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Adsorption and diffusion in nanoporous materials: the view from the nanoscale

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Nanoporous materials (pore size 1 –100 nm) are at the heart of numerous important applications: adsorption (e.g. gas sensing, chromatography), energy (e.g. hydrogen storage, fuel cells and batteries), environment (e.g. phase separation, water treatment, nuclear waste storage), etc. Among these materials, nanoporous solids which have pores ⊠ nm (e.g. active carbons, zeolites), are particularly interesting as ultraconfinement in their porosity leads to novel adsorption and transport phenomena. Thorough understanding of these effects and the underlying molecular mechanisms is critically needed to better characterize nanoporous solids. In this talk, I will present how statistical physics allows developing models for adsorption and transport in these extremely confining materials [1,2]. We will see how simple thermodynamic modeling allows rationalizing adsorption by considering reminiscent capillarity at vanishing lengthscales. Then, we will show how transport in sub-nanoporous media can be described without having to rely on macroscopic concepts such as hydrodynamics [3,4,5]. In particular, using parameters and coefficients available to experiments, we will see how transport coefficients can be rigorously upscaled using simple models such as free volume theories, etc. I will also briefly illustrate how the confinement of fluids in metallic nanoporous materials departs from what is observed for insulating materials [6].

1 B. Coasne et al., Chem. Soc. Rev. 42, 4141 (2013).
2 I. Deroche et al., Nature Comm. 10, 4642 (2019).
3 K. Falk et al., Nature Comm. 6, 6949 (2015)
4 T. Lee et al., Nature Comm. 7, 11890 (2016)
5 C. Bousige et al., Nature Comm. 12, 1043 (2021).
6 A. Schlaich et al., Nature Materials 21, 237 (2022).

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