

Program, Workshop in Hünfeld, April 11-12, 2014
“COMPUTER SIMULATION AND THEORY OF MACROMOLECULES 2014”

Friday, April 11, 2014	
11:00 – 13:00	Arrival, registration and lunch
13:00 – 13:05	Welcome
13:05 – 13:30	Mortaza Aghtar (Jacobs University Bremen) <i>A QM/MM Approach For Exciton Dynamics in Light-Harvesting Complexes</i>
13:30 – 13:55	Carl Burmeister (Max Planck Institute for Biophysical Chemistry Göttingen) <i>Excitation Energy Transfer in a Bi-chromophoric Molecule Driven by Non-adiabatic Dynamics</i>
13:55 – 14:20	Gesa Lüdemann (Karlsruhe Institute of Technology) <i>Charge Transfer in E.Coli DNA Photolyase: Understanding Polarization and Stabilization Effects via QM/MM Simulations</i>
14:20 – 14:45	Esam Abualrous (Jacobs University Bremen) <i>The Prominence of the Ligand Peptide Carboxyl Terminus in the MHC Class I Molecules Stability and Ligand Affinity</i>
14:45 – 15:10	Annalisa Arcella (Institute for Research in Biomedicine) <i>Nucleic Acids in the Gas Phase</i>
15:10 – 15:25	Coffee break
15:25 – 15:50	Johannes Foerster (University of Bayreuth) <i>Role of Electrostatic and Hydrophobic Interactions in the Encounter Complex Formation of Plastocyanin and Cytochrome</i>
15:50 – 16:15	Özlem Ulucan (University of Saarland) <i>Energetics of Hydrophilic Protein-Protein Association and Role of Water</i>
16:15 – 16:40	Christoph Kluge (Friedrich Alexander University Erlangen-Nuremberg) <i>Conformational Dynamics of the Transcriptional Regulator YvoA</i>
16:40 – 17:05	Davide Mercadante (Heidelberg Institute of Theoretical Studies) <i>An Unconventional Ultrafast Binding Mechanism of a Disordered Protein</i>
17:05 – 17:30	Siba Shanak (University of Saarland) <i>Interaction of Methylated DNA with Mecp2 and R.DpnI Proteins</i>
17:30 – 17:55	Claude Sinner (Karlsruhe Institute of Technology) <i>Effects of Energetic Heterogeneity on Protein Folding Dynamics Across Many Non-Homologous Proteins</i>
18:00 – 19:00	Dinner
19:30 –	Poster Session / Beer

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Saturday, April 12, 2014	
8:00 – 8:50	Breakfast
8:55 – 9:20	David Köpfer (Max Planck Institute for Biophysical Chemistry Göttingen) <i>Ion Permeation in K^+ Channels Proceeds Through Direct Charge-Charge Knock-On</i>
9:20 – 9:45	Maxime Louet (Heidelberg Institute of Theoretical Studies) <i>Allostery in Proteins: Cap as a Test Case</i>
9:45 – 10:10	Dennis Della Corte (Research Center Jülich) <i>Alteration of Enzyme Substrate Selectivity</i>
10:10 – 10:45	Coffee break
10:45 – 11:10	Christoph G. W. Gertzen (Heinrich Heine University Düsseldorf) <i>Joint MD Simulations and Experimental Studies Reveal Why the GPCR TGR5 Goes to the Plasma Membrane</i>
11:10 – 11:35	Po-chia Chen (Georg August University Göttingen) <i>WAXS-driven Molecular Dynamic: Prediction of Novel Transitions from Solution Scattering</i>
11:35 – 12:00	Christian Blau (Max Planck Institute for Biophysical Chemistry Göttingen) <i>Ribosomal Kinetics and Concerted Motions from Nanoseconds to Seconds</i>
12:00 – 13:00	Lunch
13:00 – 13:25	Colin Smith (Max Planck Institute for Biophysical Chemistry Göttingen) <i>Concerted Motion in Ubiquitin Highlights Similarities and Differences Between Simulation and Experiment</i>
13:25 – 13:50	Alexander Kraih (Kyoto University) <i>On the Structure and Mechanism of the Epsilon Subunit from Bacterial F-type ATP Synthases</i>
13:50 – 14:15	Timir Hajari (Technical University Darmstadt) <i>Hydrophobicity Scale based on Conditional Solvation Free Energy of Amino Acid Side-chains</i>
14:15 – 14:40	Sabine Reißer (Karlsruhe Institute for Technology) <i>3D Hydrophobic Moment Vectors as a Tool to Characterize the Surface Polarity of Amphiphilic Peptides</i>
14:40 – 15:05	Francesca Vitalini (Free University of Berlin) <i>Speed Of Force Fields</i>
15:05 – 15:20	Coffee break
15:20 – 15:45	Nuria Plattner (Free University of Berlin) <i>Adaptive Sampling Based on Markov State Models</i>
15:45 – 16:10	Benjamin Trendelkamp-Schroer (Free University of Berlin) <i>Efficient Estimation of Kinetic Quantities - Combining Enhanced Sampling and Standard MD</i>
16:10 – 16:35	Bogdan Barz (Research Center Jülich) <i>Kinetic Transition Networks Reveal Distinct Aggregation Pathways for the Amyloid Proteins $A\beta_{40}$ and $A\beta_{42}$</i>
16:35 – 17:00	Fabian Paul (Max Planck Institute of Colloids and Interfaces Potsdam-Golm) <i>Binding-Folding of PMI to MDM2: Towards a Reversible Markov Model for Nanomolar Binders</i>
17:00 – 17:30	Poster price, final remarks
18:00	Dinner / Departure

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