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Computer simulation study of structure and dynamics of supercooled water in silica nanopores[1] NICHOLAS KUON, Department of Physics, Colorado State University, BRANKA LADANYI, Department of Chemistry, Colorado State University — In narrow hydrophilic pores, interactions with pore walls and confinement dimensions allow water to remain liquid well below the normal freezing point. We investigate the properties of nanoconfined supercooled water by means of molecular simulation. The focus of our study is confinement in approximately cylindrical silica pores, with diameters in the 20-40 Å range, a model for MCM-41 materials. We use Gibbs-ensemble Monte Carlo method to determine water density in the pores in equilibrium with the bulk and molecular dynamics simulation to study the properties of confined water [1]. We study the translational and rotational mobilities of molecules in different interfacial layers and the effects on water dynamics of interfacial hydrogen bonding. We make contact with quasi-elastic neutron scattering experiments on supercooled water in MCM-14 silica pores by calculating and analyzing self-intermediate scattering functions of water hydrogens. [1] A. A. Milischuk and B. M. Ladanyi, J. Chem. Phys. **135**, 174709 (2011).

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