Program for the Hünfeld Workshop

"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES 2003"

Friday, May 9th, 2003

12.00 – 13.30 Arrival, registration, and lunch

13.30 – 14.00 **Gerald Mathias** (Ludwig Maximilians University, München)
A fast multipole method combined with a reaction field for long-range electrostatics in molecular dynamics simulations: The effects of truncation on the properties of water

14:00 – 14:30 **Frank Noe (**Heidelberg University, IWR)
Finding meaningful pathways for complex conformational changes in proteins – using ras p21 as example

14:30 – 15:00 **Matthias Schmitz** (Ludwig Maximilians University, München)
A coarse-grained description of many-particle solvation structures in liquids and its application: Monitoring temperature-induced structural transitions in water

15:00 – 15:30 **Yuguang Mu** (J. W. Goethe University, Frankfurt)
Molecular dynamics simulation of cooperative RNA-peptide recognition

15:30 – 16:00 Coffee break

16:00 – 16:30 **Yungki Park (**Saarland University, Saarbrücken)
A new residue-residue pair potential based on atomistic simulations

16:30 – 17:00 **Andrezj Szymoszek (**Institute of Molecular Biotechnology, Jena)
Reduced protein models as a tool in comparative modeling

17:00 – 17:30 **Daniel Wüstner (**Max Delbrück Center, Berlin-Buch)
Monte Carlo simulations of lipid dynamics in membranes and of lipid-DNA interactions

17:30 – 18:00 **Ronen Zangi** (University of Groningen)
Kinetics and thermodynamics of the helix-coil transition

18:00 – 19:00 Dinner

19:00 – 21:00 Poster Sessions

Saturday, May 10th, 2003

8:00 – 9:00 Breakfast

9:00 – 9:30 **Udo W. Schmitt** (Ruhr-University Bochum)
Modelling Proton Transport through Complex Hydrogen-Bonded Networks – the Multistate Empirical Valence Bond Approach

9:30 – 10:00 **Bert de Groot** (MPI for biophysical Chemistry, Göttingen)
The mechanism of proton exclusion in the membrane water channel Aquaporin-1

10:00 – 10:30 **Andreea Daniela Gruia** (Heidelberg University, IWR)
Pathways for early steps in chloride pumping by halorhodopsin

10:30 – 11:00 Coffee break

11:00 – 11:30 **Ulrich Zachariae** (MPI for Biochemistry, Martinsried)
Multi-step mechanism of chloride translocation in a strongly anion selective porin channel

11:30 – 12:00 **Wolfgang B. Fischer** (Oxford University)
Computational structure-function correlation on a viral membrane protein: Vpu from HIV-1

12:00 – 13:00 Lunch

13:00 – 13:30 **Marco Klähn** (Ruhr-University Bochum)
Simulation of IR spectra of phosphate ions in solution via a QM/MM approach

13:30 – 14:00 **Hoang Phuong Nguyen** (J. W. Goethe University, Frankfurt)
Vibrational Energy Flow in Peptides

14:00 – 14:30 **Robert Raupp-Kossmann (**Technical University, München)
Theory of pH induced changes of conformation and protonation with application to Green Fluorescent Protein

14:30 – 15:00 **Gunnar Schröder** (MPI for biophysical Chemistry, Göttingen)
Simulation of Fluorescence Spectroscopy Experiments

15:00 – 15:30 Coffee break

15:30 – 16:00 **Peter Winn** (EMBL, Heidelberg)
Analysis of the E2 ubiquitin conjugating enzymes and related proteins

16:00 – 16:30 **Jochen Farwer (**Sheffield University)
Computational studies of DNA oligomers

16:30 – 17:00 **Hao Fan (**University of Groningen)
Control of Protein Folding: Chaperones

17:00 – 17:30 **Rainer Böckmann** (MPI for biophysical Chemistry, Göttingen)
Influence of ions on structure and dynamics of lipid bilayers

17:30 Departure or

18:00 Dinner (optional)