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Unusual Properties of Water Confined in Nanoporous Silica Glasses CAMILLA KIRKEMO, University of Oslo, Physics of Geological Processes, ADARSH SHEKHAR, University of Southern California, Collaboratory for Advanced Computing and Simulations, ANDERS MALTHE-SORENSSEN, University of Oslo, Physics of Geological Processes, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, University of Southern California, Collaboratory for Advanced Computing and Simulations — The structure and dynamics of water confined in nanoporous silica are different from that of bulk water, and insight into the properties of confined water is important for our understanding of many geological and biological processes. We use reactive molecular dynamics simulations to study the structure and dynamics of nanoconfined water between 100 and 300K. The simulations are based on experimentally validated force fields for silica and water. These force fields allow dissociation of water molecules. We prepare nanoporous silica systems with pore sizes in the range 1-6 nm, and study the behavior of water in the nanopores. We observe a mixture of high-density and low-density water in the pores, and hysteresis in the energetics of water upon cooling and heating. We will present results for the structure and diffusion of water near surfaces and in the interior regions of nanopores as a function of temperature.

Camilla Kirkemo
University of Oslo, Physics of Geological Processes

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