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Respective contributions of adsorption, surface and bulk confined diffusion in molecular transport in nanoporous materials

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Numerous porous materials are made of intricate clustering of polydisperse nanoparticles. The particle organization on a length-scale ranging from nanometers to some micrometers is a cornerstone to properly understand transport properties (diffusion-permeation). A strong need to a bottom_up approach mixing SAXS, SANS and 2D -3D imagery technics is highly suitable for these types of multiscale complex systems. This multimodal structural analysis offers the possibility to use 3D reconstructions and to build constrained models mimicking observed geometrical features [1]. These models can then be used to compute transport properties allowing comparison with experimental determinations.
In this talk, we focus on a long and slow dynamics inside nanoporous porous materials essentially driven by molecular diffusion. This mechanism plays a major role to estimate the sustainability over a long period of time of numerous manufactured porous materials. We analyze the interplay between pore structure, adsorption and diffusion and how these different processes act in long term molecular transport. We show how intermittent dynamics [2] involving adsorption, surface diffusion and relocation inside the pore space induces a large part of the strong reduction of molecular diffusion inside pore network.

References

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[2] Levitz P., Bonnaud P.A., Cazade P-A, Pellenq R J-M and Coasne B. Soft Matter, 9, 8654–8663. (2013)

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Primary author: LEVITZ, Pierre (CNRS)

Presenter: LEVITZ, Pierre (CNRS)

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