Aix*Marseille université

École Doctorale des Sciences Chimiques ED250

Contrats Doctoraux **2022**

PhD title : Computational Design of Molecular Catalysts for Hydrogen Production

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- Project

The development of renewable energy sources is of crucial importance to face the energy challenge of the 21st century. As **hydrogen** is considered as an energy carrier in the search for fuels of the future, the design of catalysts for hydrogen production is fundamental to developing abundant, inexpensive and environmentally friendly renewable energy sources. In this context, we have combined the not-innocent ligand thiosemicarbazone with Earth-abundant transition metal ions to prepare a series of **bio-inspired complexes** active in electrocatalytic proton reduction. We have shown that these complexes exhibit a high electrocatalytic activity for the reduction of protons to hydrogen,[1-3] which makes these systems competitive with the most efficient **electrocatalysts** described in the literature and which are based on cobalt and nickel. However, their reaction mechanism as well as the key elements to understand, rationalize and improve their responsiveness remain unknown.[4-6] This project aims to address these issues by developing a theoretical protocol to predict the catalytic performance of bio-inspired complexes for hydrogen production. Our goal is to understand the **reaction mechanisms** of our electrocatalysts by identifying the electronic parameters that govern their reactivity and by determining the structural elements essential for efficient hydrogen production. Our strategy will lead to the determination of potential-pH diagrams that provide key information on redox-active species and will allow the study of other electrocatalysts for direct comparison with the most efficient systems described in the literature. These **theoretical studies** will therefore make possible to predict the feasibility of the conversion reaction of protons into hydrogen and will allow the **rational design** of more efficient molecular catalysts. This project will be developed under an ANR contract (CODEC, 2020-2024).

- Profile

Solid background in quantum chemistry with a special interest for bioinorganic chemistry, a good knowledge in electrochemistry and spectroscopy will be appreciated

- Procedure

Send a CV and a motivation letter to maylis.orio@univ-amu.fr before **May the 1st of 2022**

- Bibliography

1) Chem. Cat. Chem., 2017, 9, 2262-2268 ; 2) Chem. Eur. J., 2018, 24, 8779-8786; 3) Dalton Trans., 2020, 49, 5064-5073; 4) Chem. Sus. Chem., 2019, 12, 4905-4915; 5) RSC Adv., 2021, 11, 5232-5238; 6) Chem. Commun., 2021, 57, 3952.