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Raman spectroscopy and molecular polarizability at finite temperature from first principles

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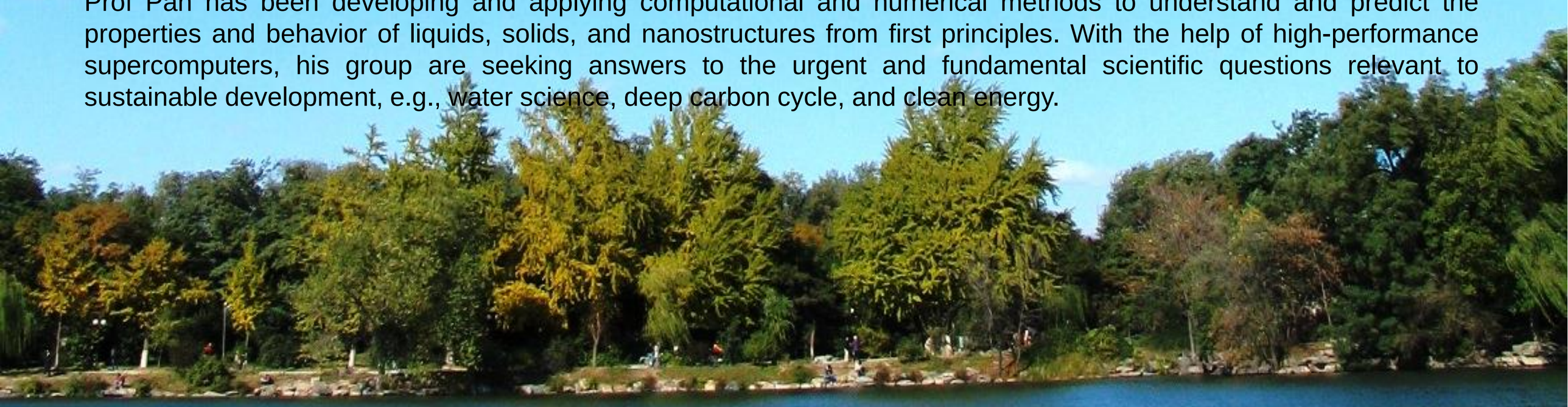
时间：12月7日（星期四）15:00—16:30

地点：北京大学物理大楼西楼202报告厅

•**摘要：** 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 the 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. We present results for molecular polarizabilities of liquid water in a wide pressure-temperature range. We found that at ambient conditions, the dipole-induced-dipole approximation is sufficiently accurate and the Clausius-Mossotti relation may be used, e.g. to obtain molecular polarizabilities from experimental refractive indexes. However, with increasing pressure this approximation becomes unreliable and in the case of ice X, where covalent bonds are present, the dipole-induced-dipole approximation breaks down. Further, we calculated the Raman spectra of (bi)carbonate aqueous solutions at supercritical conditions, and obtained the Raman scattering cross sections of carbon species at high pressures and high temperatures from first principles. We will discuss how to use our results to interpret and guide spectroscopic measurements.

•**报告人简介：** 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. After he worked as a postdoctoral researcher in the University of California at Davis (2011-2014) and the University of Chicago (2014-2016), he joined Hong Kong University of Science and Technology in 2016.

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.



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Photoed by Xiaodong Hu