Program, Workshop in Hünfeld, March 24-25, 2017
"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES"

Friday, March 24, 2017	
11:00 – 13:00	Arrival, registration and lunch
13:00 – 13:05	Welcome
13:05 – 13:30	**Jonathan Coles** (Technical University of Munich, Garching) ***An Efficient, Polarizable, Multi-Scale Molecular Dynamics Approach to Simulating Microscopic Systems***
13:30 – 13:55	**Dominik Sidler** (ETH Zurich) ***RE-EDS: A Novel Method to Estimate Multiple Free-Energy Differences from a Single Simulation***
13:55 – 14:20	**Martin Mechelke** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Bayesian Protein Structure Reconstruction from Single Molecule Scattering Experiments***
14:20 – 14:45	**Marco Reidelbach** (Free University of Berlin) ***Proton Transfer in Cytochrome c Oxidase - Calculation and Estimation of Transition Networks***
14:45 – 15:10	**Rahman Akbar** (Saarland University, Saarbrücken) ***Surface Pocket Dynamics in Splice Variants of CBD12 Domains***
15:10 – 15:25	Coffee break
15:25 – 15:50	**Wojciech Kopec** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Molecular Simulations of Ion Permeation in Potassium Channels***
15:50 – 16:15	**Duy Nguyen** (Saarland University, Saarbrücken) ***Substrates/Nonsubstrates in the MsbA Transporter***
16:15 – 16:40	**Wei Yang** (Monash University, Melbourne) ***Investigating the Protein Dynamics of the Leucyl Aminopeptidase from Plasmodium Falciparum***
16:40 – 17:05	**Csaba Daday** (Heidelberg University, IWR) ***Simulating Force Response at Cell Junctions: Desmoplakin as a Molecular Force Sensor?***
17:05 – 17:30	**Martin Voegele** (Max Planck Institute of Biophysics, Frankfurt am Main) ***Cluster Formation of Carbon Nanotubes in Lipid Membranes***
17:30 – 17:55	**Michael Feig** (Michigan State University, East Lansing) ***Protein Stability and Dynamics in Simulations of Cytoplasmic Environments***
18:00 – 19:00	Dinner
19:30 –	Poster Session / Beer

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Saturday, March 25, 2017	
8:00 – 8:50	Breakfast
8:55 – 9:20	**Oliver Lemke** (Free University of Berlin) ***Constructing Kinetic Models with Density-based Cluster Algorithms***
9:20 – 9:45	**Joseph Rudzinski** (Max Planck Institute for Polymer Research, Mainz) ***Characterization of Coarse-grained Helix-coil Transition Kinetics using Markov State Models***
9:45 – 10:10	**Simon Olsson** (Free University of Berlin) ***Augmenting and Validating Markov State Models with Experimental Data***
10:10 – 10:45	Coffee break
10:45 – 11:10	**Dusan Petrovic** (Research Center Jülich) ***Exploring Conformational Ensembles in Computational Enzymology***
11:10 – 11:35	**Roman Shevchuk** (Georg August University Göttingen) ***Bayesian Refinement of Protein Ensembles against SAXS Data Using Molecular Dynamics Simulations***
11:35 – 12:00	**Till Rudack** (University of Illinois, Urbana) ***ModelMaker: A Tool for Interactive Modeling of Complete Proteins Guided by Cryo-EM, Structure Prediction, and Molecular Dynamics***
12:00 – 13:00	Lunch
13:00 – 13:25	**Beatrix Bold** (Karlsruhe Institute of Technology) ***Active Site Structure and Absorption Spectrum of Channelrhodopsin-2 WT and C128T Mutant***
13:25 – 13:50	**Vance Jaeger** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Interpreting Interfacial Protein Spectra Using Molecular Simulation***
13:50 – 14:15	**Daniel Mann** (Ruhr University of Bochum) ***Mechanisms of GTP Hydrolysis in Heterotrimeric GTPases Elucidated via Theoretical IR Spectroscopy***
14:15 – 14:40	**Steffen Wolf** (Albert Ludwigs University of Freiburg) ***Identification and Verification of Reaction Coordinates Describing Protein Functional Motion: T4 Lysozyme as a Test Case***
14:40 – 15:05	**Gerrit Groenhof** (University of Jyvaskyla) ***Multi-Scale Molecular Dynamics Simulations of Photoactive Molecules in Optical Cavities***
15:05 – 15:20	Coffee break
15:20 – 15:45	**Narendra Kumar** (Ruhr University of Bochum) ***Insights into the Self-Cleavage Reaction of the Hairpin Ribozyme***
15:45 – 16:10	**Sonja Kirsch** (Friedrich Alexander University of Erlangen-Nuremberg, Erlangen) ***Intermolecular Interactions in the Activation of Two Pore Channels***
16:10 – 16:35	**Jeffrey Noel** (Max Delbrück Center, Berlin) ***How EF-Tu Can Contribute to Efficient Proofreading of aa-tRNA by the Ribosome***
16:35 – 17:00	**Michal H. Kolar** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Elongation of Nascent Peptides in the Ribosomal Exit Tunnel***
17:00 – 17:30	Poster price, final remarks
18:00	Dinner / Departure

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