Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

**Properties of Aqueous Electrolytes within Narrow Slit-Shaped Pores**[1] TUAN A. HO, DIMITRIOS ARGYRIS, ALBERTO STRIOLO, The University of Oklahoma, School of Chemical, Biological and Materials Engineering —
We report equilibrium molecular dynamics simulation results for structural and dynamic properties of aqueous electrolyte solutions confined within narrow pores. The slit-shaped pores are carved from cristobalite silica, corundum alumina, magnesium oxide, and other materials. The pore width is in the range 0.8 – 2.0 nm. The aqueous solutions contain NaCl, CsCl, $CaCl_2$, and $SrCl_2$ electrolytes at 1M concentration or larger. Equilibrium simulations are performed at ambient conditions within the NVT ensemble. The data suggest the formation of layered structures, which are consistent with results obtained for thin films of solution supported on free-standing surfaces. However, confinement enhances the differences in transport properties observed between those ions that are near the solid and those at the pore center. Because the self-diffusion coefficient is faster as the distance from the solid increases, the ions that are at the pore center diffuse more quickly through the pore than those adsorbed closer to the wall. Thus our results could be used to design membranes to separate, e.g., aqueous NaCl from CsCl solutions.

[1]Research supported by the Department of Energy and, in part, by the National Science Foundation.

Alberto Striolo
The University of Oklahoma

Date submitted: 23 Nov 2010 Electronic form version 1.4