# MSCA Postdoctoral Fellowships

HORIZON MSCA 2024 PF

Expression of interest









# Contact Person/Scientist in charge

Víctor A. de la Peña O'Shea & Marta Liras.

<u>victor.delapenya@imdea.org</u> / <u>marta.liras@imdea.org</u>

## Brief description of the Research Group

The main activity of the Photoactivated Processes Unit (PAPU) is the development of light-activated materials and processes for the production of sustainable fuels and other applications of interest in energy and environment. More precisely, our interest is focused on the development of devices and photoreactors, as well as in the design, synthesis and operando characterization of multifunctional materials, based on organic (conjugated polymers), inorganic (band gap engineering) and hybrid (heterojunctions and organo-inorganic coordination polymers) semiconductors, with photocatalytic activity for the production of fuels as a way for sustainable generation and storage of energy.

#### Research Area

- Chemistry (CHE)
- Information Science and Engineering (ENG)
- Physics (PHY)
- Data Scientist (ENG)

### **Applications**

Demonstrated experience:

- MOFS and COFs: Synthesis and characterization and structural determination using single crystal and powder diffraction.
- Conductive polymers: Synthesis and characterization of conductive organic polymers; Photocatalysis or photoelectrochemistry.
- Characterization and theoretical studies: In-situ characterization, including synchrotron radiation (XRD, HP-XPS, XAS); Atomic modelling and use of theoretical calculation software.
- Reactor engineering: Photocatalytic, photoelectrocatalytic or solar reactor design and operation; Process control tools; Chromatographic analytical techniques.
- Development of Machine Learning algorithms.
- Knowledge on the development of automatization environments for material synthesis.

Deadline for submission of documents: 5th of July 2024. Documents to be submitted:

CV stating background and skills

- Letter of motivation including research interests
- Two reference letters



### **Project description**

The postdoctoral fellow is expected to be involved in the development of hybrid materials for photocatalytic and photoelectrocatalytic reactions of energy and environmental interest, and proposed MSCA project may include the activities in one of the three research lines at the PAPU:

Synthesis and characterization of MOF, COF materials or conjugated organic conductive polymers (CPPs)

Synthesis of MOFs, COFs or CPPs for photocatalytic and photoelectrochemical applications.

Chemical, electrochemical, functional and optoelectronic characterization of those polymers and hybrid materials.

Application in photocatalytic reactors and photoelectrochemical cells.

Advanced experimental and theoretical characterization tools Characterization studies of different kinds of hybrid materials by standard characterization techniques.

Design, construction and use of devices for operando characterization in photocatalytic and photoelectrochemical reactions.

Theoretical studies of the structural and opto-electronic properties of hybrid materials.

Photocatalytic and photoelectrocatalytic reactor engineering

Design and set-up of photochemical and photoelectrochemical reactors for use under solar irradiation and artificial light.

Development of applications for process control in photochemical and photoelectrochemical reactors.

Operation of photochemical and photoelectrochemical reactors, including the development of analytical methods for the assessment of reaction products.

Development of artificial intelligence tools for synthesis of materials and testing on solar Fuels

Design and set-up of machine learning algorithms for managing information of database

Creation of an ontology for Solar fuels and chemical processes.

Development of applications for robotization of synthesis process and control in photoelectrochemical devices