unicat
Unifying Concepts in Catalysis

UniCat Colloquium

Please note updates of events on www.unicat.tu-berlin.de

Lecturer: **Prof. Marcus Elstner**, Karlsruhe Institute for Technology (KIT), Institute for Physical Chemistry, Theoretical Chemical Biology, Universität Karlsruhe

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

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.

- *M. Elstner, Q. Cui, Multi-scale methods for the description of chemical events in biological systems, in: Multiscale Simulation Methods in Molecular Sciences, NIC-Serie: Publikationsreihe des John von Neumann-Instituts für Computing 2009.*
- *P. Phatak, N. Ghosh, H. Yu, Q. Cui, M. Elstner, Amino acids with an intermolecular proton bond as proton storage site in bacteriorhodopsin, Proc. Natl. Acad. Sci. (USA),105, (2008) 19672.*
- *P. Phatak, J. Frähmcke , M. Wanko, M. Hoffmann, P. Strodel, J. Smith, S. Suhai, A. Bondar, M. Elstner, Long-distance proton transfer with a break in the bacteriorhodopsin active site, J. Amer. Chem. Soc. 131 (2009) 7064.*
- *T. Kubar, U. Kleinekathöfer, M. Elstner, Water Drives the Hole Transfer in DNA: a Combined TD-DFT and Classical MD Study, J. Phys. Chem B, 113 (2009) 13107.*
- *P. Woiczikowski, T. Kubar , R. Gutierrez, R. Caetano, G. Cuniberti, M. Elstner, Combined DFT and Landauer approach for hole transfer along classical MD simulations of DNA,J. Chem. Phys. 130 (2009) 215104.*

Date: **Wednesday, December 12, 2012 5:15 pm**

Location: **TU Berlin, Institute of Chemistry**
Straße des 17. Juni 115, 10623 Berlin
Building C, Lecture Hall C 264

Organizer: **Prof. Maria A. Mroginski (TUB)**

Coffee and tea will be served thirty minutes prior to the lecture start.
Guests are cordially invited to attend!

Prof. Dr. Matthias Driess, Chair of the Cluster of Excellence UniCat