Program for the Hünfeld Workshop 2009

"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES 2009"

Friday, April 17th, 2009	
11:00 – 13:00	Arrival, registration and lunch
13:00 – 13:05	Welcome
13:05 – 13:30	**Rainer Ullmann** (University of Bayreuth) *Ligand binding free energy calculations*
13:30 – 13:55	**Serena Donnini** (MPI for Biophysical Chemistry, Göttingen) *Constant pH simulations in explicit solvent using the lambda-dynamics approach*
13:55 – 14:20	**Ivan Kondov** (Forschungszentrum Karlsruhe) *Treatment of disulfide bonds in protein structure prediction and their role in protein folding*
14:20 – 14:45	**Daniel Narzi** (Saarland University, Saarbrücken) *Structure and dynamics of v-SNARE*
14:45 – 15:10	**Lars Schäfer** (University of Groningen) *Model lipid rafts at atomistic resolution: combining coarse-grained and all-atom molecular dynamics simulations*
15:10 – 15:45	Coffee break
15:45 – 16:10	**Jakob Ulmschneider** (University of Heidelberg) *Folding peptides into lipid bilayers*
16:10 – 16:35	**Christina Scharnagl** (Technical University Munich) *Sequence-specific conformational dynamics of transmembrane helices*
16:35 – 17:00	**Peter Bond** (MPI of Biophysics, Frankfurt) *Investigation of the regulatory mechanism of the ZAP-70 immunological signalling enzyme*
17:00 – 17:25	**Christian Kappel** (MPI for Biophysical Chemistry, Göttingen) *The flexibility of unbound importin-beta studied by Molecular Dynamics*
17:25 – 17:50	**Ilona Baldus** (Bioquant Heidelberg) *Nanoscale mechanism of snow crystal growth from MD simulation*
18:00 – 19:00	Dinner
19:30 –	Poster Session / Beer

Saturday, April 18th, 2009	
8:00 – 8:50	Breakfast
8:55 – 9:20	**Nadine Utz** (University of Barcelona) *Theory and simulation of DNA-nanotube contacts: geometry, electronic structure and charge transfer*
9:20 – 9:45	**Volker Knecht** (MPI of Colloids and Interfaces, Potsdam) *Peptides and pH at interfac*es
9:45 – 10:10	**Tihamer Geyer** (Saarland University, Saarbrücken) *Using Graphs to analyze spatial simulations*
10:10 – 10:45	Coffee break
10:45 – 11:10	**Ulf Hensen** (MPI for Biophysical Chemistry, Göttingen) *Estimating configurational entropies of macromolecules: The minimally coupled subspace approach*
11:10 – 11:35	**Karel Berka** (Institute of Organic Chemistry and Biochemistry, Prague) *An amino acid side-chain interaction in proteins. Comparison of ab initio QM and MM methods*
11:35 – 12:00	**Halvor S. Hansen (**ETH Zurich) *Using conformational free energies for force field parameterization*
12:00 – 13:00	Lunch
13:00 – 13:25	**Kristyna Pluhackova** (Institute of Organic Chemistry and Biochemistry, Prague) *Relative energy barriers among families of GFP tripeptide (in vacuo MD study)*
13:25 – 13:50	**Olga Bezkorovanaya** (MPI for Polymer Research, Mainz) *Conformation sampling with coarse-grained peptide models*
13:50 – 14:15	**Jan-Hendrik Prinz** (University of Heidelberg) *Temperature-dependent conformational dynamics from parallel tempering simulations*
14:15 – 14:40	**Carsten Olbrich** (Jacobs University, Bremen) *Stretching of a DNA/HU-complex in SMD simulations*
14:40 – 15:05	**Murat Cetinkaya** (MPI for Metals Research, Stuttgart) *Silk fiber mechanics*
15:05 – 15:30	Coffee break
15:30 – 15:55	**Jozica Dolenc** (ETH Zurich) *Thermodynamics of sequence-dependent stability of DNA-netropsin complexes*
15:55 – 16:20	**Martin Höfling** (Ludwig-Maximilians-University, Munich) *Adsorption of biomolecules on gold surfaces*
16:20 – 16:45	**Hao Wu** (Free University of Berlin) *Brownian dynamics based modeling and estimation of single molecule FRET experiments*
16:45 – 17:10	**Sikander Hayat** (Saarland University, Saarbrücken) *Solvent structure around the Aβ42 peptide*
17:10 – 17:35	**Camilo Andrés Aponte-Santamaría** (MPI for Biophysical Chemistry, Gött.) *The gating mechanism of yeast Aquaporin*
18:00	Dinner/Departure