Visualizing the ion hydration and transport at atomic scale

With the supports from the National Natural Science Foundation of China, Ministry of Science and Technology of China, Chinese Academy of Sciences, and Collaborative Innovation Center of Quantum Matter, the teams led by Professor Jiang Ying (江颖), Professor Xu LiMei and Professor Wang EnGe of the International Center for Quantum Materials (ICQM) of Peking University, in collaboration with Professor Gao YiQin of the College of Chemistry and Molecular Engineering of Peking University and Dr. Pavel Jelínek from the Institute of Physics, the Czech Academy of Sciences, unravel, for the first time, the microscopic structures of Na^+ ion hydrates on the NaCl surface and discover a magic-number effect on the transport of ion hydrate. This work is published in *Nature* (2018, 557: 701—705).

Ion hydration has been studied for more than one hundred years. However, many key issues are still under debate so far, such as the water number and configuration in the hydration shells, the effect of hydrated ions on the water structure and dynamics, and the microscopic factors that govern the transport of the hydrated ions. The main reason lies in the lack of experimental tools, which can really "see" and "manipulate" the hydrated ions with atomic precision. The researchers figured out a novel method to manipulate individual ions and water molecules by scanning tunneling microscopy (STM). They were able to construct individual Na^+ hydrates containing one-to-five water molecules on a NaCl (001) surface. To overcome the difficulty of disturbing the ion hydrates during imaging, the researchers developed a weakly-perturbative imaging technique, which relies on the weak high-order electrostatic force by noncontact atomic force microscopy (AFM). Such a technique yields the first-ever atomically resolved images of the Na^+ hydrates. Furthermore, they found an interesting magic-number effect: the Na^+ hydrated with three water molecules diffuses one to two orders of magnitude faster than other Na^+ hydrates (see Figure) and even much faster than the Na^+ in the dilute bulk solution. *Ab initio* calculations and MD simulations revealed that such high ion mobility arises from the degree of the symmetry match between the hydrate and substrate. Besides, they found that the magic-number effect applies for many salt ions, suggesting its generality.

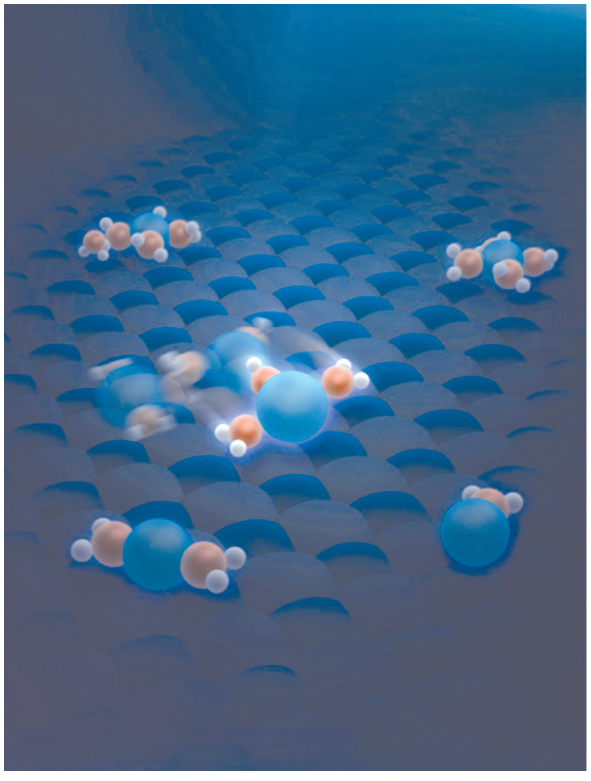

Figure Schematic showing that the Na^+ hydrated with three water molecules diffuses much faster than other Na^+ hydrates.

This work established, for the first time, direct correlation between the atomic structure and transport mechanism of hydrated ions, which may completely renovate the traditional understanding of ion transport in nanofluidic systems. Those results point out a new way to control the ion transport in nanofluidic systems by interfacial symmetry engineering, which is of great importance for an extremely wide range of technologically and biologically relevant processes.