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Ion solvation in confined water: A first-principles molecular dynamics investigation ERIC SCHWEGLER, Lawrence Livermore National Lab, GIANCARLO CICERO, Polytechnic of Torino, Italy, JEFFREY GROSSMAN, UC Berkeley, FRANCOIS GYGI, GIULIA GALLI, UC Davis — The importance of water in many areas of science has motivated an enormous number of experimental and theoretical investigations. While the properties of bulk liquid water have been relatively well characterized, much less is known about the properties of water when it is confined in a nanoscale environment. We have carried out a series of first-principles molecular dynamics simulations in order to examine how the solvation properties of simple ions are modified upon nanoscale confinement. These simulations include the aqueous solvation of cations contained within a carbon nanotube. By comparing to the properties of ions in bulk liquid water, the dynamical and structural characteristics of confined ion solvation will be discussed in detail. This work was performed under the auspices of the US Department of Energy by the University of California at the LLNL under contract no W-7405-Eng-48.

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