POSTDOCTORAL RESEARCH POSITION

Computational chemistry of functionalized Metal-Organic Frameworks for catalysis

Faculty: Laboratoire de Chimie des Processus Biologiques (LCPB), Collège de France, CNRS, Sorbonne Universités and PSL Research University

Location : 11 Marcelin Berthelot, 75231 Paris Cedex 05, France

Salary : depending on experience

Tenure : 18 months from October 2020

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Postdoctoral Position

In silico functionalization of MOFs for catalysis

Position for 18 months - Starting date from October 2020

Financial support: Agence Nationale de la Recherche

Laboratoire de Chimie des Processus Biologiques (LCPB), Collège de France, Paris

The post is available as part of the POMAC ANR research project. The objective of the project is to develop crystalline porous hybrid materials with targeted functionalization towards enhanced catalytic properties.

Porous hybrid organic-inorganic crystalline solids, known as Metal Organic Frameworks (MOFs) are built from the connection of metal clusters by polydentate organic linkers. They have proved to be an extremely attractive platform for designing catalysts thanks to their modular porosity, their versatile chemical functionalization which allows "design" strategies and their improved stability and recyclability unreached so far with homogeneous catalysts. Importantly their crystalline structures facilitate computational and theoretical approaches, whereby screening multiscale computational approaches have allowed the discovery of new materials. Overall the hybrid nature of MOFs offers the unique advantage of combining organic and inorganic moieties which can be pre-selected or functionalized for their own function, while their pores allow the immobilization of additional functional units, allowing complex multifunctional materials. Our team has developed in the last years tighly combined computational and experimental projects aiming at introducing photocatalytic activity, molecular recognition or assymetric catalysis in MOFs.

The post will build on recent publications of the team on metal-organic frameworks functionalized to perform photocatalytic reactions of interest such as OER (*Journal of the American Chemical Society* **2018**, 140, 10, 3613-3618; *ACS Applied Materials and Interfaces* **2019**, 11, 51, 47837-47845), HER (*Chemical Communications*, **2019**, 55, 4166) and CO_2RR (ChemSusChem **2015**, 8, 603-608; *ACS Catalysis* **2018**, 8, 3, 2030-2038; *Angewandte Chemie International Edition* **2020**, 59, 5116-5122, *Journal of the American Chemical Society* **2020**, 142, 20, 9428-9438) or on peptide-functionalized MOF to perform molecular recognition in view of asymmetric catalysis (*Chemistry, A European Journal* **2016**, 22, 16531-16538). Our team relies on tight interactions between theoreticians and experimentalists so as to drive the design of functional materials with interesting catalytic, photo- or electro-catalytic properties. The aim of the post-doc project is to extend our computational chemistry approach towards systematic strategies about the impact of the functionalization of the MOF (atomic and electronic structure, reactivity, photosensitivity) towards dedicated applications in catalysis in order to extract rationale and targets for more efficient materials. In other words, our ambition is thus to bring the atomic scale understanding and structure-properties rationale of such complex systems through a major step further so as to propose to synthetic chemists new families of selective and efficient functionalized MOFs for heterogeneous catalysis. This will rely on state-of-art computational methods and access to supercomputing national facilities in addition to the local ones.

Collaborations involved :
- IRCELyon – Dr. Jérôme Canivet – Covalent functionalization of MOFs
- Institut Lavoisier de Versailles (ILV)- Dr. Anne Dolbecq – Immobilization of complexes and POMs in MOFs

Potential Candidates should have a strong background in computational chemistry and catalysis:

- Expertise in computational chemistry such as DFT methods, molecular dynamics, and Monte Carlo methods etc…
- Expertise in catalysis is highly desirable together with understanding of guest response and/or catalytic function
- Relevant skills in other related areas e.g. adsorption, molecular recognition, photocatalysis are also desirable

- Excellent publication record

Your application should demonstrate the relevance and level of these skills to the project

Education, Qualifications and Training

- PhD in Theoretical Chemistry

Personal Skills

- Demonstrated ability to work as a member of a team
- Demonstrated ability to work proactively to progress a research project
- Demonstrated ability to organize own workload
- Ability to meet deadlines
- Clear and fluent report writing and oral communication
- Demonstrated ability to take ownership and responsibility for projects
- Ability to supervise and train early stage researchers

Applications: Cover letter, detailed CV and contact information for three references should be sent to Dr. Caroline Mellot-Draznieks (caroline-mellot-draznieks@college-de-france.fr). Interviews will be proposed on reception of these required documents.