

Monday 16.04

9:00-9:30 Registration

9:30-9:40 Welcome (Rebecca Wade)

Session 1 – Biological Diffusion – Experimental approaches

Chaired by Rebecca Wade (HITS, Heidelberg)

9:40 Gideon Schreiber (Weizmann, Israel) "Normal and Attenuated and Diffusion in the Cell and its effect on Activity"

10:20 Xavier Salvatella (IRB, Barcelona, Spain) "Insights from experiments and simulations into the possible roles of polyglutamine tracts in transcriptional activity"

11:00-11:20 **Coffee Break**

Chaired by Rebecca Wade (HITS, Heidelberg)

11:20 Robert Holyst (Warsaw, Poland) "Metabolism at the nanoscale in cells"

12:00 Poster presentations (3 mins x 20) (1 slides/3 mins per presenter, in the order in the abstract book)

13:00 **Group photo**

13:00-15:00 **Lunch and poster session**

Session 2 – New computational approaches

Chaired by Daria Kokh (HITS, Heidelberg)

15:00 Chia-en Chang (UC Riverside, USA) "Modeling of enhanced catalysis in multienzyme nanostructures: effect of molecular scaffolds, spatial organization, and concentration"

15:40 Maziar Heidari (MPI Polymer Research, Mainz) "Calculation of Solvation Free Energy using Hamilton Adaptive Resolution Simulations"

16:00 Gregor Weiss (Dzubiella Group, Helmholtz Zentrum Berlin, Germany) "Influence of water and charge fluctuations on ligand binding kinetics"

16:40-17:10 **Coffee Break**

Chaired by Gaurav Ganotra (HITS, Heidelberg)

17:10 Gary Huber (San Diego, USA) "Toward large-scale Brownian dynamics with bead models"

17:50 Max Linke (MPI Biophysics, Frankfurt, Germany) "Fully Anisotropic Rotational Diffusion Tensor from Simulations"

18:10 Mauricio del Razo S. (Freie Universität Berlin) "Stochastic Theory and Simulation of Diffusion-influenced Reactions in the Grand Canonical Ensemble"

18:30 Transportation to town

19:30 **Speakers Dinner - Wirtshaus zum Nepomuk**

Tuesday 17.04

Session 3 – Multiscale Simulation

Chaired by Neil Bruce (HITS, Heidelberg)

09:00 Rommie Amaro (UCSD, USA) "Molecular Simulation at the Mesoscale"

09:40 Sarah Harris (Leeds Univ, UK) "Computer Modelling of Biological Cryo-EM Data with Fluctuating Finite Element Analysis"

10:20 Giorgia Brancolini (CNR, Modena, Italy) "Modelling binding affinity for Protein-Nanoparticle co-engineering"

10:40 Kashif Sadiq (HITS, Germany) "Modelling protease-triggered HIV-1 infectivity using interaction particle-based reaction-diffusion (iPRD) simulations"

11:00-11:30 Coffee Break

Chaired by Kashif Sadiq (HITS, Heidelberg)

11:30 Art Olson (Scripps Research Institute, San Diego, USA) "Toward Whole Cell Mesoscale Models"

12:10 Neil Bruce (HITS, Heidelberg) "Efficient simulation of protein diffusion in crowded and confined solutions"

12:30 Introduction to software presentations (6 x 5 mins)

- Neil Bruce (HITS, Heidelberg) – SDA
- Moritz Hoffmann (Freie University, Berlin) – ReaDDy
- Jui-Hung Yuan (HITS, Heidelberg) – MolSurfer

These software presentations will have been introduced in talks before:

- Art Olson (Scripps) – CellPack & CellPAINT
- Sarah Harris (Univ. Leeds) – FFEA
- Gary Huber (UCSD) – Browndye

13:00-15:00 Lunch and software demos

Session 4 – Crowding

Chaired by Huan-Xiang Zhou (Florida State University)

15:00 Ralf Metzler (Potsdam, Germany) "Anomalous Diffusion in Membranes and Cytoplasm of Biological Cells"

15:40 Michael Feig (Michigan, USA) "Translational and Rotational Diffusion in Dense Protein Solutions"

16:20-16:40 Coffee Break

16:45 Transportation to town / walk via castle

19:00 Conference Dinner at the Vettters Brauhaus in the Altstadt

Wednesday 18.04

Session 5 – Cellular to multicellular diffusion

Chaired by Rommie Amaro (UCSD, USA)

9:00 Ulrich Schwarz (Bioquant, Heidelberg University, Germany) "Particle-based computer simulations of the bacterial Min-system"

9:40 Pieter Rein ten Wolde (Amsterdam University, Netherlands) "Combining Molecular Dynamics with mesoscopic Green's Function Reaction Dynamics"

10:20 Marc Joyeux (Grenoble, France) "Role of salt valency in the switch of H-NS proteins between DNA-bridging and DNA stiffening modes"

10:40 Sutapa Dutta (S.N. Bose National Center for Basic Science) "Anomalous dynamics of metal ions in presence of a bacterial protein"

11:00-11:30 Coffee Break and Poster Session/Software Demos

Session 6 – IDPs

Chaired by Ulrich Schwarz (Heidelberg University)

11:30 Huan-Xiang Zhou (Florida State University) "Rate constants and mechanisms of intrinsically disordered proteins binding to structured targets"

12:10 Fan Jin (HITS, Heidelberg) "How does phosphorylation affect intrinsically disordered proteins"

12:30 Fereydoon Taheri (DKFZ, Heidelberg) "Chromatin dynamics are governed by random motion and controlled by lamin A interconnections"

12:50-14:20 Lunch and poster sessions

Session 7 – Back to experiments

Chaired by Rebecca Wade (HITS, Heidelberg)

14:20 Jonas Ries (EMBL, Heidelberg) "High-throughput super resolution microscopy of endocytosis - linking molecular architecture and mechanics of a protein machinery"

15:00 Christian Eggeling (Oxford, UK) "New insights into molecular membrane dynamics from super-resolution microscopy"

15:40-16:00 Final discussion

16:00-16:30 Coffee Break and Departure