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Physical Properties in Confined Environments, Fundamentals & Applications

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Parrainage :

1. **SFEC** (Société Francophone d'Etude des Carbones), https://sfec-carbone.org/
2. **GDR ModMat** (Modélisation des Matériaux), http://www.cinam.univ-mrs.fr/site/modmat/
3. **GFZ** (Groupe Français des Zéolithes), http://gfz-online.fr/fr
4. **AFA** (Association Française de l'Adsorption), https://www.adsorption.fr/
5. **IRN NanoAlloys,** https://nanoalloys-irn.cnrs.fr/

The understanding, design and usage of porous medium have played a key role in human history. Caves, houses and cities are porous structures in which humans have been living for thousands of years. Porosity also plays an important role in living matter, thanks to biological membranes and tissues, ensuring transport and exchanges of water, ions, proteins and many other molecules inherent to life. The design of porous materials, being from physical or chemical routes have significantly advanced science and technology for millennia[1], and are playing increasingly important role in new technologies, especially for environmental and energy challenges that the world is facing[2].
According to the International Union of Pure and Applied Chemistry (IUPAC)[3], pores are classified into three categories: micropores (pore size < 2 nm), mesopores (in between 2 and 50 nm), and macropores (> 50 nm), with important changes in physical materials properties with their pore size. Based on adsorption phenomena (adsorbate-adsorbent interactions with pore walls), and due to the ability to tune the pore sizes and their chemistry[4,5], the past decade has seen a significant number of breakthroughs in the design and processing of novel porous materials (being natural or synthetic, organic, inorganic or hybrids)[6-8], driven by the rapid growth of emerging applications/needs, such as molecular capture, separation, energy storage and conversion, catalysis, desalination, sensors, DNA sequencing, drug delivery, and many others[9]. However, new technological applications require a high level of control over pore textural properties (pore sizes, tortuosity, topology, ...) and chemistry. For example, recent approaches based on machine learning have been proposed to identify hypothetical structures of interest for specific applications[10]. However, whilst thousand of structures such as zeolites, microporous polymers, covalent-organic frameworks or metal-organic frameworks are continuously emerging, just little is known about the role played by the ubiquitous multi-scale porosity of such materials in molecular adsorption, diffusion and transport properties[11]. Indeed, no theory or numerical algorithms are able to deal with pore sizes ranging from the nano- to the macropores. Actually, even the identification of transport mechanisms limited to nanoporosity is still a nascent field of research remaining poorly understood[12].
The objective of the mini-colloque, is devoted to both fundamental and applied approaches

in thermodynamics, kinetics and transport of multi-scale porous materials linked to applications, where structural and environmental complexity cannot be neglected. We hope to span different porous structures from both experiments (electron-tomography and microscopy, adsorption volumetry and gravimetry, ...) and simulations (Quantum computing, Density functional theory, Molecular dynamics, finite elements, ...) applied to different pore scales in applications such as CO_2 capture in metal-organic frameworks, energy storage in carbon based super-capacitors and batteries, shale gas extraction, ... We hope that such a “porous” topic, merging research and engineering will overlap interests of scientists from both academia and private sectors, sharing common interests in understanding fundamentals of porous materials for environment, energy and sustainable applications.

Such a topic mixing thermodynamics, kinetics, transport and chemistry in confined environments has been explored during the past years through the GDRI *Multi-scale Materials Under the Nanoscope* (M2UN), mainly focused on carbon, clay and silicates. The GDR *Pyrocarbon At the Nanoscale* (PYROMAN), focused on porous carbon materials, and partially through the annual meeting of *la Société Francophone d’Etude des Carbones* (SFEC), including (but not limited) to carbon nanotubes, carbon black, kerogens, cements, ... Abroad, meeting such as the *symposia of the International Conference on Materials for Advanced Technologies* (ICMAT), the *International Union of Materials Research Societies, International Conference on Advanced Materials* (IUMRS-ICAM), the *International Conference on Porous Materials and Materials Science* (ICPMMS), as well as ePorMat, InterPore, ... are organized around porosity for a large class of materials, pore scales and applications.
National CNRS laboratory and teams are specialized in different aspects of porosity in material sciences such as (but not limited) IRCE (Lyon), for the study of zeolites and Metal-Organic Frameworks, ICMN (Orléans), for porous carbons, CINaM (Marseille) for the characterization of porous carbons, clay, silicates, PHENIX (Paris), for the study of interfacial properties in nano-systems, or the Laboratoire de Physique de l’ENS (Paris), in theoretical research linking condensed matter, fluid dynamics and nano-science, ... Industries like TotalEnergies also perform R&D spanning both fundamentals and applications in Metal-Organic frameworks for CO_2 capture, electrodes for CO_2 conversion, CO_2 geological storage, battery electrodes, *etc*. Furthermore, the proposal is supported by several French meeting organized each year as SFEC, ModMat, GFZ and the IRN NanoAllaoys.

Références

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