Program, Workshop in Hünfeld, March 22-23, 2019
"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES"

Friday, March 22, 2019	
11:00 – 13:00	Arrival, registration and lunch
13:00 – 13:05	Welcome
13:05 – 13:30	**Markus Rainer Hermann** (Georg August University of Göttingen) *Restrained-Ensemble Simulations of Intrinsically Disordered Proteins with the Maximum Entropy Principle*
13:30 – 13:55	**Matthias Post** (Albert Ludwigs University of Freiburg) *Principal Component Analysis of Non-Equilibrium Molecular Dynamics Simulations*
13:55 – 14:20	**Mazen Ahmad** (Max Planck Institute for Informatics, Saarbrücken) *Relative Principal Components Analysis: Application to Analyzing Biomolecular Conformational Changes*
14:20 – 14:45	**Daniel Nagel** (Albert Ludwigs University of Freiburg) *Dynamical Coring of Markov State Models*
14:45 – 15:10	**Leonard Heinz** (Max Planck Institute for Biophysical Chemistry, Göttingen) *Charting the Hydrophobic Effect: Computing Spatially Resolved Absolute Hydration Shell Entropies*
15:10 – 15:25	Coffee break
15:25 – 15:50	**Pratiti Bhadra** (University of Macau, China) ***Force field parameterization for protein simulations on Hydrophobic Self-Assembled Monolayers***
15:50 – 16:15	**Sören von Bülow** (Max Planck Institute of Biophysics, Frankfurt/Main) *Dynamic Cluster Formation Determines Viscosity and Diffusion in Dense Protein Solutions*
16:15 – 16:40	**Ariane Nunes Alves** (Heidelberg Institute for Theoretical Studies (HITS)) *Effects of Macromolecular Crowding on the Diffusion Rates of Enzyme Substrates and Drug Molecules*
16:40 – 17:05	**Christopher Paeslack** (Ruhr University of Bochum) *Effect of Cholesterol on Collective Motions in Lipid Bilayers*
17:05 – 17:30	**Sonja Kirsch** (Friedrich Alexander University of Erlangen-Nuremberg) *Membrane Domain Formation and Enhanced Electroporation near Phase Transition*
17:30 – 17:55	**Xue Wang** (Research Center Jülich) *Simulations of the Interactions Between Membrane Binding Proteins and Lipids: the Cases of Guanylate Binding Proteins and GABARAP*
18:00 – 19:00	Dinner
19:30 –	Poster Session / Beer

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Saturday, March 23, 2019	
8:00 – 8:50	Breakfast
8:55 – 9:35	**Jeremy Smith** (Oak-Ridge National Laboratory, USA) ***Computational Drug Discovery***
9:35 – 10:00	**Dirk Matthes** (Max Planck Institute for Biophysical Chemistry, Göttingen) *The Molecular Basis of anle138b Interactions with Beta-sheet Rich Oligomers*
10:00 – 10:25	**Kara Grotz** (Max Planck Institute of Biophysics, Frankfurt/Main) *Optimized All-Atom Force Fields for Mg2+ Based on Water Exchange Properties*
10:25 – 10:45	Coffee break
10:45 – 11:10	**Annie Westerlund** (Royal Institute of Technology (KTH), Solna/Stockholm, Sweden) *Free Energy Clustering with Gaussian Mixtures*
11:10 – 11:35	**Luca Donati** (Free University of Berlin) *Girsanov Reweighting for Metadynamics **Simulations***
11:35 – 12:00	**David Hartich** (Max Planck Institute for Biophysical Chemistry, Göttingen) *Extreme Value Statistics from First Passage Concepts in Free Energy Landscapes*
12:00 – 13:00	Lunch
13:00 – 13:25	**Lucie Delemotte** (Royal Institute of Technology (KTH), Solna/Stockholm, Sweden) *Determining the Molecular Basis of Voltage Sensitivity in Membrane Proteins*
13:25 – 13:50	**Johann Biedermann** (Leibniz Institute for Molecular Pharmacology, Berlin) *Investigation of Cation Permeation through AMPA Receptor Channels by Molecular Dynamics Simulations*
13:50 – 14:15	**Wojciech Kopec** (Max Planck Institute for Biophysical Chemistry, Göttingen) *Molecular Simulations of Ion Permeation, Gating and Selectivity in K+ channels*
14:15 – 14:40	**Vinaya Kumar Golla** (Jacobs University of Bremen) *Permeation of Phosphonic Acid Antibiotics Across Bacterial Pores*
14:40 – 15:05	**Simon Menig** (Technical University of Munich) *Predicting Substrates of the Intramembrane Protease Gamma-Secretase from Coarse-Grained Simulations*
15:05 – 15:20	Coffee break
15:20 – 15:45	**Fan Jin** (Heidelberg University and Heidelberg Institute of Theoretical Studies (HITS)) *Molecular Mechanism for Phosphorylation of Intrinsically Disordered Proteins: Insights from Computer Simulations and Implications for Biological Function*
15:45 – 16:10	**Maxim Igaev** (Max Planck Institute for Biophysical Chemistry, Göttingen) *Mechanical Strain and Long-Range Coupling in the Microtubule Lattice*
16:10 – 16:35	**Benedikt Rennekamp** (Heidelberg Institute for Theoretical Studies (HITS)) *Bond Scission in Tensed Collagen: A Hybrid Monte Carlo / Molecular Dynamics Approach*
16:35 – 17:00	**Massimiliano Anselmi** (Georg August University of Göttingen) *The Role of the Ligand-Induced Conformational Changes in the Activation Mechanism of SHP2 Tyrosine Phosphatase*
17:00 – 17:30	Poster prize, final remarks
18:00	Dinner / Departure