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Adsorption, intrusion and freezing in porous silica: The view from the nanoscale

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Abstract

I will present the state of the art of molecular simulation and theory of adsorption, intrusion and freezing in porous silica. Both silica pores of a simple geometry and disordered porous silica's which exhibit morphological and topological disorders are considered. I will provide a brief description of the numerical models of porous silica's available in the literature and present the most common molecular simulation and theoretical methods. Adsorption in regular and irregular pores will be discussed in the light of classical theories of adsorption and capillary condensation in pores. I will also present the different evaporation mechanisms for disordered systems: *pore blocking* and *cavitation*. The *criticality* of fluids confined in pores, which is still the matter of debate, will then be discussed. I will review theoretical results for intrusion/extrusion and freezing in silica pores and discuss the validity of classical approaches such as the Washburn-Laplace equation and Gibbs-Thomson equation to describe the thermodynamics of intrusion and in-pore freezing. The validity of the most widely used characterization techniques will also be discussed. Finally, I will report some concluding remarks and suggest directions for future work.

Biography

Benoit Coasne obtained his PhD in Physics on capillary condensation in nanoporous materials (Paris, 2003). Then, he worked as a postdoc with Keith Gubbins on freezing of nanoconfined systems (North Carolina, USA). In 2005, he was appointed French CNRS researcher in Montpellier, France. He is currently working in the CNRS/MIT joint department on MultiScale Material Science for Energy and Environment located on MIT campus. He is member of the bureau of the French Zeolite Society and Cofounder and President of the French Adsorption Society. His research focuses on the adsorption and dynamics of systems confined in porous materials.