

MOFs/COFs, porous polymers French Conference, Paris 2023

Final Program

Tuesday 23^d May

9.30 – 10.00: Welcome

10.00 – 12.00: Oral session 1 – Synthesis – Chair: C. Serre

- 10.00 – 10.20 : Alexandre Legrand, *UCCS, Université de Lille* - Stimuli-responsive gelation of linked metal-organic cages using pH and light
- 10.20 – 10.40 : Pauline Salaun, *UMET, Université de Lille* - Cooperative synthesis of raspberry-like covalent organic frameworks-polymers particles with a radial single-crystal grain orientation
- 10.40 – 11.00 : Saly Hawila, *IRCELYON, Université Claude Bernard Lyon 1* - New 1D and 2D d¹⁰ Coinage Metal Organic Chalcogenolate Coordination Polymers
- 11.00 – 11.20 : Xingze Wang, *ENS, ESPCI Paris, Université PSL* - Heterometallic (M^{IV}/M^{II}) MOFs as a versatile platform for the photocatalytic overall water-splitting reaction
- 11.20 – 11.40 : Ahmad Sousaraei, *University of Madrid, Spain* - Synergistic Binding Sites in a Metal-Organic Framework for the Optical Sensing of Nitrogen Dioxide
- 11.40 – 12.00 : Jean-Michel Rueff, *ENSICAEN* - Synthesis and structural study of Zn((HO)O₂P-C₁₂H₆S-PO₂(OH)) a new porous metallophosphonate with honeycomb structure

12.00 – 1.30 pm: Lunch Break

1.30 – 2.30: Plenary Lecture Dr Hana Bünzen, *University of Augsburg, Germany* – Challenges and opportunities of nano-sized metal organic frameworks in medicine - **Chair: FX Coudert**

2.30 – 3.10: Oral session 2 – Theory – Chair: FX Coudert

- 2.30 – 2.50 : Louis Vanduyfhuys, *University of Ghent* - How to efficiently simulate adsorption at ab initio accuracy?
- 2.50 – 3.10 : Pedro Brântuas, *Université de Montpellier* - VOCs capture and detection by MOFs : a synergetic experimental and computational approach

3.10 – 3.30: Coffee Break

3.30 – 4.30: Oral session 2 – Theory – Chair: FX Coudert

- 3.30 – 3.50 : Lionel Zoubritzky, *Chimie Paris, Université PSL* - Easy and fast identification of crystalline topologies with CrystalNets.jl
- 3.50 – 4.10 : Ambroise De Izarra, *ENS, Université PSL* - Molecular simulation of aqueous electrolyte solution insertion in porous materials in the osmotic ensemble
- 4.10 – 4.30 : Roberta Poloni, *Université Grenoble Alpes* - Optical properties of azobenzene-functionalized metal-organic frameworks via many body perturbation theory

4.30 – 6.30 : Poster Session

5.45 – 7.00 : Cocktail

Wednesday 24th May

8.45: Welcome

9.00 – 10.00: Plenary Lecture, Prof. Tomislav Friscic, *Birmingham university, UK* –MOF Extravaganza: Exploration of Unusual MOF Designs, Compositions, and Origins - **Chair: G. Maurin**

10.00 – 10.20 : Yann Magnin, *TotalEnergies* - Water effects on CO₂ adsorption & diffusion in MOF for carbon capture

10.20 – 10.40 : Romuald Dez, *Micromeritics* - Solutions pour la caractérisation des MOFs

10.40 – 11.00: Coffee Break

11.00 – 12.00: Oral session 4 - Biomedical applications - Chair: H. Bünzen

- 11.00 – 11.20 : Rosana Pinto, *University of Lisbon, Portugal* - Biocompatible MOFs as therapeutic vehicles for the delivery of nitric oxide
- 11.20 – 11.40 : Joanna Christodolou, *Université Paris-Saclay* - Nanoscale Iron-Based Metal-Organic Frameworks: Incorporation of Functionalized Drugs and Degradation in Biological Media
- 11.40 – 12.00 : Jonathan Bachir, *Université Paris-Saclay, UVSQ* - Integrating Metal-Organic Framework in Alginate hydrogel for Protein Encapsulation

12.00 – 1.30 pm: Lunch Break

1.30 – 3.10: Oral Session 5 – Other applications - Chair: T. Friscic

- 1.30 – 1.50 : Alisa Ranscht, *IRCELYON, Université Claude Bernard Lyon 1* - Polyoxometalate embedded in porous cationic polymers for photocatalytic oxidation reactions
- 1.50 – 2.10 : Inderdip Shere, *Institut Charles Gerhardt Montpellier* - A Computational Strategy to Explore the Potential of MOF/PHI Heterojunctions for Catalytic CO₂ Conversion
- 2.10 – 2.30 : Talal Mallah, *Université Paris-Saclay* - Unraveling the electronic structure of the Ni₃HHTP₂ ferromagnet, where are the single electrons ?
- 2.30 – 2.50 : Cédric Viravaux, *Université Paris-Saclay, UVSQ* - Temperature sensors based on europium polyoxometalate and metal-organic frameworks
- 2.50 – 3.10 : Thomas Devic, *Université de Nantes* - Is there any benefit of coating Si particles for negative electrode material of Li-ion batteries with MOFs? The case of Al-fumarate
- 3.10 – 3.30 : D. Dell'Angelo, *Université de Nancy* - Tuning van der Waals interactions in two dimensional metal organic frameworks for photodetector applications

3.30 – 3.45: Round table

3.45 – 4.00: Best poster and presentation prizes, Closing