Program, Online Workshop, April 23-24, 2021

"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES"

Times given in CEST: Central European Summer Time (UTC+2)

2021-04-09

Friday, April 23, 2021	
09:00 – 09:10	Welcome Volkhard Helms
	Chair Bert de Groot
09:10 – 09:35	Mila Vladimirova Krämer Karlsruhe Institute of Technology (KIT), Germany *Charge and Exciton Transfer Simulations driven by Machine Learned Models*
09:35 – 10:00	Suman Samantray Forschungszentrum Jülich, Germany *Computational Studies on the Effects of Different Cellular Environments on Amyloid-beta Aggregation*
10:00 – 10:25	Miloš Ivanović University of Zurich, Switzerland *Combining Single-Molecule FRET Data with Multiscale MD Simulations of Intrinsically Disordered Proteins*
10:25 – 10:40	Break
	Chair Aljaz Godec
10:40 – 11:05	Marius Wenz Free University of Berlin, Germany *Identification and Characterisation of the Interaction Interface Between h-FBP21 and SmB/B'*
11:05 – 11:30	Gianmarco Lazzeri Frankfurt Institute for Advanced Studies, Kronberg im Taunus, Germany *Atomically Detailed Characterisation of RNA Folding by Means of Biased Molecular Dynamics Simulations*
11:30 – 11:55	Pedro Reis Faculty of Sciences, University of Lisbon, Portugal *Accelerating Electrostatics-Driven pKa Predictions with Fast and Interpretable Deep Learning Models*
11:55 – 13:00	Break
13:00 – 16:00	Poster Sessions
	Chair Ilia Solov'yov
16:00 – 16:25	Faidon Brotzakis University of Cambridge, United Kingdom *A Method of Incorporating Rate Constants as Kinetic Constraints in Molecular Dynamics Simulations*
16:25 – 16:50	Kristian Blom Max Planck Institute for Biophysical Chemistry, Göttingen, Germany *Criticality in the Mechanical Regulation of Cell Adhesion*
16:50 – 17:15	Benjamin Lickert University of Freiburg, Germany *Langevin Modeling of Multisecond Dynamics Based on Atomistic Simulations*
17:15 – 17:40	Cristina Paissoni University of Milan, Italy *SAXS-Driven MD Simulations to Investigate the Dynamics of Biomolecules*

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Saturday, April 24, 2021	
	Chair Ulrich Kleinekathöfer
09:00 – 09:25	Chen Song Peking University, China *Molecular Dynamics Simulations on the Mechanosensitive Ion Channel NompC*
09:25 – 09:50	Koushik Choudhury KTH Royal Institute of Technology, Stockholm, Sweden *Opening and Inactivation of Bacterial Sodium Channel: Insights from Molecular Dynamics Simulations*
09:50 – 10:15	Weria Pezeshkian University of Groningen, The Netherlands *Simulating Realistic Membrane Shapes*
10:15 – 10:40	Hanne Antila Max Planck Institute of Colloids and Interfaces, Potsdam, Germany *How Realistic are the Lipid Conformational Dynamics in Contemporary Molecular Dynamics Models?*
10:40 – 10:55	Break
	Chair Lars Schäfer
10:55 – 11:20	Yong Wang University of Copenhagen, Denmark *Lipid Transport and Specificity in a Phospholipid Flippase*
11:20 – 11:45	Carmelo Tempra Institute of Organic Chemistry and Biochemistry, Prague, Czech Republic *Unrevealing the Interplay Between Ca2+, Calmodulin, and a Model Lipid Membranes in Early Calcium Signaling Events*
11:45 – 12:10	Ruth Helena Tichauer University of Jyväskylä, Finland *Polaritonic Protein Lasers: Insights from Multi-Scale Molecular Dynamics Simulations*
12:10 – 13:10	Break
	Chair Gerhard Stock
13:10 – 13:35	Leonie Chatzimagas Saarland University, Saarbrücken, Germany *Simulation of Liquid Jet Explosions and Shock Waves Induced by X-Ray Free-Electron Lasers*
13:35 – 14:00	Pratiti Bhadra Saarland University, Saarbrücken, Germany *How Does Sec63 Affect the Conformation of Sec61 in Yeast?*
14:00 – 14:25	Martin Reinhardt Max Planck Institute for Biophysical Chemistry, Göttingen, Germany *The Variationally-Derived Intermediates Method to Calculate Free Energy Differences*
14.25 – 14:40	Break
	Chair Jochen Hub
14:40 – 15:05	Luise Jacobsen University of Southern Denmark, Odense, Denmark *Development of an Improved and Automated Virtual Drug Screening Procedure*
15:05 – 15:30	Sebastian Wingbermühle Ruhr University Bochum, Germany *Capturing the Flexibility of a Protein-Ligand Complex: Binding Free Energies from Different Enhanced Sampling Techniques*
15:30 – 15:55	Yuriy Khalak Max Planck Institute for Biophysical Chemistry, Göttingen, Germany *Absolute Binding Free Energy: Alchemical Calculations at a Large Scale*

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15:55 – 16:10	Break
	Chair Thorsten Koslowski
16:10 – 16:35	Cong Liu Stony Brook University, Nesconset, United States *Computing Poses of Ligands Bound to Proteins using MELD Accelerated Molecular Dynamics*
16:35 – 17:00	Maria Bzówka Silesian University of Technology, Gliwice, Poland *Analysis of Molecular Dynamics Simulations from the "Intramolecular Voids" Perspective with the Use of Small Molecular Probes*
17:00 – 17:25	Abhishek Acharya Jacobs University Bremen, Germany *Exploration of Free Energy Landscape for Antibiotics Permeation Using Temperature Accelerated Sliced Sampling*
17:25 – 17:50	Dhiman Ray University of California Irvine, United States *Kinetics and Free Energy of Protein-Ligand Interaction Using Weighted Ensemble Milestoning (WEM)*
17:50 – 18:10	Final Remarks Helmut Grubmüller