

Abstract Submitted
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Adsorption of Electrolytes within Narrow Slit-Shaped Silica Pores: Molecular Dynamics Simulation Results to Design Separation Strategies¹ ALBERTO STRIOLO, The University of Oklahoma, DIMITRIOS ARGYRIS, OU MOLECULAR SCIENCE AND ENGINEERING TEAM — 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 and show various degrees of hydroxylation. The pore width is in the range 0.8 – 2.0 nm. The aqueous solutions contain NaCl, CsCl, CaCl₂, and SrCl₂ electrolytes at 1M concentration or larger. Simulations are performed at ambient conditions within the NVT ensemble. The results are analyzed in terms of density profiles away from the solid substrates, self diffusion coefficients in the direction parallel to the solid substrate, and residence time at contact with the solid substrate. The data suggest the formation of layered structures, consistent with results obtained for thin films of solution supported on free-standing surfaces. 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. Further, our results are important for exploring and understanding Hofmeister effects under confinement, and also for deploying a number of practical applications including water desalination, remediating nuclear waste sites, and designing nanofluidic devices.

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