Electronic structure and molecular dynamics of hydrated water ions

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Time: 10:00am, July. 27, 2017 (Thursday)

时间：2017年7月27日 （周四）上午10:00

Venue: w563, Physics building, Peking University

地点：北京大学物理楼，西563会议室

Abstract

Proton transfer via hydronium and hydroxide ions in water is ubiquitous. It underlies acid-base chemistry, certain enzyme reactions, and even infection by the flu. Despite two-centuries of investigation, the mechanism underlying why hydronium diffuses faster than hydroxide in water is still not understood. Herein, we employ state of the art Density Functional Theory based molecular dynamics, with corrections for nonlocal van der Waals interactions, and self-interaction in the electronic ground state, to model water and the hydrated water ions. At this level of theory, structural diffusion of hydronium preserves the previously recognized concerted behavior. However, by contrast, proton transfer via hydroxide is dominated by stepwise events, arising from a stabilized hyper-coordination solvation structure that discourages proton transfer. Specifically, the latter exhibits non-planar geometry, which agrees with neutron scattering results. Asymmetry in the temporal correlation of proton transfer enables hydronium to diffuse faster than hydroxide and may underlie observed isotope anomalies.

About the Speaker

Prof. Roberto Car's research focusses on the understanding of the atomistic, the electronic structures, and the dynamics in materials. His methodology roots in theoretical physics, and particularly in quantum and statistical mechanics. For people doing molecular simulations, he/she must have or will be benefited from a groundbreaking invention of Car and Parrinello in 1985, known as ab initio molecular dynamics, which has completed changed the way we understand many problems in condensed matters, in chemical physics, in material sciences, and in geosciences, etc. Due to contributions like this, he is currently a member of NAS, a professor in Princeton University, a Raman lecturer at Argonne National Lab, a Berni Alder CECAM prize winner, a Dirac medal winner of ICTP, etc. In this talk, he will tell us a story on the electronic structure and molecular dynamics of hydrated water ions.

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