Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

Wednesday, September 25th, 2019 – 14:00 pm
CFEL Seminar room IV (Bldg. 99)

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Full Quantum Nature of Water on Salt Surface

Despite water being a ubiquitous substance, it is surprising that some basic questions are still debated. Here using a combination of experimental (cryogenic STM) and theoretical (first-principle electronic structures and molecular dynamics) methods, we systematically studied the unusual structure and dynamics of water molecules on NaCl surface. More interestingly, for the first time, we observe the full quantum effect and magic number hydrates in water system. These results shed light on our understanding of water at atomic scale.

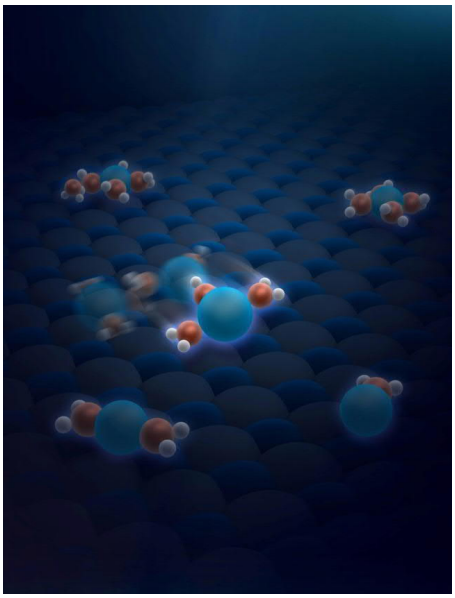

Figure We constructed individual sodium ion (Na+) hydrates on a NaCl(001) surface by progressively attaching single water molecules (one to five) to the Na+ ion using a combined scanning tunnelling microscopy and noncontact atomic force microscopy system. It is found that the Na+ ion hydrated with three water molecules diffuses orders of magnitude more quickly 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 energy barrier.

Host: Angel Rubio

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