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Theoretical Chemistry Colloquium

April 9, 2013 (Tue), 16:00-17:00

Chemistry Gallery, RCMS 2nd floor

Multi-Scale Methods for the Investigation of Biological Structures and Processes

Prof. Dr. Marcus Elstner
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Abstract: *In the last years, we have combined ab initio quantum chemistry and density functional theory (DFT) methods with semi-empirical (SCC-DFTB), empirical force field and continuum electrostatic methods in so called Multi-Scale approaches in order to study biological structures and processes on different time and length scales. This includes also the use of QM/QM/MM methods as well as polarizable force fields and a variety of sampling methods, which allow to overcome the limitations of direct molecular dynamics simulations.*
One major field of application concerns the rhodopsin family of proteins. Here, we have studied in particular the mechanisms of color tuning as well as proton transport pathways in Bacteriorhodopsin. We used a variety of spectroscopic methods like UV/vis, IR, Raman, NMR in order to clarify details of the molecular structures, not resolved by experiment. A second major field of application is concerned with electron/hole transfer in complex molecular systems. Due to the immense system size of several hundreds of atoms, which have to be treated quantum mechanically, we have developed a coarse-grained quantum/classical methodology within the framework of time-dependent DFT. This methodology allows to describe the dynamics of the electronic system coupled to the dynamics of DNA or proteins in water solvent and shows, that solvent fluctuations are a major driving force of hole transfer. Currently, we extend this methodology towards organic electronics applications.

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