



## **IMAP Seminar on July 24th 2025**

## **Guillaume Maurin & Mohamad El-Roz**

Horizon Europe MOF2H2 Project dissemination of results

Free admission • No registration • Available via zoom, write to roxane.solomovici@espci.psl.eu to obtain the link 🖂





#### 10:00 CET

Guillaume MAURIN,

# "Computational approaches to MOFs based-Sorbents Catalysts and and Membranes"

This presentation will deliver our latest achievements in the computational-aided development of MOFs as sorbents, catalysts and membranes for addressing a wide range of societal challenges, e.g. indoor air pollutants trapping, natural gas/biogas purification, water-sorption heat transfer,  $CO_2$  capture and photocatalytic conversion, hydrogen photocatalytic production, purification and storage.

#### Guillaume MAURIN, Institut Charles Gerhardt Montpellier (ICGM)

Guillaume Maurin is a Full Professor at the University of Montpellier and a distinguished Senior Chair at the Institut Universitaire de France. His research focuses on developing and applying advanced modelling/numerical simulation tools to aid the design of innovative nanoporous materials for energy and environmental applications.



#### 11:00 CET

Mohamad EL-ROZ,

### "Photocatalytic Hydrogen Production using Cu-Based MOFs: Insights into the mechanism"

Photocatalysis is a promising strategy for solar energy conversion and environmental remediation, but its potential is often limited by a lack of understanding of the dynamic processes occurring on the photocatalyst surface under realistic conditions. Operando techniques, particularly operando-FTIR, provide advanced characterization methods to monitor these processes in real-time. By coupling FTIR with photocatalytic reactors, reaction intermediates and adsorbed species can be detected, revealing the roles of surface sites in photocatalytic reactions. This approach offers insights into reaction pathways and catalyst performance, while also enhancing our understanding of how variables like light intensity and environmental conditions affect efficiency. My lecture will focus on the use of operando techniques such as FTIR, and XAS for investigating reaction mechanisms in photocatalytic hydrogen production from liquid organic hydrogen carriers (LOHCs), such as formic acid, using Cu-based MOFs photocatalysts. I will provide new mechanistic insights into metal cations restructuring in MOFs and underscores the importance of their structure-tailoring for sustainable light-driven applications.

#### Mohamad EL-ROZ, Catalysis & Spectrochemistry Laboratory (LCS)

Mohamad EL-Roz is a researcher at the French National Center of Scientific Research (CNRS). His research focuses on the preparation of photocatalysts and the investigation of photocatalytic reaction mechanisms using various spectroscopic techniques, including operando FTIR spectroscopy.





