Program, Theory Workshop in Hünfeld, April 15-16, 2011
"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES 2011"

Friday, April 15th, 2011	
11:00 – 13:00	Arrival, registration and lunch
13:00 – 13:05	Welcome
13:05 – 13:30	**Jacek Czub** (Max Planck Institute for Biophysical Chemistry, Göttingen) *Mechanism of energy transmission in F1-ATPase*
13:30 – 13:55	**Aliaksei Krukau** (Technical University Munich) *Specific versus non specific binding in protein complexes. Molecular dynamics study*
13:55 – 14:20	**Carl Burmeister** (Max Planck Institute for Biophysical Chemistry, Göttingen) *Simulation of Primary Electronic Dynamics in Molecules upon Photoionization*
14:20 – 14:45	**Stephanie de Beer** (VU University, Amsterdam) *Structural rationalization of selective cytochrome P450 BM3 metabolism*
14:45 – 15:10	**Tihamér Geyer** (Saarland University, Saarbrücken) *On the Importance of Hydrodynamic Interactions in Coarse-Grained Protein Models*
15:10 – 15:45	Coffee break
15:45 – 16:10	**Silke Andrea Wieninger** (University of Bayreuth) *ATP binding enables broad antibiotic selectivity of aminoglycoside phosphotransferase - an elastic network analysis*
16:10 – 16:35	**Andrea Vaiana** (Max Planck Institute for Biophysical Chemistry, Göttingen) *Ribosomal translocation as seen from a combination of cryo-EM and molecular dynamics simulations*
16:35 – 17:00	**Sundar Raman Subramanian** (HITS gGmbH, Heidelberg) *The mode of action of collagen degradation by collagenase: A structural perspective*
17:00 – 17:25	**Laura Riccardi** (University of Freiburg, Institute of Physics) *Functional dynamics of a minimalistic riboswitch binding aminoglycosides*
17:25 – 17:50	**Jan Henning Peters** (Max Planck Institute for Biophysical Chemistry, Göttingen) *Dynamic Properties of Ubiquitin in Complexes*
18:00 – 19:00	Dinner
19:30 –	Poster Session / Beer

Saturday, April 16th, 2011	
8:00 – 8:50	Breakfast
8:55 – 9:20	**Jan-Hendrik Prinz** (Free University Berlin) *Robust Estimation of Timescales from Low-Dimensional Experimental Data*
9:20 – 9:45	**Moritz Wolf** (Karlsruhe Institute of Technology) *Efficient time-resolved conformational sampling using a Kinetic Monte Carlo approach*
9:45 – 10:10	**Nick Kepper** (Universty of Heidelberg; Kirchhoff-Institut für Physik and BioQuant) *Force spectroscopy of chromatin fibers: extracting energetics and structural information from Monte Carlo simulations*

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10:10 – 10:45	Coffee break
10:45 – 11:10	**Martin Brieg** (Karlsruhe Institute of Technology) *Power Born Radii: A fast accurate method for calculating Born Radii*
11:10 – 11:35	**Daniel Klose** (University of Osnabrueck) *Comparative DEER- & FRET distance determination in simulation & experiment*
11:35 – 12:00	**Martin Höfling** (Max Planck Institute for Biophysical Chemistry, Göttingen) *FRET through Atomistic Simulation and Monte Carlo*
12:00 – 13:00	Lunch
13:00 – 13:25	**Abhinav Jain** (University of Freiburg, Institute of Physics) *Resolving the free-energy landscape of folding proteins*
13:25 – 13:50	**Lipi Thukral** (University of Heidelberg) *Common folding mechanism revealed using multiple microsecond-long MD simulations*
13:50 – 14:15	**Chetan Poojari** (Forschungszentrum Juelich) *Modelling transmembrane structures of Alzheimer's Abeta 1-42 peptide: Peptide insertion and Abeta-membrane interactions*
14:15 – 14:40	**Katharina Meier** (ETH Zuerich) *On the effect of a variation of the force field, spatial boundary condition and size of the QM region in QM/MM MD simulations*
14:40 – 15:05	**Olujide Olubiyi** (German Research School for Simulation Sciences, Jülich) *Molecular simulation studies on the prevention of amyloid aggregation of Alzheimer's Abeta peptide by D-peptides*
15:05 – 15:25	Coffee break
15:25 – 15:50	**Maarten Wolf** (Max Planck Institute for Biophysical Chemistry, Göttingen) *Unexpected hydrolysis of carbohydrate based sulfonamide inhibitors by Carbonic anhydrase*
15:50 – 16:15	**Timo Strunk** (Karlsruhe Institute of Technology) *Analysis of amino acid specific energy contributions to native conformations in high-resolution protein structures*
16:15 – 16:40	**Nadine Utz** (Institute for Research in Biomedicine (IRB) Barcelona) *Understanding the antagonist mechanism of Peroxisome Proliferator-Activated Receptor gamma*
16:40 – 17:05	**Shirley Siu** (University Erlangen-Nuremberg) *Reparametrization of OPLS/AA Force Field for Hydrocarbons*
17:05 – 17:30	**Rodolfo Briones** (Max Planck Institute for Biophysical Chemistry, Göttingen) *Lipid-Protein interactions by Molecular Dynamics Simulations*
18:00	Dinner/Departure