北京大学量子材料科学中心
International Center for Quantum Materials, PKU

Weekly Seminar

A first-principles method to determine speciation with Raman spectroscopy and molecular polarizability

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Time: 4: 00 Pm, Dec. 4, 2019 (Wednesday)

时间：2019年12月4日 （周三）下午4:00

Venue: Room W563, Physics building, Peking University

地点：北京大学物理楼，西563会议室

Abstract

We present a strategy, based on first-principles simulations, to determine ratios of Raman scattering cross sections of aqueous species, thus providing a key quantity that can be used, in conjunction with Raman measurements, to predict chemical speciation in aqueous fluids. Due to the ever-growing importance of the Earth's carbon cycle both in the atmosphere and the Earth interior, we focused on carbonate and bicarbonate ions, as these represent one of the major dissolved carbon species at extreme conditions. Knowledge of molecular polarizabilities in condensed phases provides important information about molecular crystals, and in general about materials composed of molecular or nano-building blocks. It is of great importance for Raman spectroscopy. We propose a first-principles method based on electronic densities to compute molecular polarizabilities in condensed phases. The method includes all multipole interactions in addition to the dipole-dipole one, and it is applicable to any semiconductor or insulator.

References:

[1] Nore Stolte, Ding Pan, J. Phys. Chem. Lett. **10**, 5135 (2019)

[2] Ding Pan, Marco Govoni, and Giulia Galli, J. Chem. Phys. **149**, 051101 (2018)

About the speaker

Prof. Ding Pan obtained BS in physics in the 00 Class (SCGY) at University of Science and Technology of China in 2005, and ScD at Institute of Physics, Chinese Academy of Sciences in 2011. During the ScD study, he was a visiting researcher at the Fritz-Haber-Institute of the Max Planck Society in Berlin, Germany and a Thomas Young Centre Junior Research Fellow at the University College London, UK. Before he joined HKUST in 2016, he worked as a postdoctoral researcher in the University of California at Davis (2011-2014) and the University of Chicago (2014-2016). He was honored with the Croucher Innovation Award in Hong Kong in 2018 and the Deep Carbon Observatory Emerging Leader Award in the US in 2019.

Prof. Pan has been developing and applying computational and numerical methods to understand and predict the properties and behavior of liquids, solids, and nanostructures from first principles. With the help of high-performance supercomputers, his group are seeking answers to the urgent and fundamental scientific questions relevant to sustainable development, e.g., water science, deep carbon cycle, and clean energy.