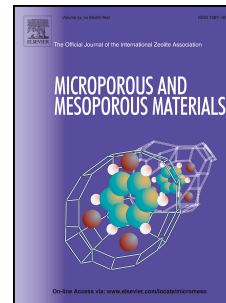


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Effects of Chemical and Physical Heterogeneity on Confined Phase Behavior in Nanopores

Evan Lowry*, Mohammad Piri

Abstract

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

Keywords:

nanopores, capillary condensation, phase behavior

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