Program, Hybrid Workshop in Hünfeld, April 19-20, 2024
"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES" 2024-04-05

Friday, April 19, 2024 **Times given in CEST: Central European Summer Time (UTC+2)**	
11:00 – 13:00	Arrival, registration and lunch
13:00 – 13:05	Welcome
13:05 – 13:30	**Rita Ann Roessner** (University of Montpellier, France) ***Exploring the Conformational Landscape of a Class A G Protein-Coupled Receptor with Biased Molecular Dynamics Simulations and Markov State Modeling***
13:30 – 13:55 online	**Saha Satvati** (Instituto Italiano di Tecnologia, Genoa, Italy) ***Molecular Dynamics Simulations of Bacterial Membrane Interaction with Double and Tetra Branched Antimicrobial Peptides***
13:55 – 14:20	**Katharina Spies** (Karlsruhe Institute of Technology, Germany) ***Proton Coupled Electron Transfer in Biomimetic Peptides***
14:20 – 14:45	**Daniel Szöllösi** (Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany) ***Simulation of Ion Mobility Spectrometry Experiments***
14:45 – 15:10	**Saumyak Mukherjee** (Ruhr University Bochum, Germany) ***Microscopic Dynamics of an Intrinsically Disordered Protein in a Condensate***
15:10 – 15:25	Coffee break
15:25 – 15:50	**Sanjoy Paul** (Max Planck Institute of Biophysics, Frankfurt, Germany) ***Delineating the Shape of COPII Coated Membrane Bud***
15:50 – 16:15	**Arya Changiarath Sivadasan** (Johannes Gutenberg University, Mainz, Germany) ***Condensate Coexistence in Gene Transcription: Molecular Dynamics Insights***
16:15 – 16:40	**Aleksandr Zlobin** (Leipzig University, Germany) ***Charges and Boundary Terms: Easy Ways to Spoil Your QM/MM(MD) Results***
16:40 – 17:05	**Isabell Louise Grothaus** (University of Bremen, Germany) ***The Third Dimension of the Sugar Code under the Computational Microscope***
17:05 – 17:30	**Marius Trollmann** (Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany) ***One Ring to Rule Them All: Lugdunin's Disruptive Effects***
17:30 – 17:55	**Patrick Quoika** (Technical University of Munich, Germany) ***Evaporation Behavior of Common Water Models in Molecular Dynamics Simulations***
18:00 – 19:00	Dinner
19:30 –20:30	Poster Presentations: **odd numbers**/ Beer
20:30 – 21:30	Poster Presentations: **even numbers**/ Beer

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Saturday, April 20, 2024 **Times given in CEST: Central European Summer Time (UTC+2)**	
8:00 – 8:50	Breakfast
8:55 – 9:35	**Invited Speaker: Pavel Jungwirth** (IOCB Prague, Czech Republic) ***Charge Scaling Force Fields for Biomolecular Simulations: Do Free Lunches Exist?***
9:35 – 10:00	**Steffen Schultze** (Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany) ***Bayesian Electron Density Determination from Single-Molecule X-ray Scattering***
10:00 – 10:25	**Leif Seute** (Heidelberg Institute for Theoretical Studies, Germany) ***Learning a State of the Art MM Force Field***
10:25 – 10:45	Coffee break
10:45 – 11:10	**Sudarshan Behera** (Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany) ***Understanding Errors in Relative Binding Free Energy Calculations***
11:10 – 11:35	**Alejandro Martínez-León** (Saarland University, Saarbrücken, Germany) ***Absolute Binding Free Energy Calculations: A Systematic Force Field Comparison by a Newly Designed Computational Pipeline***
11:35 – 12:00	**Ahmed Ali** (University of Freiburg, Germany) ***Allosteric Communication in PDZ3 Studied by Nonequilibrium Simulations and Markov State Model***
12:00 - 13:00	Lunch
13:00 – 13:25	**Mislav Brajković** (Heidelberg Institute for Theoretical Studies (HITS), Heidelberg, Germany) ***Investigation of Effect of Loop Motion on the Residence Time of Histamine-1-Receptor (H1R) Antagonists by τRAMD***
13:25 – 13:50	**Chenggong Hui** (Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany) ***Effects of Charge Scaling on Potassium Channel Simulations, Conductance, Ion Occupancy, Voltage Response, and Selectivity***
13:50 – 14:15	**Lisa Sophie Kersten** (Heinrich Heine University, Düsseldorf, Germany) ***Atomistic Mechanism of Copper Transfer to Plant Receptor ETR and Structural Receptor Dynamics after Binding of Ethylene and 1-Methylcyclopropene***
14:15 – 14:40	**Jonathan Hungerland** (Carl von Ossietzky University, Oldenburg, Germany) ***Introducing the Automated Ligand Searcher***
14:40 – 15:05	**Sara Gabrielli** (Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany) ***Rest Assured: Programmed Translational Stalling Studied by Means of MD Simulations***
15:05 – 15:20	Coffee break
15:20 – 15:45	**Chetan Poojari** (Saarland University, Saarbrücken, Germany) ***Molecular Mechanisms Unveiling Virus-Host Interactions Steering Membrane Fusion***
15:45 – 16:10	**Yanna Gautier** (CNRS, Paris, France) ***High-Pressure Response of the Coupled Dynamics of Lipids and Membrane Proteins***
16:10 – 16:35	**Beatrice Caviglia** (Université de Paris Cité, University of Perugia, Paris, France) ***Investigation on the Protein Dynamics at Extreme Temperatures***
16:35 – 17:00	**Gustavo Enrique Olivos Ramirez** (Institute of Fundamental Technological Research, Polish Academy of Sciences, Warsaw, Poland) ***Accessing the Conformational Space of Viral Protein Models by GōMartini 3 Approach***
17:00 – 17:25	**Balázs Fábián** (Max Planck Institute for Biophysics, Frankfurt am Main, Germany) ***Molecular Modeling of the SARS-CoV-2 Nucleocapsid Protein Using Martini***
17:30 – 17:55	Poster prize, final remarks
18:00	Departure