

Abstract Submitted
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Probing the Structure of Salt Water Under Confinement with Computation HEATHER KULIK, Stanford University, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, GIULIA GALLI, University of California, Davis — We have investigated the structure of liquid water around cations (Na^+) and anions (Cl^-) confined inside a (19,0) carbon nanotube with first principles molecular dynamics (FPMD) and theoretical X-ray absorption spectroscopy (XAS). We study the distribution of ions and nature of the ion solvation shells under confinement from molecular dynamics. We also examine the XAS signal of water molecules surrounding Na^+ and Cl^- upon confinement and relate these spectral fingerprints to those of solvated ions in bulk water. We observe unusual trends in the XAS upon confinement of cations and anions that likely stems from variation in the number of acceptor hydrogen bonds in the first solvation shell for the two species. The rigid first solvation shell of Na^+ is rigid whether in bulk or confined solution, disrupting the overall hydrogen bonding network of the rest of the confined water. The solvation shell of Cl^- is considerably more flexible and adapts under confinement to accommodate roughly the same number of acceptor bonds. In our nanotube, we observe an inner bulk-like shell of water and outer shell of interfacial waters, as observed through both FPMD and XAS properties.

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