Simulation of Electric Dipole in Complex System

SPEAKER: Jun Jiang, University of Science and Technology China
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VENUE: Room 264, Geography Building, Zhongbei Campus
HOST: Fei Xia, East China Normal University

ABSTRACT OF THE TALK

Based on density functional theory simulations, we have proposed that the electric dipole, a parameter deduced from the distribution of ground or excited states, is a useful descriptor to describe and evaluate the structure-property relationship of complex systems. It helps people to understand the electron kinetics in for various physics or chemistry applications, and thereby enable the manipulation of electron-photon interactions, energy/electron transfer, and material conversion processes. By developing quantum chemistry and deep learning techniques to compute the electric dipole moment, we have demonstrated it as an efficient knob to improve the rational design of catalyst, solar cell, smart materials, and so on.

BIOGRAPHY

Jun Jiang, Professor of Physical Chemistry, School of Chemistry and Materials Science at University of Science and Technology of China. He received a Ph.D. degree in Theoretical Chemistry under the tutelage of Prof. Yi Luo in 2007 at Royal Institute of Technology, Sweden, and a Ph.D. degree in Solid State Physics under the tutelage of Prof. Wei Lu in 2008 at Shanghai Institute of Technical Physics, Chinese Academy of Science. From 2009 to 2011, he worked as Post-doc at the University of California Irvine, USA with Prof. Shaul Mukamel. He joined the University of Science and Technology of China in 2011. His major research interests focus on the development and employment of multi-scale modeling methods for exciton kinetics in complex system, while targeting on a wide range of physics or chemistry applications such as Photocatalysis, Biochemistry, Photochemistry, Molecular electronics and photonics.