

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

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