



PHYSICAL COLLOQUIUM INVITATION

Monday, 25.01.2021, 4.15 p.m.,
video conference: <https://meeting.uol.de/b/anj-2vc-j6s-fwe>

speaks

Prof. Dr. Ulrich Kleinekathöfer
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about

“Transport in biomolecular systems: On light harvesting and nanopores”

Transfer and transport processes in biomolecular systems are important and ubiquitous. Depending on the actual nature of the respective processes, many techniques from theoretical physics starting at classical mechanics, over electrodynamics and statistical physics to quantum mechanics are necessary to describe them adequately at the molecular level. In the present talk, I will focus on two quite different processes, i.e., excitation energy transfer in light harvesting as well as ion and molecule transport through nanopores. For light-harvesting complexes a multi-scale approach of (quantum) molecular dynamics simulations and electronic structure calculations can be employed. The results of such a treatment can subsequently be used to determine the respective energy transfer scenarios using ensemble-averaged wave function or density matrix approaches. Examples of such a treatment for bacterial and plant light-harvesting systems will be shown. Concerning the transport of ions and molecules through nanopores, classical molecular dynamics simulations are often sufficient but one often needs to determine multi-dimensional Gibbs Free Energy surfaces for such systems. The calculation of such Free Energy surfaces for realistic systems is a formidable numerical task. To this end, I will focus on channels in membranes of bacteria which 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 permeation will be presented.

All interested persons are cordially invited.

Sgd. Prof. Dr. Ilia Solov'yov