



Seminar Topic: Simulating Dynamics in Molecular Systems: From Light Harvesting to Transport across Bacterial Membranes

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Abstract

Excitation energy as well as charge transfer processes are important and ubiquitous in biological and man-made systems but at the same time complicated to model at the molecular level. For many systems a multiscale approach of classical molecular dynamics simulations and electronic structure calculations along the trajectory can to be employed. The result of such a treatment can subsequently be used to determine the respective charge and energy transfer scenarios as well as optical responses. As examples, excitation energy transfer in a light-harvesting system and charge transport through a DNA molecule will be detailed.

Molecular dynamics simulations are often sufficient to model the transport of ions and substrate molecules across bacterial membrane pores. Channels in the outer membrane of Gram-negative bacteria provide essential pathways for the controlled and unidirectional transport of ions, nutrients and metabolites into the cell. At the same time the outer membrane serves as a physical barrier for the penetration of noxious substances such as antibiotics into the bacteria. Examples of ion and substrate translocation will be presented.

Biography

Professor Ulrich Kleinekathöfer received his diploma in Physics in 1993 and PhD in 1996 from the University of Göttingen. He joined Weizmann Institute of Science in Israel as a postdoctoral fellow from 1996 to 1997. In subsequent years he was Research Assistant in Chemnitz and habilitation in 2002. He had several research stays at the University of Illinois at Urbana-Champaign. He became Associate Professor at Jacobs University Bremen in 2006 and was promoted to Full Professor in 2017. His research focuses on simulating the quantum as well as classical dynamics in Biomolecular systems.

**Tuesday, 27 August 2019 || Time: 10:30 am – 11:30 am ||
Venue: MSE Meeting Room (N4.1-01-28)
Hosted by: Associate Professor Zhao Yang**