Program, Hybrid Workshop in Hünfeld, March 7-8, 2025
"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES"

Friday, March 7, 2025 **Times given in CET: Central European Time (UTC+1)**	
11:00 – 13:00	Arrival, registration and lunch (starts **11:30**)
13:00 – 13:05	Welcome
13:05 – 13:30	**Carlos A. Ramos-Guzmán** (University of Bristol , United Kingdom) ***Decoding Carbapenem Resistance: From Room-Temperature X-Ray Crystallography to QM/MM Mechanistic Insights***
13:30 – 13:55	**Saeed Norouzi** (Technical University of Darmstadt, Germany) ***Multiscale Insights into Gecko Adhesive Mechanics: Molecular Dynamics and Continuum Coupling Approach***
13:55 – 14:20	**Michel Mom** (University of Stuttgart, Germany) ***A Computational Study on the Detection of Citrulline Modifications Using an Aerolysin Nanopore***
14:20 – 14:45	**Noora Aho** (Saarland University, Germany) ***Molecular Dynamics Simulations of a Protein-Detergent Complex to Model Contrast-Variation SAXS Experiments***
14:45 – 15:10	**Edward Francisco Mendez Otalvaro** (Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany) ***Effect of Activators on the Gating of a K2P Channel***
15:10 – 15:35	Coffee break
15:35 – 16:00	**Anja Marquardt** (Hanover Medical School, Germany) ***Exploring the Biochemical Impact of the β-Actin G74S Mutation and Associated Histidine Methylation Deficiency via Molecular Dynamics Simulations***
16:00 – 16:25	**Alen Thykkoottathil Mathew** (Ghent University, Belgium) ***Unlocking the Molecular Gates: Choline Import and the Dynamics of a Bacterial Transporter***
16:25 – 16:50	**Alp Tegin Sahin** (University of Dundee, United Kingdom) ***Characterization of Ligand Gating, Ion Conduction and the Ion Selectivity Mechanism in the Endo-Lysosomal Ion Channel hTPC2***
16:50 – 17:15	**Reinier de Vries** (Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany) ***Molecular Mechanism of Calcium Block in the MthK Potassium Channel***
17:15 – 17:40	**Florian Leidner** (Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany) ***How Loop Dynamics Control Activity and Selectivity in an Alcohol Dehydrogenase***
17:40 – 18:05	**Paolo Rossetti** (Friedrich-Alexander University Erlangen-Nuremberg, Germany) ***An Atlas of Membrane-Driven Antibiotic Resistance: Insights from Molecular Dynamics Simulations***
18:05 – 19:30	Break / **Dinner starts at 18:30**
19:30 –20:30	Poster Presentations: **odd numbers**
20:30 – 21:30	Poster Presentations: **even numbers**

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Saturday, March 8, 2025 **Times given in CET: Central European Time (UTC+1)**	
8:00 – 9:00	Breakfast
9:00 – 9:40	**Invited Speaker: Kresten Lindorff-Larsen** (University of Copenhagen, Denmark) ***Structure Prediction and Design of Intrinsically Disordered Proteins***
9:40 – 10:05	**Kush Coshic** (Max Planck Institute of Biophysics, Frankfurt a. M., Germany) ***Multi Resolution Modeling of Large Nucleic Acid Systems: Physical Virology and Beyond***
10:05 – 10:30	**Eliane Briand** (Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany) ***Constant pH Molecular Dynamics Simulation with FMM Electrostatics in GROMACS: Design and Applications***
10:30 – 10:55	Coffee break
10:55 – 11:20	**Varun Mandalaparthy** (Technical University of Darmstadt, Germany) ***A Generic Model for pH-Sensitive Collapse of Hydrophobic Polymers***
11:20 – 11:45	**Julia Keil** (Technical University of Darmstadt, Germany) ***Buffer-Specific Interactions of Imidazolium with Elastin-Like Polypeptides***
11:45 – 12:10	**Mengmeng Wu** (Max Planck Institute for Polymer Research, Mainz, Germany) ***Porous Particles Formation in the Drying of Polymer Solution Droplets***
12:10 - 13:15	Break / **Lunch starts at 12:30**
13:15 – 13:40	**Joana-Lysiane Schäfer** (Free University Berlin, Germany) ***Girsanov Reweighting in OpenMM and Deeptime***
13:40 – 14:05	**Simon Holtbrügge** (Ruhr University Bochum, Germany) ***Rotational Diffusion of Proteins from MD***
14:05 – 14:30	**Leif Seute** (Max Planck Institute for Polymer Research, Mainz, Germany) ***Learning the Boltzmann Distribution of Protein Backbones***
14:30 – 14:55	**Rodrigo Fedrizzi Dillenburg** (Max Planck Institute for Polymer Research, Mainz, Germany) ***Grand Canonical Simulations of IDPs: Investigating Microstructure Formation***
14:55 – 15:20	**Dafna Knani** (Braude College, Karmiel, Israel) ***Simulation of the Co-Assembly of Peptide Amphiphiles***
15:20 – 15:45	Coffee break
15:45 – 16:10	**Joel Chavarria Rivera** (Saarland University, Germany) ***Free Energies of Stalk Formation - Comparison Between All-Atome and MARTINI simulations***
16:10 – 16:35	**Kamonthira Wichai** (Technical University of Darmstadt, Germany) ***Molecular Simulation of Pectin Mucilage Adhesion on a Flat Substrate***
16:35 – 17:00	**Mohsen Sadeghi** (Free University Berlin, Germany) ***Large-Scale Mesoscopic Simulations: From Membranes to Human Cytomegalovirus***
17:00 – 17:20	Poster prize, final remarks and departure

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