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Fachbereich für Physik

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Herr Prof. Dr. Ulrich Kleinekathöfer

Dept. of Physics and Earth Sciences, Jacobs University Bremen, Germany

über

Simulating dynamics in molecular systems: From light harvesting to transport across bacterial membranes

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 [1,2] and charge transport through a DNA molecule will be detailed [3].

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 [4-6].

References

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