Prof. Yi Zhao
State Key Laboratory of Physical Chemistry of Solid Surfaces,
College of Chemistry and Chemical Engineering, Xiamen University, China

Prof. Yi Zhao is a Professor of Chemistry in State Key Lab. of Physical Chemistry of Solid Surfaces and Dept. of Chemistry, Xiamen University. He received his PhD in Physical Chemistry at Dalian Institute of Chemical Physics, Chinese Academy of Sciences, and Hong Kong University of Science & Technology in 1997. After postdoctoral and visiting studies at Free University-Berlin, UIUC and UC Berkeley, he joined University of Science & Technology of China in 2003 as a professor. In 2004, he visited Institute of Molecular Sciences, Japan supported by JSPS for a year. In 2008, he moved to Xiamen University. Research of his group focuses on rate theories for adiabatic, nonadiabatic chemical reactions and charge transfer, photo-physics properties of organic functional materials.

Theoretical Ssimulation of Carrier Quantum Dynamics in Organic Materials

Yi Zhao

State Key Laboratory of Physical Chemistry of Solid Surfaces,
College of Chemistry and Chemical Engineering, Xiamen University, China

The carriers in organic materials commonly follow hopping-type motions because of strong carrier-phonon interactions. However, they can also present a band-like behaviour in well-performed organic crystals or mixed inorganic-organic materials. Therefore, their dynamics should be described by a unified way covering from band-like to hopping-type motions. Development of such a method for large systems is interesting in theoretical chemistry and still meets a great challenge. Focusing on this problem, we have proposed a time-dependent wavepacket diffusion method. In the method, the effects of carrier-phonon interaction and inter- or intra-molecular electronic couplings are considered as the fluctuations on carrier dynamics. Based on this concept, we have also proposed a rigorous hierarchy of stochastic Schrödinger equation, and the relationship between two methods are built. We further present how to combine electronic structure calculations with these quantum dynamics methods to reveal the carrier dynamics in realistic organic semiconductors, such as exciton energy relaxation and singlet fission.