

## Ph.D student call in “Time-resolved X-ray spectroscopy in biological and chemical catalysis”

### 1. Scientist in Charge

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### 2. Institution

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### 3. Brief description of the Research Group

Our research group is focused on the development and application of advanced spectroscopic tools for the design of active catalysts for water oxidation, proton reduction, and methane to methanol production processes. Currently the development of artificial photosynthetic assemblies and biological mimics of naturally methane oxidizing enzymes is of great interest, and has drawn significant attention by exploring molecular catalysts based on 3d transition metal complexes. However in spite of emerging design principles, there is an urgent need to correlate the performance and stability of a catalyst to its geometric structure and electronic configuration for its rational development.

In this regard, we are interested in the development of static and time-resolved X-ray based spectroscopic approaches, including X-ray absorption (XAS) and X-ray emission spectroscopy (XES), to understand the critical electronic, energetic and geometric requirements of the water splitting and methane oxidation reactions necessary for achieving economically feasible catalysts. Our research is particularly oriented towards ultrafast pump (laser), X-ray probe studies of metal noble-free photosensitizers, and multimolecular photocatalytic systems for artificial photosynthesis in the femtosecond-microsecond time regime. Combined analysis of experimental data on structures, electronic configurations and spin states provide valuable information to understand the operation mechanism. Further selectivity is achieved through resonant XES or resonant inelastic X-ray scattering spectroscopy.

Synchrotron-based techniques employed in our group are complemented with laboratory-based spectroscopic methods such as UV-Visible spectroscopy, Resonance Raman, Electron Paramagnetic Resonance, Optical transient absorption spectroscopy, and Atomic Force Microscopy. Our studies involve the interplay of several disciplines including synthetic inorganic chemistry, electrochemistry, kinetics, and spectroscopy.

#### 4. Project description

The project will consist in studying solar fuel catalysts through static and ultrafast *in-situ* X-ray spectroscopy and electrochemistry. The main objectives of the project will be to probe the electronic and structural changes occurring near the active catalytic site through X-ray absorption, emission and resonant inelastic scattering spectroscopy. The student will also be trained in Raman, EPR, Scanning Tunneling Microscopy and X-ray photoelectron spectroscopy.

The Ph.D student will assist in writing the beamtime proposals, and carrying out the synchrotron and laboratory-based experiments, data analysis and interpretation.

Required Qualifications:

1. M.S in chemistry, Physics or Biological Science
2. Experience in synthesis
3. Strong analytical skills, written and verbal communication skills

#### 5. Research Area

Chemistry (CHE)

Social Sciences and Humanities (SOC)

Economic Sciences (ECO)

Information Science and Engineering (ENG)

Environmental Sciences and Geology (ENV)

Life Sciences (LIF)

Mathematics (MAT)

Physics (PHY)

#### 6. Applications (documents to be submitted and deadline)

Candidates are required to submit a complete and updated CV with a brief description of the previous research and a motivation letter. Applications should be sent to the email [dooshaye.moonshiram@imdea.org](mailto:dooshaye.moonshiram@imdea.org) before **October 15<sup>th</sup>**.