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

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The talk 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 silicas which exhibit morphological and topological disorders are considered. A brief description of the numerical models of porous silicas available in the literature and present the most common molecular simulation and theoretical methods will be discussed. Adsorption in regular and irregular pores will be discussed in the light of classical theories of adsorption and capillary condensation in pores. The discussion 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. Theoretical results for intrusion/extrusion and freezing in silica pores will be reviewed and 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 will be discussed. The validity of the most widely used characterization techniques will also be discussed. Finally, some concluding remarks and directions for future work will be reported.

Biography

Benoit Coasne obtained his Ph.D. 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.

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