Program, Workshop in Hünfeld, April 28-29, 2023
"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES"

Friday, April 28, 2023	
11:00 – 13:00	Arrival, registration and lunch
13:00 – 13:05	Welcome
13:05 – 13:30	**Saber Shakibi** (University of Groningen, The Netherlands) ***A One-Bead-Per-Saccharide (1BPS) Model for Multiscale Modelling of the Brain ECM***
13:30 – 13:55	**Thomas Tarenzi** (University of Trento, Italy) ***Exploring and Leveraging the Interplay Between System Properties and Model Resolution***
13:55 – 14:20	**Lorenzo Petrolli** (University of Trento, Italy) ***The In Silico Assessment of DNA Lesions by Radiations***
14:20 – 14:45	**Bart Bruininks** (University of Helsinki, Finland) ***Challanges and Solution for Molecular Dynamics Simulations at the Mesoscale***
14:45 – 15:10	**Erik Poppleton** (Max Planck Institute for Medical Research, Heidelberg Institute for Theoretical Studies (HITS), Germany) ***Coarse-Grained Modeling of DNA Origami Structures Using oxDNA***
15:10 – 15:25	Coffee break
15:25 – 15:50	**Hana Zupan** (Free University of Berlin, Germany) ***Grid-Based State Space Exploration for Molecular Binding***
15:50 – 16:15	**Yixin Chen** (Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany) ***A Minimal Markov Model for Rotary Catalysis of F1-ATPase***
16:15 – 16:40	**Emanuele Zippo** (Johannes Gutenberg University of Mainz, Germany) ***Towards Markov State Models of Chemically Driven Non-Equilibrium Steady States***
16:40 – 17:05	**Debora Monego** (Heidelberg Institute for Theoretical Studies (HITS), Germany) ***Size-dependent Sedimentation of Nanocrystals: The Role of the Ligand Shell Structure***
17:05 – 17:30	**Johanna-Barbara Linse** (Saarland University, Saarbrücken, Germany) ***Scrutinizing the Protein Hydration Shell from MD Simulations against Experimental Solution Scattering Data: Effects of Water Models, Force Fields, and Surface Compositions***
17:30 – 17:55	**Tobias Marcel Prass** (Ruhr University Bochum, Germany) ***Residue-Specific Protein-Cosolvent Interactions in All-Atom and Coarse-Grained MD Simulations***
18:00 – 19:00	Dinner
19:30 –	Poster Session / Beer

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Saturday, April 29, 2023	
8:00 – 8:50	Breakfast
8:55 – 9:35	**Frauke Gräter** (Heidelberg Institute for Theoretical Studies (HITS), Germany) ***Incorporating Chemistry Into Classical Molecular Dynamics Simulations by Machine Learning***
9:35 – 10:00	**Anders Frederiksen** (Carl von Ossietzky Universität Oldenburg, Germany) ***Modeling the Electron Transfer Activation of European Robin Cryptochrome 4***
10:00 – 10:25	**Katharina Leitmann** (Ruhr University Bochum Germany) ***Refining Active Sites of Proteins to Sub-Ångström Resolution by Combining Theoretical and Experimental Infrared Spectroscopy***
10:25 – 10:45	Coffee break
10:45 – 11:10	**Tobias Hüfner** (Max Planck Institute of Biophysics, Frankfurt/Main, Germany) ***Automated and Systematic Derivation of Parameter Type Definitions for Molecular Mechanics Force Fields***
11:10 – 11:35	**Benjamin Eltzner** (Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany) ***Maximum Entropy Force Field Refinement***
11:35 – 12:00	**Jayashrita Debnath** (Max Planck Institute of Biophysics, Frankfurt/Main, Germany) ***Clustering Molecular Dynamics Trajectories Using Density and Flux***
12:00 - 13:00	Lunch
13:00 – 13:25	**Lars V. Bock** (Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany) ***Mechanisms of Ribosome Stalling and Unstalling Studied by MD Simulations***
13:25 – 13:50	**Anna Jäckering** (Research Center Jülich, Germany) ***Engineering PET-Degrading Enzymes – Targeting the Energy Barrier for PET Binding***
13:50 – 14:15	**Andrei Mironenko** (Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany) ***Effect of Selectivity Filter Mutations on K+ Permeation Mechanism in the KcsA Channel: A Molecular Dynamics Study***
14:15 – 14:40	**Richard Kullmann** (Max Planck Institute of Colloids and Interfaces, Potsdam, Germany) ***Investigating Amylose-Amylomaltase Binding with H-REMD Simulations***
14:40 – 15:05	**Matthias Post** (University of Freiburg, Germany) ***Path Separation of Dissipation-Corrected Targeted Molecular Dynamics Simulations of Protein-Ligand Unbinding***
15:05 – 15:20	Coffee break
15:20 – 15:45	**Ferdinand Horvath** (JKU Linz, Austria) ***Pathways of Dimerization of STIM1 Transmembrane Helices***
15:45 – 16:10	**Leonhard Starke** (Saarland University, Saarbrücken, Germany) ***The Influence of Lipid Composition on the Free Energy of Membrane Pore Formation***
16:10 – 16:35	**Matthias Pöhnl** (University of Erlangen-Nürnberg, Erlangen, Germany) ***Lipid Bicelles in the Study of Biomembrane Characteristics***
16:35 – 17:00	**Abhik Ghosh Moulick** (S N Bose National Centre For Basic Sciences, Kolkata, India) ***Microscopic Understanding of Fatty Acid Binding with α-Lactalbumin at Molten Globule State***
17:00 – 17:25	**Miloš Ivanović** (University of Zurich, Switzerland) ***Protein Dynamics in a Biomolecular Condensate***
17:30 – 17:55	Poster prize, final remarks
18:00	Dinner / Departure

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