559a Molecular Models of Mcf and Sba-15 and Gas Adsorption: a Molecular Simulation Study

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We have developed both mesoscale and atomistic models of templated mesoporous silicas such as Mesostructured Cellular Foams (MCF) and SBA-15. The first part of this work involves mimicking the synthesis process of these materials using Lattice Monte Carlo simulations, by equilibrating mixtures of surfactant, oil, water and inorganic oxides at a constant temperature. Depending on the solvent concentrations, we have observed the formation of spherical mesocells connected through windows resembling the MCF structure, as well as hexagonal phases mimicking the SBA-15 porous structure. The mesoscale pore models are then converted into atomistic models by carving out of silica blocks the pore morphologies generated from Lattice Monte Carlo simulations [1,2]. In our model, both the pore surface heterogeneity and the micropores (for the case of SBA-15) are derived from the mimetic mesoscale simulations. The simulated TEM and pore size distribution of the models qualitatively resemble the real materials.

In the second part of our work, we have studied argon adsorption inside the atomistic pores using GCMC simulations. As an example, for the case of SBA-15, a comparison of adsorption behavior has been made among several different pore models: (1) a regular cylindrical pore, (2) our model pore removing the microporosity, (3) our model pore with the micropores. We have also calculated the isosteric heats of adsorption and compared our simulation results with experimental data [3].

[1] S. Bhattacharya, B. Coasne, F. R. Hung and K. E. Gubbins, Stud. Surf. Sci. Catal., submitted (2005)

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[3] A. Galarneau, H. Cambon, F. Di Renzo and F. Fajula, Langmuir, 17 (2001) 8328.