Visualizing interfacial ion hydration and transport at molecular level

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Ion hydration and transport at interfaces are relevant to a wide range of applied fields and natural processes. Interfacial effects are particularly profound in confined geometries such as nanometre-sized channels, where the mechanisms of ion transport in bulk solutions may not apply. The main difficulty in correlating atomic structure with transport properties of hydrated ions lies in the interfacial inhomogeneity as well as the complex competing interaction among ions, water and surfaces, which requires detailed molecular-level characterization. Using a combined scanning tunneling microscopy and noncontact atomic force microscopy system [1], here we were able to construct individual Na^+ hydrates on a NaCl(001) surface by progressively attaching single water molecules (one to five) to the Na^+. We found that the Na^+ hydrated with three water molecules diffuses orders of magnitude faster than other ion hydrates. Ab initio calculations revealed that such high ion mobility arises from the existence of a metastable state, in which the three water molecules around the Na^+ ion can rotate collectively with a rather small barrier. The above picture applies even at room temperature according to the classical molecular dynamics simulations. Our work suggests that anomalously high diffusion rates for specific hydration numbers of ions is generally determined by the degree of symmetry match between the hydrates and the surface lattice [2].

References:

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