16. Computational Design of Mesoporous Silica for CO_2 sequestration: controling nanoconfined supercritical fluids.

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An understanding of the phenomena of interface and transport of ions and molecules (H_2O and CO_2) in confined geometries is crucial, especially in the context of CO_2 sequestration. Atomistic calculations can provide interesting ways to address these issues. Here, we apply molecular dynamics calculations to study the effects of confinement on the wettability and transport phenomena of CO_2 within SiO_2 mesostructures. Knowing the effects of nanoconfinament of CO_2 in silica can lead to production of mesostructures "tailored" to optimize the specific separation and CO_2 capture. We started from extensive silica amorphous (106 atoms) to generate mesoporous structures. Voids have been created within this matrix, minimizing the surface area and pore energy. Optimizing the radius and geometry of the voids, we can generate any topology and sub-networks of pores embedded in the matrix. The porous were filled by supercritical CO_2 under different thermodynamic conditions (T=300K and pressure range of 50 to 500 atm). In this first phase, channels has been modeled with three forms of ellipsoids joined two by a reduction in diameter at the center, an ellipsoid and a cylinder. Our MD calculations indicate that the radial function of pairs decreases with increasing pressure and an accumulation of CO_2 near the surface. The surface tension increases as the pressure increase (from 0.92 to 0.96 N/m) and the diffusion coefficient was found to be lower in the channel at a reduced diameter in the center and decreases from the interface to the channel's center.