北京大学量子材料科学中心

International Center for Quantum Materials, PKU

Seminar

First-principles molecular dynamics simulations of liquid water and lithium

Mohan Chen

Temple University

Time: 2:00pm, Nov. 17, 2017 (Friday)

时间：2017年11月17日 （周五）下午2:00

Venue: Room W663, Physics building, Peking University

地点：北京大学物理楼，西663会议室

Abstract

We perform first-principles molecular dynamics (MD) simulations on liquid water and lithium based on Kohn-Sham density functional theory (KSDFT) and orbital-free density functional theory (OFDFT), respectively. Water is of the utmost importance for life and technology. However, a genuinely predictive ab initio model of water has eluded scientists. We demonstrate that a fully ab initio approach, relying on the strongly constrained and appropriately normed (SCAN) density functional, provides such a description of water. Furthermore, we model the hydrated water ions (hydronium and hydroxide) with corrections for nonlocal van der Waals interactions and self-interaction in the electronic ground state. We provide theoretical explanations to why hydronium diffuses faster than hydroxide, which has been a puzzle for over two centuries. Liquid lithium (Li) attracts scientific interest due to its substantial advantages in being a plasma-facing component. We accurately predict the melting point of Li; diffusivities and viscosities of liquid Li are also obtained. In addition, we develop algorithms to enable peta-scale computations of OFDFT in efficiently modeling systems consisting of more than one million atoms.

About the speaker

Dr. Mohan Chen obtained his B.S. and Ph.D. degrees in the Department of Physics at the University of Science and Technology of China in 2007 and 2012, respectively. After that he joined the Mechanical and Aerospace Engineering department at Princeton University as a postdoc from 2012 to 2016. Dr. Chen became a postdoctoral fellow at the Department of Physics at Temple University since 2016. His current research mainly focuses on developing predictive computational algorithms within the framework of both Kohn-Sham and orbital-free density functional theories, and applying them to study liquid water and liquid metals.