Program Hybrid Workshop COMPUTER SIMULATION AND THEORY OF MACROMOLECULES
Hünfeld, April 08-09, 2022

Friday, April 08, 2022 Times given in CEST: Central European Summer Time (UCT+2)	
10:00	Arrival, registration
11:30 - 13:00	Lunch (depending on individual arrival time)
13:00 – 13:05	**Welcome** Helmut Grubmüller
13:05 – 13:30	**Georg Diez** Albert Ludwig University of Freiburg, Germany *Identifiying Collective Motion in Proteins - Divide and Conquer the Feature Space*
13:30 – 13:55 online	**Hugo McGrath** University of Chemistry and Technology, Prague, Czech Republic *Peptide Deformylase as a Probe of Long-Range Allostery Through the Ribosomal Protein uL22*
13:55 – 14:20	**Raphaëlle Versini** Sorbonne University, PSL Research University, University of Paris, France *Structural Basis of the Transmembrane Domain of the Yeast Mitofusin Fzo1*
14:20 – 14:45 online	**Maximilian Vossel** Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany *Local Mode Softening versus Hardening Underpins Specific Allosteric Responses*
14:45 – 15:10	**Claudia Leticia Gomez Flores** Karlsruhe Institute of Technology, Germany *Thiol-Disulfide Exchange Reactions Using an Artificial Neural Network Corrected DFTB/MM Methodology*
15:10 – 15:30	Coffee break
15:30 – 15:55 online	**Chun Kei Lam** Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany *Identification of Gating Sensitive Residues in TREK-2*
15:55 – 16:20	**Callum Ives** University of Dundee, United Kingdom *A Cooperative Knock-On Mechanism Underpins Ca2+-Selective Cation Permeation in TRPV Channels*
16:20 – 16:45 online	**Nabanita Mandal** National Institute of Technology, Warangal, India *Mechanistic Insights into the Differential Dynamics of SARS-CoV-2 Variants of Concern (VOC)*
16:45 – 17:10	**Terra Sztain** Free University Berlin, Germany *Weighted Ensemble Simulations of SARS-CoV-2 Glycosylated Spike Opening*
17:10 – 17:35	**Stefan Schäfer** Max-Planck-Institute for Biophysics, Frankfurt/Main, Germany *Anchoring of the SARS CoV-2 Fusion Peptide in Host Membranes*
17:40 – 18:25	Dinner 1 (45 min)
18:40 – 19:25	Dinner 2 (45 min)
19:30 –	Poster Session on-site and online

Saturday, April 09, 2022 Times given in CEST: Central European Summer Time (UCT+2)

7:35 – 8:05	Breakfast 1 (30 min)
8:20 – 8:50	Breakfast 2 (30 min)
8:55 – 9:35	**Invited speaker** **Gerhard Hummer** Max Planck Institute for Biophysics, Frankfurt/Main, Germany *Towards Cell-Scale Molecular Simulations*
9:35 – 10:00	**Pavel Buslaev** University of Jyväskylä, Finland *Constant pH MD in GROMACS*
10:00 – 10:25	**Eliane Briand** Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany *Constant pH Molecular Dynamics in GROMACS using Lambda Dynamics and the Fast Multipole Method*
10:25 – 10:45	Coffee break
10:45 – 11:10	**Aleksander Durumeric** Free University Berlin, Germany *Towards Quantitatively Accurate Neural Network CG Force-fields*
11:10 – 11:35	**Hendrik Jung** Max Planck Institute for Biophysics, Frankfurt/Main, Germany *Artificial Intelligence for Molecular Mechanism Discovery*
11:40 – 12:25	Lunch 1 (45 min)
12:40 – 13:25	Lunch 2 (45 min)
13:25 – 13:50	**Melanie König** University of Groningen, The Netherlands *Membrane Curvature Induced Lipid Sorting in Coarse-Grained Simulations*
13:50 – 14:15	**Xavier Prasanna Anthony Raj** University of Helsinki, Finland *Mechanistic Insight into Seipin's Activity During Initial Stages of Lipid Droplet Formation*
14:15 – 14:40 online	**Ebru Çetin** Sabanci University, Istanbul, Turkey *Manipulation of a Cryptic Site on DHFR to Combat Trimethoprim Resistance in E. coli*
14:40 – 15:05	**Anna Selina Juber** Ruhr University Bochum, Germany *Thermodynamic Driving Forces of Guest Confinement in a Photoswitchable Cage*
15:05 – 15:25	Coffee break
15:25 – 15:50	**Christian Faber** Research Center Jülich, Germany *A New Measure for Contact Maps*
15:50 – 16:15	**Batuhan Kav** Research Center Jülich, Germany *Does the Inclusion of Polarisability Lead to a Better Modelling of Peptide Aggregation?*
16:15 – 16:40	**Maxim Igaev** Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany *Bending-Torsional Elasticity and Energetics of the Plus-End Microtubule Tip*
16:40 – 17:05	**Jeremy Lapierre** Saarland University, Saarbrücken, Germany *DNA Opening During Transcription Initiation by RNA Polymerase II in Atomic Detail*
17:05 – 17:30	**Nicholas Michelarakis** Heidelberg Institute for Theoretical Studies, Germany *Avidity of the Malaria Adhesin VAR2CSA is Mechano-Controlled by Exposure of a Second Cryptic CSA Sugar Binding Site*
17:30 – 17:55	**Poster prize, final remarks** Volkhard Helms
18:00	Dinner / Departure