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How does confinement affect the structure and dynamics of water and other liquids? ANATOLI MILISCHUK, BRANKA LADANYI, Department of Chemistry, Colorado State University, Fort Collins, Colorado 80523-1872 — We studied the effects of confinement on static and dynamical properties of liquids including water, acetonitrile, and benzene in amorphous silica nanopores in equilibrium with the bulk liquid at ambient conditions. The model pores are approximately cylindrical, with diameters ranging from 20 to 40 Å. The filled pores are prepared using grand canonical Monte Carlo simulation and molecular dynamics simulation is used to calculate liquid structure and dynamics. Our studies of dynamics included translational mean squared displacements, orientational time correlations, and survival probabilities in interfacial shells. We also studied polarizability anisotropy time correlations that are related to experimentally observed optical Kerr effect response functions. We found that there is layering and preferential orientational ordering of solvent molecules in the interfacial region. Molecular translational and rotational mobility is reduced in the layers near the interface. Confinement leads to slowdown of the polarizability anisotropy relaxation in agreement with experimental findings.

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