

Aqueous Solutions on Silica Surfaces: Structure and Dynamics from Simulations

Alberto Striolo^{C, S}, Dimitrios Argyris and Naga Rajesh Tummala

The University of Oklahoma, School of Chemical, Biological and Materials Engineering, Norman, OK, U.S.A.

We are interested in understanding the properties of aqueous electrolyte solutions at interfaces. The fundamental questions we seek to answer include: (A) how does a solid structure perturb interfacial water? (B) How far from the solid does this perturbation persist? (C) What is the rate of water reorientation and exchange in the perturbed layer? (D) What happens in the presence of simple electrolytes? To address such topics we implemented atomistic molecular dynamics simulations. Recent results for water and simple electrolytes near silicon dioxide surfaces of various degrees of hydroxylation will be presented. The simulations are analyzed in terms of density profiles away from the solid surfaces, residence times for water and/or ions at contact with the surface, and structure and dynamics of the hydrogen bond network at the interface. The data suggest the formation of a layered aqueous structure near the interface. The density profile of interfacial water seems to dictate the density profiles of aqueous solutions containing NaCl, CaCl₂, CsCl, and SrCl₂ near the solid surfaces. These results suggest that ion-ion and ion-water correlations are extremely important factors that should be considered when it is desired to predict the distribution of electrolytes near a charged surface. Our results will benefit a number of practical applications including water desalination, exploitation of the oil shale in the Green River Basin, nuclear waste sites remediation, and design of nanofluidic devices.