

Abstract Submitted
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Salt Solutions in Carbon Nanotubes: The Role of Cation- π Interactions¹ TUAN ANH PHAM, Lawrence Livermore Natl Lab, GOLAM MORTUZA, School of Mechanical and Materials Engineering, Washington State University, BRANDON WOOD, EDMOND LAU, TADASHI OGITSU, Lawrence Livermore Natl Lab, STEVEN BUCHSBAUM, ZUZANNA SIWY, Department of Physics and Astronomy, University of California, Irvine, FRANCESCO FORNASIERO, ERIC SCHWEGLER, Lawrence Livermore Natl Lab — Understanding the structure of aqueous electrolytes at interfaces is essential for predicting and optimizing device performances for a wide variety of emerging energy and environmental technologies. In this work, we investigate the structure of two common salt solutions, NaCl and KCl, at a hydrophobic interface within narrow carbon nanotubes (CNTs). Using a combination of first-principles and classical molecular dynamics simulations, we find that the solvation structure of the cations in the CNTs can deviate substantially from the conventional weakly interacting hydrophobic picture. Instead, interactions between solvated ions and the π -orbitals of the CNTs are found to play a critically important role, with the ion solvation structure ultimately determined by a subtle interplay between cation- π interactions and the intrinsic flexibility of the solvation shell. In the case of K^+ , these effects result in an unusually strong propensity to partially desolvate and reside closer to the carbon wall than either Na^+ and Cl^- , in sharp contrast to the known ion ordering at the water-vapor interface.

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