



Fourth Biological Diffusion and Brownian Dynamics Brainstorm Meeting April 16-18, 2018

Program

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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 Jonas Ries (EMBL, Heidelberg) High-throughput super resolution microscopy of endocytosis - linking molecular architecture and mechanics of a protein machinery
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)
13:00 Group photo
13:00-15:00 Lunch and poster session

Session 2 - New computational approaches

Chaired by Gaurav Ganotra (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)
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



Want to contact us?

If you have any question or want to contact us, please send us a note:

bdbdb@h-its.org



Chaired by Ulrich Schwarz (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)
- 11:00-11:30** Coffee Break
- 11:30** Art Olson (Scripps Research Institute, San Diego, USA) Toward Whole Cell Mesoscale Models
- 12:10** Neil Bruce (HITS, Heidelberg)
- 12:30** Introduction to software presentations (6 x 5 mins)
- 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)
- 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** Neil Bruce (HITS, Heidelberg)

- 11:30** Huan-Xiang Zhou (Florida State University) Rate constants and mechanisms of intrinsically disordered proteins binding to structured targets
- 12:10** Xavier Salvatella (IRB, Barcelona, Spain) Insights from experiments and simulations into the possible roles of polyglutamine tracts in transcriptional activity
- 12:30** Fan Jin (HITS, Heidelberg) How does phosphorylation affect intrinsically disordered proteins
- 12:50-14:30** Lunch and poster sessions

Session 7 - Back to experiments**Chaired by** Rebecca Wade (HITS, Heidelberg)

- 14:30** Fereydoon Taheri (DKFZ, Heidelberg) Chromatin dynamics are governed by random motion and controlled by lamin A interconnections

- 14:50** Christian Eggeling (Oxford, UK) New insights into molecular membrane dynamics from super-resolution microscopy
- 15:30-16:00** Final discussion
- 16:00-16:30** Coffee Break and Departure