Complex behaviour of fluids in confined spaces of soft porous materials

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Recent years have seen a large increase of the research effort focused on framework materials, including the nowadays-ubiquitous metal–organic frameworks, but also porous coordination polymers, covalent organic frameworks, and molecular frameworks. A large number of these frameworks flexible, or stimuli-responsive, i.e. their structure can undergo changes of large amplitude in response to physical or chemical stimulation. We will explore the recent advances in the understanding of the behaviour of fluids in the pores of these materials, and the interplay between fluid and host material.

Our group has put together a "toolbox" of theoretical approaches to shed light into these materials' properties and the behaviour of confined fluids. By means of molecular simulation at varying scale, we can now probe, rationalize and predict the behaviour of stimuli-responsive materials, producing a coherent description of Soft Porous Crystals from the unit cell scale all the way to the behaviour of the whole crystal. We also apply these methods to the understanding of bulk liquid phases, ionic or molecular, with complex solvation structures. In particular, I will discuss the examples of liquid metal-organic frameworks, and the solvation of CO2 in molten calcium carbonate.

References

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