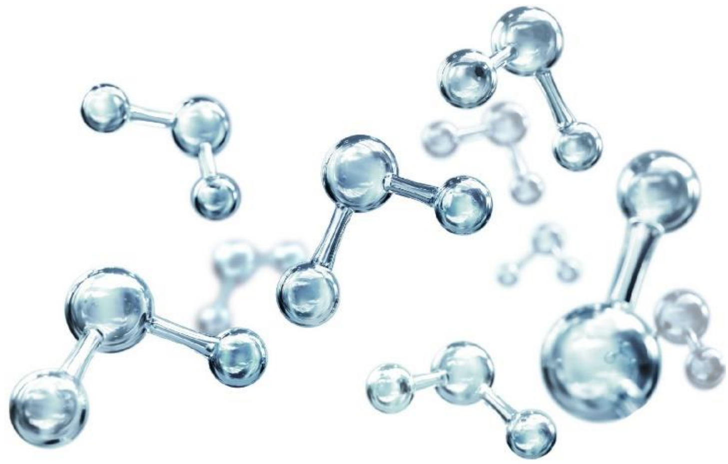
Seminar

CMWS Centre for Molecular Water Science

15th of January 2026
12:00 h

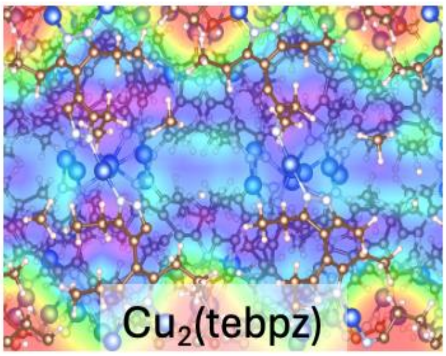
Zoom Virtual Meeting:
https://tuhh.zoom.us/j/82631283465
Meeting-ID: 826 3128 3465
Password: 978444



Simone Meloni

University of Ferrara, Italy

Water in the pointland: Unusual chemistry in confining MOFs' cavities



Contrary to intuition and bulk behavior, water confined inside Cu_2(tebpz) shows regions with density as large as twice the corresponding value in the bulk alternated to strongly depleted domains. Adapted from *J. Am. Chem. Soc.* 2024, **146**, 13236.

Metal–organic frameworks (MOFs) have recently gained major visibility following the 2025 Nobel Prize in Chemistry awarded to Susumu Kitagawa, Richard Robinson, and Omar M. Yaghi. As highlighted by the Royal Swedish Academy of Sciences, *"The Nobel Prize laureates in chemistry 2025 have created molecular constructions with large gaps through which guest molecules and other chemicals can flow. These constructions, metal–organic frameworks, can be used to harvest water from desert air, capture carbon dioxide, store toxic gases, or catalyze chemical reactions."* In this talk, I will focus on water confined within the narrow cavities of selected MOFs.

Water in MOFs (and other porous media) exhibits rich and unconventional thermodynamic and interfacial behaviors, enabling energy storage, wetting control, and stimuli-responsive phenomena at the nanoscale. When confined within these media, water's properties deviate sharply from those of the bulk phase: water in nanobottles is completely different from that in regular bottles on our table. Confinement alters the balance between cohesive and interfacial forces, reshaping transport mechanisms, free-energy landscapes, and ultimately phase equilibria. This raises fundamental questions as to whether familiar solid, liquid, and vapor phases remain well defined under extreme confinement. Understanding these deviations is essential to exploit confined water for future technologies.

Liquid intrusion and extrusion in hydrophobic MOFs and other nanoporous frameworks can be regarded as a confined thermodynamic cycle capable of energy storage, controlled dissipation, and energy conversion. We have exploited these effects to develop oil- and spring-free shock absorbers that convert mechanical energy—normally lost as heat—into electrical energy, offering a strategy to recharge batteries in electric vehicles and extend their driving range.

Confinement also profoundly modifies the supercritical state of water. In this regime, the interplay between density fluctuations and hydrogen-bond disruption produces a supercritical-like state at temperatures approximately 300 K below the bulk critical point, a striking departure from conventional phase behavior. Low-temperature "confined" supercritical water enables the design of micro- and mesoscopic Kamine-type cycles capable of harvesting low-grade heat using entirely aqueous working fluids. Moreover, mild-condition oxidation of persistent pollutants, such as PFAS, becomes feasible, suggesting compact, water-based treatment processes with reduced energy demands.

I will present our research on water confined in MOFs, emphasizing both fundamental insights and emerging technological opportunities. I will discuss the consequences of confinement for phase behavior, energy transduction, and reactivity, demonstrate how nanoscale wetting controls chemical reactivity, and outline emerging engineering challenges in harnessing confined fluids for sustainable technologies.