

Postdoctoral position in quantum chemistry at Aix-Marseille University

Theoretical investigation of bio-inspired hydrogen evolution catalysts

Description

The NiFemim project aims at developing bio-inspired hydrogen evolution catalysts to contribute to the full understanding of the catalytic mechanism of the NiFe hydrogenases. The main objective of NiFemim is to develop efficient mimics of this enzyme that model the structure and function of the active site as well as its reactivity. This project, funded by the ANR/DFG program, is an international cooperation between France and Germany which requires staff able to handle computational approaches for the modeling part in order to explore the field in an efficient way within a reasonable time. The present proposal is a **12 month-postdoctoral funding** starting during the **first semester of 2019**. The recruited candidate will work on deciphering the reaction mechanism of proton reduction by dithiolato-bridged heterobimetallic NiFe complexes. For that purpose, quantum chemical tools mainly based on Density Functional Theory (DFT) will be used to understand the catalytic activity of the bio-inspired complexes by unraveling the key-steps of their reaction mechanism. The goal of this computational study is to identify the electronic parameters that govern the reactivity of known catalysts and determine the crucial structural elements to achieve efficient hydrogen production and guide the design of new synthetic targets.

Keywords

hydrogenase, proton reduction, quantum chemistry, mechanism, catalysis

References

- [1] D. Brazzolotto, M. Gennari, N. Queyriaux, T. R. Simmons, J. Pecaut, S. Demeshko, F. Meyer, M. Orio, V. Artero and C. Duboc, *Nat. Chem.* 2016, 8, 1054–1060.
- [2] D. Brazzolotto, L. Wang, H. Tang, M. Gennari, N. Queyriaux, C. Philouze, S. Demeshko, F. Meyer, M. Orio, V. Artero, M. B. Hall, C. Duboc, *ACS Catal.*, 2018, DOI: 10.1021/acscatal.8b02830.

Profile

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

Duration

1 year, starting as soon as possible

Send a CV and a motivation letter to maylis.orio@univ-amu.fr before **January 2019 the 31th**

Contact

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