Program for the Hünfeld Workshop 2006

"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES 2006"

Friday, May 19th, 2006	
11:00 – 13:00	Arrival, registration and lunch
13:00 – 13:05	Welcome
13:05 – 13:30	**Susanne Eyrisch** (Saarland University) *Frequent and fast appearance of pockets on surfaces of proteins involved in protein-protein interactions*
13:30 – 13:55	**Nadine Homeyer** (University of Erlangen-Nuremberg) *Insights into the Role of Phosphorylation in Molecular Recognition Processes by Molecular Dynamics Simulations*
13:55 – 14:20	**Jochen Hub** (MPI for biophysical Chemistry) *Does CO_2 permeate through Aquaporin-1?*
14:20 – 14:45	**Frank Noe** *(IWR, University of Heidelberg)* *Transition Networks for Protein Structural Change*
14:45 – 15:10	**Hari Leontiadou (**University of Groningen) *Antimicrobial Action*
15:10 – 15:45	Coffee break
15:45 – 16:10	**Ulrich Kleinekathoefer (**Technical University Chemnitz) *Molecular modeling of transport through OmpF channels*
16:10 – 16:35	**Ulrich Zachariae** (MPI for biophysical Chemistry) *Prediction of a RanGTP-Induced Conformational Switch in the Exportin CAS/Cse1p by Molecular Dynamics Simulations*
16:35 – 17:00	**Shirley Siu** (Saarland University) *Electric Fields & Membranes: Gramicidin A as a Test Ground*
17:00 – 17:25	**Andrew Aird (**University of Stuttgart) *Evaluation of a possible pathway for Quinone shuttling in the Photosynthetic Unit of the Purple Bacterium Rhodospirillum rubrum*
17:25 – 17:50	**Alexander Benedix** (Saarland University) *Fast Free Energy Prediction of Mutants*
18:00 – 19:00	Dinner
19:30 –	Poster Session / Beer

Saturday, May 20th, 2006	
8:00 – 8:50	Breakfast
8:55 – 9:20	**Pascal Baillod (**EPFL, Swiss Federal Institute of Technology) *Prion Protein Misfolding: Towards the Scrapie Isoform*
9:20 – 9:45	**Edgar Luttmann (**Stanford University) *Protein Folding Simulations ? Application in beta-Amyloid Aggregation*
9:45 – 10:10	**Isabella Daidone (**IWR, University of Heidelberg) *Solvent treatment effects on peptide folding: microsecond timescale molecular dynamics simulations*
10:10 – 10:45	Coffee
10:45 – 11:10	**Martin Stumpe** (MPI for biophysical Chemistry) *Hindered Refolding as Mechanism for Urea-Induced Unfolding of the Cold Shock Protein*
11:10 – 11:35	**Rainer Hegger** (University of Frankfurt) *Nonlinear data analysis of peptide dynamics*
11:35 – 12:00	**Edda Kloppmann (**University of Bayreuth) *Extended Dead-End Elimination: an algorithm to find the global energy minimum and the next higher states in a discretized energy landscape*
12:00 – 13:00	Lunch
13:00 – 13:25	**Jürgen Haas** (MPI for biophysical Chemistry) *Probing the Energy Landscape governing Protein Motions*
13:25 – 13:50	**Henrik te Heesen (**University of Bochum) *Empirical rules facilitate the search for binding sites on protein surfaces*
13:50 – 14:15	**Dietmar Paschek (**University of Dortmund) *Reversible Folding of a Miniprotein in an Explicit Solvent: Effect of the Water Model*
14:15 – 14:40	**Jan Saam (**Charite Berlin) *PARATOOL - Convenient generation of force field parameters for arbitrary molecules*
14:40 – 15:05	**Wei Gu** (Saarland University) *Protonation equilibria of solvated acetic acid studied by Q-HOP molecular dynamics simulation*
15:05 – 15:30	Coffee
15:30 – 15:55	**Prasad Phatak (**University of Paderborn) *QM/MM simulations of the last proton transfer step in the bacteriorhodopsin Photocycle*
15:55 – 16:20	**Petra Imhof (**IWR, University of Heidelberg) *Quantum Mechanical/Molecular Mechanical Simulations of the Restriction Enzyme catalyzed DNA Cleavage*
16:20 – 16:45	**Roman Gorbunov (**University of Frankfurt) *Quantum-classical calculations of infrared spectra of peptides*
18:00	Dinner/Departure