Contribution ID: **3**   Type: **Oral**

On De Gennes Narrowing of Fluids Confined in Nanoporous Materials

Monday, 2 June 2025 15:45 (15 minutes)

Beyond well-documented confinement and surface effects arising from the large internal surface and severely confining porosity of nanoporous hosts, the transport of nanoconfined fluids remains puzzling by many aspects. With striking examples such as memory, i.e. non-viscous, effects, intermittent dynamics and surface barriers, the dynamics of fluids in nanoconfinement challenges classical formalisms (e.g. random walk, viscous/advective transport) – especially for molecular pore sizes. In this context, while molecular frameworks such as intermittent brownian motion, free volume theory and surface diffusion are available to describe the self-diffusion of a molecularly confined fluid, a microscopic theory for the collective diffusion (i.e. permeability) – which characterizes the flow induced by a thermodynamic gradient – is lacking.

Here, to fill this knowledge gap, we invoke the concept of "De Gennes narrowing" which relates the wavevector-dependent collective diffusivity $D0(q)$ to the fluid structure factor $S(q)$ [Kellouai et al. J. Chem. Phys. 160, 024113 (2024)]. First, using molecular simulation for a simple yet representative fluid confined in a prototypical solid (zeolite), we unravel an essential coupling between the wavevector-dependent collective diffusivity and the structural ordering imposed on the fluid by the crystalline nanoporous host. Second, despite this complex interplay with marked Bragg peaks in the fluid structure, the fluid collective dynamics is shown to be accurately described through De Gennes narrowing. Moreover, in contrast to the bulk fluid, departure from De Gennes narrowing for the confined fluid in the macroscopic limit remains small as the fluid/solid interactions in severe confinement screen collective effects and, hence, weaken the wavevector dependence of collective transport.

Primary author: Dr KELLOUAI, Wanda

Co-authors: Prof. BARRAT, Jean-Louis; JUDEINSTEIN, Patrick (LLB, CNRS, CEA, Université Paris Saclay); PLAZANET, Marie (Laboratoire Interdisciplinaire de Physique); COASNE, Benoit (CNRS/Univ. Grenoble Alpes)

Presenter: COASNE, Benoit (CNRS/Univ. Grenoble Alpes)

Session Classification: Contributed talks