Program for the Hünfeld Workshop 2007

"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES 2007"

Friday, April 20th, 2007	
11:00 – 13:00	Arrival, registration and lunch
13:00 – 13:05	Welcome
13:05 – 13:30	**Marcus Kubitzki** (MPI for biophysical Chemistry, Göttingen) *Temperature Enhanced Essential dynamics Replica Exchange*
13:30 – 13:55	**Daniele Narzi** (Center for Bioinformatics Saar, Saarbrücken) *Dynamic Protonation State Analysis of Dsb Proteins*
13:55 – 14:20	**Marcus Hennig** (MPI for biophysical Chemistry, Göttingen) *Entropy Calculations of Protein Solvent Shells*
14:20 – 14:45	**Alexandros Altis** (J.W. Goethe University, Frankfurt) *Applications of Dihedral Angle Principal Component Analysis to Biomolecules*
14:45 – 15:10	**Karine Voltz** (IWR, University Heidelberg) *Study of global motions and correlations in the nucleosome using a coarse-grained model*
15:10 – 15:45	Coffee break
15:45 – 16:10	**Birgit Strodel** (University of Cambridge) Exploring the energy landscape of amyloid formation from Discrete Path Sampling
16:10 – 16:35	**Lothar Reich** (MPI for Colloids and Surfaces, Potsdam) *Kinetic clustering analysis of unfolding simulations of the PinWW domain*
16:35 – 17:00	**Harald Lanig** (University Erlangen-Nuernberg) *On the stability and self-interaction of the human guanylate-binding protein 1*
17:00 – 17:25	**Domantas Motiejunas** (EML Research, Heidelberg) *Following the path of protein-protein association towards the bound complex structure*
17:25 – 17:50	**Sampath Koppole** (University of Heidelberg) *Structural coupling between ATPase activation and recovery-stroke in the Myosin II motor*
18:00 – 19:00	Dinner
19:30 –	Poster Session / Beer

Saturday, April 21th, 2007	
8:00 – 8:50	Breakfast
8:55 – 9:20	**Guillem Portella** (MPI for biophysical Chemistry, Göttingen) *Determinants of water permeation in single-file peptidic model pores*
9:20 – 9:45	**David Nutt** (University of Heidelberg) *Molecular Dynamics Simulations of Antifreeze Proteins and the Role of the Water Model*
9:45 – 10:10	**Frauke Gräter** (Columbia University, New York) *Hydrophobic collapse of unfolded proteins under force*
10:10 – 10:45	Coffee break
10:45 – 11:10	**Prasad Phatak** (Technical University Braunschweig) *Quantum Mechanics/Molecular Mechanics simulations of the proton-transfer pathways at the extracellular side of bacteriorhodopsin*
11:10 – 11:35	**Elena Herzog** (MPI of Biophysics, Frankfurt) *Studying Proton Transfer in Quinol Fumarate Reductase*
11:35 – 12:00	**Christoph Pfisterer** (University of Heidelberg / IWR) *Halorhodopsin maximises the motive force for chloride pumping while preventing unproductive decay of the first photocycle intermediate*
12:00 – 13:00	Lunch
13:00 – 13:25	**Cristina Pereira** (ETH-Zürich**)** *Sugars and Biomolecular Stabilization - What MD Simulations Can Tell Us*
13:25 – 13:50	**Beate Griepernau** (Center for Bioinformatics Saar, Saarbrücken) *1-Alkanols and Membranes: A Story of Attraction*
13:50 – 14:15	**Outi Salo-Ahen** (EML Research, Heidelberg) *Targeting human thymidylate synthase - can MD simulations reveal putative binding pockets at the dimer interface?*
14:15 – 14:40	**Tihamer Geyer** (Saarland University, Saarbrücken) *Brownian Dynamics with Explicit Ions and their Effects on Protein Association*
14:40 – 15:05	**Torsten Becker** (Bioinformatics, University Bayreuth) *Dynamical Monte Carlo Simulations of Electron Transfer in the C-Subunit of the Photosynthetic Reaction Center*
15:05 – 15:30	Coffee break
15:30 – 15:55	**Tomas Kubar** (Technical University Braunschweig) *Selected thermodynamic features of non-covalent DNA?drug complexes*
15:55 – 16:20	**Alessandra Villa** (J.W. Goethe University, Frankfurt) *Structure, dynamics and stability of RNA hairpins*
16:20 – 16:45	**Gerrit Groenhof** (MPI for biophysical Chemistry, Göttingen) *Photostability of DNA*
18:00	Dinner/Departure