometallates (POMs), have proven to be very interesting, effective and inexpensive for catalysing this reaction. However, some of these systems are not very stable in aqueous environments. One way to stabilise them is to immobilise them in biological matrices such as proteins. This produces artificial enzymes that can have remarkable catalytic activities.

The objective of this thesis project, which lies at the interface between inorganic chemistry, catalysis, and biology, will first be to develop new hybrid systems combining metal-sulphur (e.g., Mo-S and/or Fe-S) clusters with POMs. Both compounds are recognized for their exceptional electron and proton storage properties, as well as for their capacity to interact with proteins. In a second step, we will seek to stabilise these molecular systems in biological matrices such as proteins to form artificial enzymes either through a covalent chemical link or electrostatic interactions. The objective of this study is to develop stable and functional assemblies that operate in aqueous environments. An example illustrating this strategy through a covalent bond is given in figure below.



Example of an engineering strategy proposed for the generation of new artificial metalloenzymes for hydrogen production in aqueous media. In this example, a molybdenum complex is covalently grafted to a cysteine located in the caviy of an artificial protein αRep.

The molecular compounds and hybrid systems obtained will be characterised in Versailles using the extensive range of equipment available at ILV, including IR, RAMAN, UV-Visible, mass spectrometry, NMR, XRD, microscopy, electrochemistry, XPS. In particular, advanced characterisation techniques such as flow NMR, unique in the Ile-de-France region, and coupled RAMAN/electrochemistry and electrochemistry/GCMS techniques will enable in-depth study of the catalytic mechanisms involved in the targeted reactions.

References. 1) Zee *et al*, *Chem. Res*. **2015**, 48, 2027 ; 2) Rao *et al*., *Catal. Sci. Technol.* **2015**, 5, 233 ;. 3) B. Keita, et al., *J. Phys. Chem. C*, **2008**, 112, 1109 ; 4) J. Buils et al., *Dalton Trans*. **2025**, 54, 10381 ; 5) Y. Smortsova et al., *Chem. – Eur. J.*, **2021**, 27, 17094–17103 ; 6). Kariyawasam, *et al*. *Chem. Eur. J.*, **2020**, *26*, 14929 ; 7) Kariyawasam *et al*, *Biotechnol. Appl. Biochem.*, **2020**, *67*, 563.

Profile. The candidate must demonstrate a strong interest in the project and be comfortable with the field at the interface of chemistry and biology. Solid experience in coordination chemistry, as well as skills in spectroscopy and/or electrochemistry, will be particularly valued.
Salary : approximately €1800 net per month (possibility of additional salary if teaching assignment).
Duration : 36 months from October 1, 2026.
Supervisors / contacts if you are candidate : Dr Maxime Laurans (maxime.laurans@uvsq.fr), Dr Nada Savic (nada.savic@uvsq.fr), Pr. Sébastien Floquet (sebastien.floquet@uvsq.fr), Dr Mohamed Haouas (mohamed.haouas@uvsq.fr).