Program for the Hünfeld Workshop 2008

"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES 2008"

Friday, April 18th, 2008	
11:00 – 13:00	Arrival, registration and lunch
13:00 – 13:05	Welcome
13:05 – 13:30	**Marcel Baer** (Ruhr University Bochum) *QMMM study of the Schiff Base and the complex counter ion in the ground and L state of Bacteriorhodopsin*
13:30 – 13:55	**Jan Stephan Frähmcke** (Technical University Braunschweig) *Spectral Tuning in Rhodopsin and Cone Visual Pigments Calculated with QM/MM-Methods*
13:55 – 14:20	**Tomas Kubar** (Technical University Braunschweig) *What governs the charge transfer in DNA? The role of DNA conformation and environment*
14:20 – 14:45	**Thomas Steinbrecher** (The Scripps Research Institute, San Diego) *Direct observation of fast electron transfer in DNA via QM/MM simulations*
14:45 – 15:10	**Hiroshi Fujisaki** (J.W. Goethe University, Frankfurt) *Dynamic treatment of vibrational energy relaxation in biomolecules*
15:10 – 15:45	Coffee break
15:45 – 16:10	**Udo W. Schmitt** (MPI for Biophysical Chemistry, Göttingen) *Unified framework for first-principle minimum free energy pathway computation*
16:10 – 16:35	**Jürgen Lampe** (MPI for Biophysical Chemistry, Göttingen) *Structural and dynamical aspects of membrane-bound protons*
16:35 – 17:00	**Steffen Wolf** (Ruhr University Bochum) *From light to power - simulations of a GPCR homology model predict dynamic features and ligand binding site*
17:00 – 17:25	**Phuong H. Nguyen** (J.W. Goethe University, Frankfurt) *Molecular dynamics simulation of aggregation of Aβ peptide*
17:25 – 17:50	**Daniel Seeliger** (MPI for Biophysical Chemistry, Göttingen) *Geometry-based sampling of conformational transitions in proteins*
18:00 – 19:00	Dinner
19:30 –	Poster Session / Beer

Saturday, April 19th, 2008	
8:00 – 8:50	Breakfast
8:55 – 9:20	**Frank Noe** (Free University Berlin) *Metastability, Folding pathways and Experimental Observables from Markov transition networks of Peptide and Protein Dynamics*
9:20 – 9:45	**Bettina Keller** (ETH Zürich) *Identification of metastable conformers using kinetics vs. using conformational similarity - can we trust conformational cluster algorithms?*
9:45 – 10:10	**Iris Antes** (MPI for Informatics, Saarbrücken) *DynaDock: Protein-peptide docking including receptor flexibility*
10:10 – 10:45	Coffee break
10:45 – 11:10	**Ling Wang** (Saarland University, Saarbrücken) *Graph-theoretical identification of dissociation pathways on free energy landscapes of biomolecular interaction*
11:10 – 11:35	**Elodie Laine** (Pasteur Institute, Paris) *Modeling the effect of Ca2+ through the residue network of the complex between the adenylyl cyclase EF and calmodulin*
11:35 – 12:00	**Shirley Siu** (Saarland University, Saarbrücken) *Biomolecular simulations of membranes: Physical properties from different force fields*
12:00 – 13:00	Lunch
13:00 – 13:25	**Senbo Xiao** (Heidelberg University) *Force distribution explains toughness of silk-like crystalline units*
13:25 – 13:50	**Jochen Hub** (MPI for Biophysical Chemistry, Göttingen) *Mechanism of Selectivity in Aquaporins and Aquaglyceroporins*
13:50 – 14:15	**Mazen Ahmad** (Saarland University, Saarbrücken) *Mechanism of ultra-fast peptide binding to SH3 domains*
14:15 – 14:40	**Soroosh Pezeshki** (Jacobs University Bremen) *Simulation of Transport through OmpF Channels*
14:40 – 15:05	Coffee break
15:05 – 15:30	**Carla Haid** (MPI for Informatics, Saarbrücken) *A new Sampling Approach for Ligand Binding Site Identification including Protein Flexibility*
15:30 – 15:55	**Maik Götte** (MPI for Biophysical Chemistry, Göttingen) *No lead to gold - modern alchemy of ligand binding: Influence on stability, desolvation and non-equilibrium free energy calculations*
15:55 – 16:20	**Konstantin Klenin** (Forschungszentrum Karlsruhe) *Free-energy based all-atom protein modelling with worldwide distributed computational resources*
16:20 – 16:45	**Caroline Becker** (Saarland University, Saarbrücken) *Prediction of Protein-Protein Binding Affinity*
18:00	Dinner/Departure