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Structure and adsorption of water in non-uniform cylindrical nanopores GREG LAKATOS, Department of Chemistry, University of British Columbia, GLENN TORRIE, Department of Chemistry and Chemical Engineering, Royal Military College, GREN PATEY, Department of Chemistry, University of British Columbia — Grand canonical Monte Carlo simulations are used to examine the adsorption and structure of water in the interior of cylindrical nanopores with non-uniform surfaces. Nanopores with radii in the range of 0.45 to 1.2nm are considered, and the axial symmetry of the nanopores is broken by varying the radius as a function of position along the pore axis, or by introducing regions where the strength of the water-nanopore interaction is reduced. Water in filled pores with a 0.6nm radius, exists in either a weakly structured fluid-like state, or a structured polarized state, with a pentagonal cross section. This structured state can be disrupted by creating hydrophobic regions on the nanopore surface, and the degree of disruption can be controlled by adjusting the size of these regions. Similarly, spatial variation in the nanopore radius can produce two condensation transitions, and vapor-liquid, and solid-liquid co-existences at points along the filling isotherm. This ability to control water structure through nanopore surface modification holds promise for the development of tunable nanoscale fluid conduits and storage devices.

Greg Lakatos
Department of Chemistry, University of British Columbia

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