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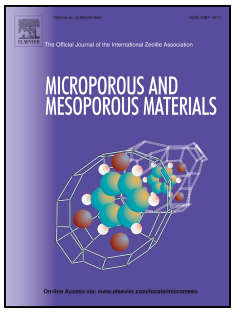

Effects of chemical and physical heterogeneity on confined phase behavior in nanopores

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Effects of Chemical and Physical Heterogeneity on Confined Phase Behavior in Nanopores

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Abstract

It is well known that fluids confined within nanoporous media often experience drastic and unexpected changes in thermodynamic properties. Recent research has focused on uncovering the mechanisms as well as pore size dependent effects. Unfortunately, very little insight is available for how pore wall chemistry and heterogeneity affect the fluid phase behavior. In this study, grand canonical Monte Carlo (GCMC) simulations were employed to investigate the effects of three different pore types on the fluid phase behavior and thermodynamic properties of ethane. Pores were created in sizes ranging from 3nm to 6nm and composed of either carbon or amorphous silica. Thermodynamic properties were calculated using particle number fluctuations, energy, and the grand canonical partition function. Results showed that ethane experienced a notable reduction in entropy due to layering effects within the carbon pores composed of a face centered cubic lattice structure. This layering effect was not observed in the amorphous silica pores. The combination of atomic disorder, chemical dissimilarity and lessened pore-fluid potential resulted in less reduction of the critical temperature within confinement. The results concluded that the pore structure leads to distinct shifts in the confined critical temperature depending upon the level of pore material disorder and surface chemistry. Both higher levels of atomic disorder and increasing chemical differences between the surface and adsorbate resulted in less critical point depression as compared to the ordered carbon pores which are commonly used in the literature. This paper showed that the effects of surface chemistry and atomic disorder are non-negligible factors when considering adsorption at the nanoscale.

Keywords:
nanopores, capillary condensation, phase behavior

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