

Water in hydrophobic micropores : dynamical behavior

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The study of interactions between porous materials and gases or liquids confined in them can be achieved by different methods. Numerical studies by means of molecular dynamics simulations and neutron scattering provide, for example, microscopic information about either the structure of the confined fluid or that of the porous matrix. This couple of methods may thus fit in the *bottom up* description of matter. The present talk will describe an experimental and somewhat more *top-down* approach to the study of the behavior of liquids confined in micro-mesoporous matrices in the case where the liquid does not wet the porous surface. Such an interface is said to be *lyophobic*, or hydrophobic in the particular case of water and aqueous solutions.

The experimental studies of lyophobic nanoporous materials coupled with liquids under hydrostatic pressure has provided the scientific community with several facts regarding this kind of systems. Thus, it is now established that the pressure at which water enters the porous volume is given by the Laplace-Washburn law of capillarity for mesoporous materials with pore diameters of size down to a few nanometers with a negligible impact of the intrusion velocity [1]. For smaller pores, Michelin-Jamois experimentally shown that this behavior breaks, in particular when considering electrolyte aqueous solutions. For most saline solutions combined with ZIF-8 microporous matrix, the intrusion pressure of liquid is observed to follow the same trend as with pure water but with an offset pressure found to obey the Van't Hoff osmotic pressure law [2]. Moreover we have recently shown with this system that the intrusion time scale has a significant impact on the intrusion and extrusion pressure: in this case, pressures should not be understood solely under the assumption of equilibrium thermodynamics. In particular when decreasing temperature close to 0°C an unusual pressure-volume characteristic is observed in dynamical regime, with a non monotonic decrease of pressure during the extrusion process.

[1] L. Guillemot, T. Biben, A. Galarneau, *et al.* Activated drying in hydrophobic nanopores and the line tension of water, Proc. Natl. Acad. Sci. **109**, 19557 (2012),

[2] M. Michelin-Jamois, C. Picard, G. Vigier *et al.*, Giant osmotic pressure in the forced wetting of hydrophobic nanopores, Phys. Rev. Lett. **115**, 036101 (2015).

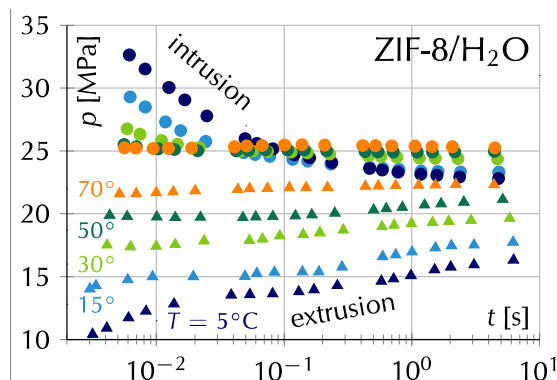


Figure 1 : Evolution of intrusion/extrusion pressures over the time at which pressure is applied for the ZIF-8/water lyophobic system at various temperatures.