Mechanical response of a nanopore saturated with fluid: molecular simulation results

Joel Puibasset*[1]

[1]Interfaces, Confinement, Materiaux, Nanostructures (ICMN) – CNRS : UMR7374, Université d'Orléans – 1b rue de la férollerie, 45071 ORLEANS CEDEX 2, France

Abstract

We present molecular simulations of a simple Lennard-Jones fluid saturating a deformable nanopore. The simulations allow to obtain the deformation of the nanopore as a function of the liquid pressure, in a way similar to what is done experimentally to measure the effective elastic moduli of the walls of the porous solid. The results show unexpected discrepancy between the observed deformation and that deduced from the direct stress-strain curves of the solid matrix. This effect is correlated with the fluid structure at the interface with the solid, and could be relevant to experimental data analysis.

*Speaker