量子材料科学中心
International Center for Quantum Materials

Seminar

Ab-initio path-integral molecular dynamics: theory and applications

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- **Venue: Room 607, Conference Room A , Science Building 5**

Abstract

Ab-initio molecular dynamics method allows finite temperature statistic properties of real materials to be addressed in a predictive manner. The standard treatment is to calculate the electronic states quantum mechanically and address the nuclei as classical point-like particles. In hydrogen and hydrogen-bonded systems, the small mass of the nuclei and the inherent importance of issues like quantum tunneling and zero-point motion mean that one needs to go beyond this approximation in many cases. In solving such a problem, state-of-the-art technique, i.e. ab-initio path-integral molecular dynamics, uses the idea of the part-integral method proposed by Feynman [1] and implementation in the molecular dynamics manner originally done by Marx and Tuckerman [2-4]. In the last two years, we used this technique and investigated the importance of quantum nuclear effects in a series of systems. In this talk, I will show two examples: a path-integral investigation of water-metal interfaces [5] and a systemic study on the impact of quantum nuclear effects on hydrogen bond strength [6]. Our study presents a new mechanism for the proton transfer process in water-metal interfaces and gives a rule of thumb to estimate the impact of quantum nuclear effects on the strength of hydrogen bonds.

[1] R. P. Feynman and A. R. Hibbs, Quantum Mechanics and Path Integrals, New York: McGraw-Hill (1965)
[2] D. Marx and M. Parrinello, Zeitschrift fur Physik B-Cond. Mat. 95, 143 (1994)
[3] Tuckerman et al. J. Chem. Phys. 104, 5579 (1996)
[4] D. Marx and M. Parrinello, Nature 375, 6528 (1995)
[5] X. Z. Li et al. Phys. Rev. Lett. 104, 066102 (2010)
[6] X. Z. Li et al. submitted.