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Confinement effects on collective water dynamics: Molecular dynamics study of optical Kerr response in silica nanopores[1] ANATOLI MILISCHUK, BRANKA LADANYI, Department of Chemistry Colorado State University — We report the results of the study of the effects of confinement on collective dynamical properties of water in model nanopores at ambient conditions. The main focus is on approximately cylindrical pores composed of amorphous silica, with diameters ranging from 20 to 40 Å, designed to represent MCM-41 materials. Results for hydrophilic and hydrophobic pores of similar dimensions, but with roughness reduced compared to silica nanopores, are also considered. The main quantity studied is the polarizability anisotropy time correlation function (TCF), which is related to the experimentally-observed optical Kerr effect (OKE) nuclear response. We investigate the effects on this TCF of the reduced molecular translational and rotational water mobility in the layers near the interface. We find that these effects lead to pore diameter dependent slowdown of polarizability anisotropy relaxation, in agreement with OKE experiments.

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