Program, Workshop in Hünfeld, May 27-28, 2016
"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES"

Friday, May 27, 2016	
11:00 – 13:00	Arrival, registration and lunch
13:00 – 13:05	Welcome
13:05 – 13:30	**Natacha Gillet** (Karlsruhe Institute of Technology) ***QM/MM Study of L-Lactate Oxidation by Flavocytochrome b2***
13:30 – 13:55	**Marten Priess** (Ruhr University of Bochum) ***Elucidating the Mechanism of ATP Hydrolysis by means of QM/MM simulations***
13:55 – 14:20	**Stevan Aleksic** (Free University of Berlin) ***Dynamic Regulation of Ca2+ Binding to C-type Lectin Langerin by an Allosteric Network***
14:20 – 14:45	**Karunakar Reddy Pothula** (Jacobs University Bremen) ***Molecular Basis of Selectivity and Permeation in OccK channels***
14:45 – 15:10	**Catarina Carvalheda** (University of Dundee) ***Water Dynamics and Proton Translocation in Cytochrome cbb3 Oxidase***
15:10 – 15:25	Coffee break
15:25 – 15:50	**Mehmet Ali Öztürk** (Heidelberg Institute for Theoretical Studies) ***Conformational Selection and Dynamic Adaptation Upon Linker Histone Binding to the Nucleosome***
15:50 – 16:15	**Rodrigo Casasnovas Perera** (Research Center of Jülich) ***Prediction of Ligand-Protein Unbinding Kinetics from Metadynamics Simulations***
16:15 – 16:40	**Pauline Delcroix** (Institute of Organic Chemistry and Biochemistry, Praha) ***Effect of Calcium on Structure and Dynamics of Calmodulin in Solution***
16:40 – 17:05	**Tomas Bastys** (Max Planck Institute for Informatics, Saarbrücken) ***Mutation Effect On Inhibitor Affinity in HIV-1 Protease***
17:05 – 17:30	**Pavel Oborsky** (Swiss Federal Institute of Technology Zürich) ***The Surprisingly Simple Rules Governing the Conformational Preferences of Disaccharides in Water***
17:30 – 17:55	**Falk Hoffmann** (Ruhr University of Bochum) ***How Much Entropy is Contained in Generalized S2 Order Parameters?***
18:00 – 19:00	Dinner
19:30 –	Poster Session / Beer

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Saturday, May 28, 2016	
8:00 – 8:50	Breakfast
8:55 – 9:20	**Benjamin von Ardenne** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Structure Determination from Few Photon Single Molecule X-Ray Scattering Experiments***
9:20 – 9:45	**Tatjana Braun** (Research Center of Jülich) ***Protein Structure Modelling using Cryo-EM Data***
9:45 – 10:10	**Mykola Dimura** (Heinrich Heine University of Düsseldorf) ***Toolkit for Multi-conformation Biomolecular Structure Determination by High-precision FRET and Molecular Simulations***
10:10 – 10:45	Coffee break
10:45 – 11:10	**Dirk Matthes** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***An Atomistic View of Amyloidogenic Self-assembly: Structure and Dynamics of Heterogenous Conformational States in the Pre-nucleation Phase***
11:10 – 11:35	**Angélica Sandoval-Perez** (Friedrich-Alexander University of Erlangen-Nürnberg, Erlangen) ***Comparison of Biomembrane Force Fields: Protein-Lipid interactions***
11:35 – 12:00	**Neha Awasthi** (Georg August University of Göttingen) ***Free Energies of Trans-Membrane Pore Formation: Reaction Coordinates and Effects of Peptides***
12:00 – 13:00	Lunch
13:00 – 13:25	**Gregory Bubnis** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Directing Membrane Pore and Stalk Formation in MD Simulations Using Embedded Mechanical Devices***
13:25 – 13:50	**Colin Smith** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Simulating Protein Motion by Incorporating Timescale Information from NMR Spectroscopy***
13:50 – 14:15	**Martin Carballo Pacheco** (Research Center Jülich and RWTH Aachen University) ***Comparison of Modern Force Fields for Protein Aggregation***
14:15 – 14:40	**Vladimir Palivec** (Academy of Sciences of the Czech Republic, Prague) ***Neurotransmitters Serotonin and Dopamine as Possible In Vivo Phenolic Ligands of Insulin Hexamer***
14:40 – 15:05	**Sebastian Buchenberg** (University of Freiburg) ***Signal Transport in Allosteric Proteins: From Nonequilibrium Simulations to Dynamic Networks***
15:05 – 15:20	Coffee break
15:20 – 15:45	**Jan Henning Peters** (Free University of Berlin) ***Adaptive Resolution Simulations of Polymer Chains***
15:45 – 16:10	**Aoife Fogarty** (Max Planck Institute for Polymer Research, Mainz) ***Including Atomistic Detail in the Active Site of Coarse-grained Enzyme Models***
16:10 – 16:35	**Luca Donati** (Free University of Berlin) ***Markov State Models with Reweighting***
16:35 – 17:00	**Alexander Götz** (Technical University of Munich, Freising) ***Multiscale Modeling of Transmembrane Domain Dynamics: From Normal Modes to Markov State Models***
17:00 – 17:30	Poster prize, final remarks
18:00	Dinner / Departure