**597a Development of Realistic Models of MCM-41 Materials for Gas Adsorption Studies**

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Siliceous mesoporous materials MCM-41 and SBA-15 attract a great deal of attention because of their possible uses as adsorbents or catalytic supports for gas adsorption, phase separation, catalysis, preparation of nano-structured materials, drug delivery, etc. [1] From a fundamental point of view, these materials are considered as model systems to investigate the effect of nano-confinement on the thermodynamic properties of fluids. As a result, many experimental, simulation, and theoretical works have been reported on gas adsorption in these materials [2]. In most simulation and theoretical studies, MCM-41 materials are modeled as pores of a regular cylindrical geometry. Recent studies [3-6] have investigated the behavior of fluids confined in atomistic models of these materials. However, it is not clear whether these models are realistic representations of the morphology of MCM-41 pores, due to the lack of conclusive experiments regarding their surface roughness and morphology.

One possible approach to modeling porous solids is to mimic the synthesis process of the real material, a strategy used in the past [7] to develop realistic models for Vycor and controlled pore glasses. Recently, Siperstein and Gubbins [8,9] reported mimetic on-lattice Monte Carlo simulations of surfactant – solvent – silica systems that were able to reproduce the formation of hexagonal structures resembling the arrangement of MCM-41 pores. In this work, we report the preparation of atomistic silica mesopores that keep the morphological features of the MCM-41 lattice model developed by Siperstein and Gubbins. The porous material is generated by carving out of a silica block, the skeleton of a MCM-41 pore that was obtained by lattice Monte Carlo simulations. We also present Grand Canonical Monte Carlo simulations of Ar and Xe adsorption in this model. We discuss the effect of the pore shape by comparing the adsorption isotherm and the isosteric heat curves with those obtained for an atomistic, regular cylindrical nanopore having a similar pore diameter. Comparison with adsorption and neutron scattering experiments suggests that our model of MCM-41 pores is too rough at the molecular scale, but reproduces reasonably the surface disorder of real MCM-41 at larger length scales.

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