

## Three year PhD in Marseille: Bio-inspired Ni complexes for efficient H<sub>2</sub> oxidation and production

### Description

The performance of a catalyst is always considered in terms of speed (turnover frequency, TOF). Reversible catalysts are desirable, because they do not dissipate the chemical or electrical energy that is input to drive the transformation. In particular, understanding what makes some catalyst “reversible” is crucial in the solar fuels field, where efficient and cheap catalysts, based on transition metals, are needed to store in the form of chemicals (such as dihydrogen) the energy collected from intermittent sources<sup>1,2</sup>. Reversible catalysts are common in Nature: The enzymes hydrogenases, which produce and oxidized H<sub>2</sub>, are reversible catalysts. However, it has been difficult to characterize experimentally and to engineer in molecular catalysts<sup>3</sup>. Leger and coworkers have recently proposed the first kinetic models that allow the use of electrochemical methods to decipher the catalytic mechanism of synthetic, bidirectional redox catalysts, and to understand what makes them function (ir)reversibly<sup>4</sup>. This new methodology will be applied to a series of synthetic bio-inspired nickel complexes that have the rare property of functioning reversibly for the conversion between protons and H<sub>2</sub> (ref 3). The target complexes will be synthesized and chemically modified to help their attachment to electrodes. Upon a proper evaluation as molecular electrocatalysts, the systems will be investigated in deep using dynamic electrochemistry to get insight into their reaction mechanism. This synergic project will involve both the bioinorganic chemists from the laboratory iSm<sup>2</sup><sup>5,6</sup> and the electrochemists from the laboratory BIP<sup>1-4</sup>.

### References

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5. Orio M. *et al*, *Dalton Trans.*, 2020, 49, 5064-5073.
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### Keywords

bioinspired complex, electrocatalysis, coordination chemistry, reaction mechanism, energy

### Required skills

Background in organic synthesis, coordination chemistry and electrochemistry

### Contact

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