Program, Workshop in Hünfeld, April 20-21, 2012
"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES 2012"

Friday, April 20, 2012	
11:00 – 13:00	Arrival, registration and lunch
13:00 – 13:05	Welcome
13:05 – 13:30	**Mikolaj Feliks** (University of Bayreuth) *QM and QM/MM Modeling of Mechanisms of Glycyl-Radical Enzymes: B12-Independent Glycerol Dehydratase and 4-Hydroxyphenylacetate Decarboxylase*
13:30 – 13:55	**Till Rudack** (Ruhr University Bochum) *Catalysis of GTP Hydrolysis by 10 Orders of Magnitude by Ras-RasGAP Revealed at Atomic Detail by Combining QM/MM Simulations and FTIR Spectroscopy*
13:55 – 14:20	**Ludger Inhester** (Max Planck Institute for Biophysical Chemistry, Göttingen) *Auger Spectrum of a Water Molecule After Single and Double Core Ionization by XFEL Radiation*
14:20 – 14:45	**Michal Kolar** (Institute of Organic Chemistry and Biochemistry AS CR, Prague) *Treatment of Halogen Bonding by Current Biomolecular Empirical Force Field*
14:45 – 15:10	**Thorsten Will** (Saarland University, Saarbrücken) *Finding Low Energy Conformations in a Haystack of Tautomers*
15:10 – 15:25	Coffee break
15:25 – 15:50	**Christian Hanke** (Heinrich Heine University Düsseldorf) *Influence of Mg^{2+} on the Structure and Dynamics of the Guanine-Sensing Riboswitch*
15:50 – 16:15	**Alexander Krah** (Max Planck Institute of Biophysics, Frankfurt) *Binding-Site Gating in a Mitochondrial F_0 Rotor Induced by Environment Changes: Implications for the Mechanism of Proton Translocation by ATP Synthases*
16:15 – 16:40	**Lars Bock** (Max Planck Institute for Biophysical Chemistry, Göttingen) *Dynamic, Energetic, and Kinetic Determinants of Ribosomal Translocation*
16:40 – 17:05	**Martin Vesper** (Max Planck Institute for Biophysical Chemistry, Göttingen) *Collective Dynamics Underlying Allosteric Transitions in Hemoglobin*
17:05 – 17:30	**Mari Chikvaidze** (Heidelberg University) *The Power of Two: A Molecular Dynamics Study of Mono and Dimeric Forms of the Enzyme Alkaline Phosphatase*
17:30 – 17:55	**Thomas Steinbrecher** (Karlsruhe Institute of Technology) *Lipid Bilayer Insertion and Stability of Small Toxic Peptide tisB*
18:00 – 19:00	Dinner
19:30 –	Poster Session / Beer

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Saturday, April 21, 2012	
8:00 – 8:50	Breakfast
8:55 – 9:20	**Chen Song** (Max Planck Institute for Biophysical Chemistry, Göttingen) *Dermcidin Oligomer in Action*
9:20 – 9:45	**Niraj Modi** (University of Bremen) *Transport of Ions Through Bacterial Porins*
9:45 – 10:10	**Paul Strodel** (German School for Simulation Sciences, Jülich) *Investigations on Small Ion Permeation Through a Bacterial Porin*
10:10 – 10:45	Coffee break
10:45 – 11:10	**Camilo Aponte-Santamaria** (Heidelberg Institute for Theoretical Studies) *Molecular Driving Forces Defining Lipid Positions Around Aquaporin-0*
11:10 – 11:35	**Hiroshi Watanabe** (Karlsruhe Institute of Technology) *Structural Modeling of Channelrhodopsin*
11:35 – 12:00	**Shijun Xiao** (Heidelberg Institute for Theoretical Studies) *Forces at Protein-Mineral Interfaces and Flaws: The Case of Nacre*
12:00 – 13:00	Lunch
13:00 – 13:25	**Antonia Mey** (Free University Berlin) *Efficient Estimation of Equilibrium Expectations from Multi-Ensemble Simulations*
13:25 – 13:50	**Davide Branduardi** (Max Planck Institute for Biophysics, Frankfurt) *Probing New Dimensions in Free Energy Through String Method*
13:50 – 14:15	**Abhinav Jain** (University of Freiburg) *Identifying Metastable States of Folding Proteins*
14:15 – 14:40	**Felix Rausch** (Institute of Plant Biochemistry, Halle) *Protein Modeling and Molecular Dynamic Studies of Two New Surfactant Proteins*
14:40 – 15:05	**Kenneth Osborne** (Research Center Jülich) *Replica Exchange Studies of Amyloidogenic Peptide Aggregation*
15:05 – 15:25	Coffee break
15:25 – 15:50	**Ignacio Faustino** (Institute for Research in Biomedicine, Barcelona) *B-DNA Polymorphisms at the Base Pair Step Level: The CG Step Case*
15:50 – 16:15	**Ruben Vosmeer** (VU University Amsterdam) *Plasticity Models for Binding Affinity Prediction to Human Cytochrome P450 2D6*
16:15 – 16:40	**Manuel Glaser** (Technical University Munich) *Structure-Based Prediction of MHC-Peptide Binding*
16:40 – 17:05	**Andrzej Rzepiela** (University of Freiburg) *Configurational dynamics of BPTI explored with a multidimensional Langevin model*
17:05 – 17:45	Poster price, final remarks
18:00	Dinner / Departure