# Bio-inspired Ni complexes for efficient H2 oxidation and production


## Keywords
Hydrogen, catalysis, biomimetic chemistry, electrochemistry, solar-fuels



## Summary
The performance of a catalyst (be it a synthetic molecular catalyst, a surface, an enzyme or even a biological motor) is most often considered in terms of speed (turnover frequency). A distinct figure of merit of any catalyst is related to how much thermodynamic driving force must be applied to make it work at a significant rate; we and others have called “reversible” the catalysts that function at a high rate in response to even a small departure from equilibrium (1-4). Reversible catalysts are desirable, because they do not dissipate (waste as heat) the chemical or electrical energy that is input to drive the transformation. In particular, understanding what makes some catalyst function reversibly 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 (2,3). Reversible catalysis is common in Nature: the enzymes hydrogenases, which produce and oxidize H2, are reversible catalysts. However, catalytic reversibility has been difficult to characterize experimentally and to engineer in molecular catalysts (3). We 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 (4). We will apply this new methodology to a series of recently discovered bio-inspired nickel complexes that have the rare property of converting reversibly protons and H2 (3). The target complexes will be synthetized and chemically modified to help their attachment to electrodes, and thoroughly investigated using dynamic electrochemistry to understand how they work. This synergic project will involve both the bioinorganic chemists at iSm2 (5,6) and the electrochemists at BIP (1,2,4).


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## Locations
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## Doctoral school
Chemical Sciences (ED 250, https://ecole-doctorale-250.univ-amu.fr/ ), Aix-Marseille Université

## Expected profile of the candidate
The candidate will have an experience in inorganic chemistry or electrochemistry.