

Monday 11 October 2010**10.30 – 10.50 Registration and Coffee**10.50 – 11.00 Andreas Reuter and Rebecca Wade - **Welcome**

11.00 Session 1a - [Chaired by Rebecca Wade]

- Gary Pielak - *Slides*: Effects of proteins on protein diffusion, *Poster*: -, Recording
- Jörg Langowski - *Slides*: Multiscale Modeling of Chromatin Dynamics, *Poster*: Mobility of proteins in the chromatin network, Recording
- Martin Held - *Slides*: Mechanisms of protein-ligand association and its modulation by protein mutations, *Poster*: -, Recording

13.00 Group photo**13.00 – 14.00 Lunch**

14.00 Session 2a - [Chaired by Jörg Langowski]

- James Weisshaar - *Slides*: Protein Diffusion in Live E. coli, *Poster*: Protein Diffusion in Live E. coli, Recording
- Johannes Seibert - *Slides*: Spatiotemporal model of particle diffusion in the primary rod vision signal transduction, *Poster*: Spatiotemporal model of particle diffusion in the primary rod vision signal transduction, Recording

15.00 – 15.45 Poster Session**15.45 – 16.15 Coffee Break**

16.15 Session 2b - [Chaired by Jörg Langowski]

- Matthias Weiss - *Slides*: Crowding and anomalous diffusion in vivo, in vitro, and in silico, *Poster*: -, Recording
- Yossi Klafter - *Slides*: -, *Poster*: -, Recording

18.00 Session 3b - **Video conference session** - [Chaired by Rebecca Wade]

- J. Andrew McCammon - *Slides*: Gated diffusional binding of ligands to proteins, *Poster*: -, Recording
- Adrian Elcock - *Slides*: Large-scale Brownian Dynamics Simulations of the Cytoplasm, *Poster*: -, Recording
- Poster presentations
 - Mykhaylo Berynskyy *Slides*: -, *Poster*: Analysis Tool for Brownian Dynamics Simulations
 - Stefan Richter *Slides*: -, *Poster*: Simulation of Diffusional Association (SDA) Software Release 6
 - Anna Feldman-Salit *Slides*: -, *Poster*: Structure determination by Brownian dynamics simulation: the Cysteine Synthase complex
 - Pawel Zielinski - *Slides*: -, *Poster*: Dealing with hydrodynamics in Brownian dynamics simulations CPU vs. GPU
 - Peter Kekenyes-Huskey - *Slides*: -, *Poster*: Multiscale modeling in rabbit ventricular myocytes

- Martin Kenward - *Slides*: -, *Poster*: Twist propagation in nucleosome arrays: A Monte Carlo and Brownian Dynamics study
- Balaji Vaidyanathan - *Slides*: -, *Poster*: Role of Chromatin Remodeling and Associated Flexibility Modifications on Gene Expression

20.00 – 21.00 **Dinner**

Tuesday 12 October 2010

09.00 Session 3a - [Chaired by Matthias Weiss]

- Maxim Petoukhov - *Slides*: Modern methods for solution scattering data analysis from biological macromolecules, *Poster*: -, Recording
- Gideon Schreiber - *Slides*: Transient complexes along the association reaction of proteins in solution and in the crowd, *Poster*: -, Recording

10.30 – 11.00 **Coffee Break**

11.00 Session 3b - [Chaired by Matthias Weiss]

- Johan Elf - *Slides*: Probing Intracellular Kinetics at the level of Single Molecule, *Poster*: -, Recording
- Daria Kokh - *Slides*: Brownian dynamics simulation of protein binding to solid surfaces, *Poster*: *Brownian Dynamics simulation of protein binding to solid state surfaces* -, Recording
- Maciej Dlugosz - *Slides*: From single molecules to dense biomolecular systems - Brownian dynamics simulations with the BD_BOX package, *Poster*: -, Recording

13.00 – 14.00 **Packed lunch**

14.30 – 15.30 **Guided Excursion to the Castle**

17.30 – 18.00 **Coffee Break**

18.00 Session 4a - **Video conference session** - [Chaired by Paolo Mereghetti]

- Gary Huber - *Slides*: Recent and future developments in the Browndye package, *Poster*: -, Recording
- Joanna Trylska - *Slides*: On the structure and aggregation of N-terminal Huntingtin fragments, *Poster*: -, Recording
- Barry Grant - *Slides*: Electrostatically biased binding of kinesin to microtubules, *Poster*: -, Recording
- Patricia Bauler - *Slides*: Channeling by Proximity; The Catalytic Advantages of Active Site Colocalization Using Brownian Dynamics, *Poster*: -, Recording

20.00 – 21.00 **Dinner**

Wednesday 12 October 2010

09.30 Session 5a - [Chaired by Daria Kokh]

- Gerhard Naegele - *Slides*: Dynamics in concentrated dispersions of colloids and biomolecules: Theory, simulation and experiment, *Poster*: -, Recording

- Paolo Mereghetti - *Slides*: Brownian Dynamics Simulations of Protein Solutions, *Poster*: Brownian Dynamics Simulations of Protein Solutions, Recording

10.30 – 11.00 **Coffee Break**

11.00 Session 5b

- Jose Garcia de la Torre - *Slides*: Recent advances and applications in the prediction of dilute-solution properties of macromolecules and nanoparticles: hydrodynamic calculations and Brownian dynamics simulation, *Poster*: -, Recording
- Tihamer Geyer - *Slides*: Coarse-Grained Simulations of a Small Peptide: Effects of Finite Damping and Hydrodynamic Interactions, *Poster*: Graph Measures Reveal Fine Structure of Complexes Forming in Multi-Particle Simulations, Recording
- Elfriede Friedmann - *Slides*: Spatio-temporal simulations of the JAK2/STAT5 pathway in CFU-E and NIH3T3 cells, *Poster*: Spatio-temporal simulations of the JAK2/STAT5 pathway in CFU-E and NIH3T3 cells, Recording

13.00 – 14.00 **Lunch**

14.30 – 15.30 **Excursion to the Carl Bosch Museum**

16.00 – 16.30 **Coffee Break**

16.45 Session 6a - [Chaired by –]

- Yuji C. Sasaki - *Slides*: High-speed Observations of Intramolecular Brownian motions on Functional Proteins using X-rays and Electrons, *Poster*: yuji_c._sasaki.pdf, Recording
- Huan-Xiang Zhou - *Slides*: Theory and Simulation of Diffusion-Influenced Bimolecular Reactions, *Poster*: -, Recording

18.00 Session 6b - **Video conference session** - [Chaired by Rebecca Wade]

- Olga Dudko - *Slides*: Biomolecules under mechanical stress: New insights from the hopping-over-a-barrier problem , *Poster*: -, Recording
- Joanna Sulkowska - *Slides*: Tightening of knots in proteins, *Poster*: -, Recording
- Gaurav Arya - *Slides*: Using force to interrogate single molecules, *Poster*: -, Recording
- Johan Hake - *Slides*: Modeling of Ca dynamics in the dyadic cleft: Mixing continuous description of the diffusive process with discrete channel dynamics, *Poster*: -, Recording

19.30 – 20.00 **Round Table**

20.00 – 21.00 **Dinner**

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