POSTDOCTORAL RESEARCH POSITION

(ARTIFICIAL PHOTOSYNTHESIS : CHARACTERIZATION OF POROUS MATERIALS)

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

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

Salary : 2100 € net from RESPORE funding (http://www.respore.fr)

Tenure : 12 months from October 2018

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Postdoctoral Position

Noble metal-free POM@MOFs photocatalytic systems : in-depth structural characterization and development of thin films

Position for 12 months - Starting date: from October 2018 - Financial support: DIM RESPORE

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

Scientific context: Recently, we have combined for the first time the three realms of porphyrins antenna, polyoxometalates (POMs) and metal-organic frameworks (MOFs), which had remained unexplored so far, to provide a proof-of-concept "three-in-one" photocatalysts: the Co-POM@MOF-545, where the catalytically active Co-POM is immobilized into the porphyrin-based MOF-545 possesses remarkable water oxidation activities and recyclability (G. Paille et al. *J. Am. Chem. Soc*. **2018**, *140*, 3613). Our unique noble metal-free photosystem benefits from the confinement of the catalytic POMs into the pores, making further structural characterizations a crucial while challenging issue.

Aim of the post-doc project: Along a first line, our ambition is to bring the atomic scale understanding and structure-properties rationale of such complex systems through a major step further. Indeed, the direct structural characterization of cat@MOFs composites possessing immobilized catalytic species has been neglected in all studies reported since it is not accessible using conventional diffraction techniques due to their positional/statistical disorder of encapsulated/immobilized species. Here, PDF (pair distribution function) techniques are appropriate for locally probing the POM and its environment by collecting POM@MOF pair distribution functions. In depth structural characterization of cat@MOF composite photosystems has never been achieved so far at the atomic level. This project thus aims to leverage that limit by precisely identifying and locating POMs of interest for Water Oxidation Catalysis (WOC) or Hydrogen Evolving Reaction (HER) within MOFs pores thanks to last generation PDF techniques. Along a second line of innovative character, thin films technology applied to MOF-based photosystems is indeed a burgeoning area. We control the thin film synthesis of Co-POM@MOF-545 to produce a versatile easy-to-use photochemical heterogeneous setup. EXAFS/XANES runs at SOLEIL, SAMBA line, will allow us gaining further local structural details, using our initial existing structural models derived from DFT calculations.

POM@MOFs systems : The selected MOF will be the porphyrinic MOF-545. For PDF studies on powders, the immobilized POM will be the sandwich-type POM $[(PW_9O_{34})_2Co_4(H_2O)_2]^{10-}$ (known as a photocatalyst for WOC) and its analogue with Mn (known as a photocatalyst for HER). The preparation of the POM@MOF powder composite is already well handled by impregnation as well as its deposition in thin films. The objectives of the project are to explore PDF techniques and possibly EXAFS/XANES techniques to push forwards the atomic scale characterization of this POM@MOFsystem and similar ones.

Collaborations involved :
- Laboratoire de Chimie de la Matière Condensée de Paris (LCMCP) – Dr. Capucine SASSOYE
- Institut Lavoisier de Versailles (ILV)- Dr. Anne DOLBECQ

Potential Candidates should have a strong background in materials science. Previous experience in PDF (pair distribution function) techniques is mandatory. Previous experience in EXAFS/XANES is desirable.

Applications are invited for an ambitious scientist with an excellent track record in hybrid organic-inorganic materials and their structural characterization under ex-situ or in situ environment using X-Ray scattering and X-Ray absorption methods (PDF, EXAFS/XANES). The project required an integrated array of complementary skills to allow the characterization and evaluation of new materials for artificial photosynthesis, understanding their structures and properties arising from both computations and experiments carried in collaboration with other researchers.

The principal investigator is Caroline Mellot-Draznieks at the Collège de France who is an expert in the porous materials and adsorption properties using integrated computational and experimental approaches. The CDF has at hand a whole range of techniques available allowing to evaluate new porous materials for their performances in

artificial photosynthesis. CMD also works in collaboration with Dr. Anne Dolbecq (Versailles), an expert in multifunctional molecular polyoxometalates and their incorporation in hybrid porous host. The project co-investigator, Dr. Capucine Sassoye, at Sorbonne Université, currently focuses her research efforts on laboratory PDF measurements for investigating amorphous solids and nanoparticles. The post will suit a scientist motivated to produce step-change advance in new photocatalysts characterizations.

Profile requirements

Experience

- Expertise in data collection and analysis of Pair Distribution Functions (PDF) and X-ray absorption techniques (EXAFS/XANES) at synchrotron or laboratory facilities in ex-situ and in-situ environments
- Excellent technical competence and knowledge of porous materials (e.g., metal-organic frameworks or porous coordination polymers, zeolites) and their characterization relevant to the project goal
- Good understanding of guest response and/or catalytic function of porous materials is highly desirable (metal-organic framework or porous materials, porous polymers)
- Experience in computational chemistry approaches is highly desirable
- Relevant skills in other related areas e.g. adsorption, catalysis, photocatalysis are also desirable
- Past experience in thin films (spin coating, drop casting, electrophoresis etc…) will be useful although not mandatory
- Excellent publication record

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

Education, Qualifications and Training

- PhD in Chemistry or Materials Science

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

Ability to contribute to broader management and administrative processes (applications to runs at SOLEIL)

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.