

3rd Status Symposium on New trends in simulating biological systems and soft matter

Seminaris SeeHotel Potsdam
February 22nd to 24th, 2012

Wednesday, February 22

Registration and Lunch (12:00 – 1:45 pm)

1:45 – 2:00 **Dr. Wilhelm Krull** (Volkswagen Stiftung, Hannover)
Opening remarks

Session 1 (2:00 pm – 3:45 pm): Simulations of biomolecular systems

2:00 – 2:45 **Charles L. Brooks** (University of Michigan, Ann Arbor)
Multi-scale explorations of virus maturation dynamics and mechanics

2:45 – 3:05 **Markus Miettinen** (Universität Potsdam)
Kinetic stabilities of suggested polyglutamine aggregation initiating conformers

3:05 – 3:25 **Ilpo Vattulainen** (Tampere University of Technology)
Cholesteryl ester transfer protein interacting with lipoproteins and anacetrapib

3:25 – 3:45 **Christoph Globisch/Venky Krishnamani**
(Max-Planck-Institut für Polymerforschung, Mainz/Carnegie Mellon University, Pittsburgh)
Atomistic and coarse grained simulations of viral capsids

Coffee break

Session 2 (4:15 pm – 6:00 pm): Simulations of soft matter I

4:15 – 5:00 **Ard Louis** (Oxford University)
Coarse-grained model for self-assembling DNA

5:00 – 5:20 **Ernst-Walter Knapp** (Freie Universität Berlin)
Influence of Spacer-Receptor Interactions on the Stability of Bivalent Ligand-Receptor Complexes

5:20 – 5:40 **Agur Sevink** (Universiteit Leiden)
A hybrid method for efficiently modeling lipid membranes with molecular resolution

5:40 – 6:00 **Jonathan James Ward** (European Molecular Biology Laboratory, Heidelberg)
Physical principals underlying the morphogenesis of the fission yeast spindle

Buffet and Poster Session (6:15 pm – late)

Thursday mornings, February 23

Breakfast

Session 3 (9:00 am – 10:25 am): Modeling of active systems I

9:00 – 9:45 Lev Tsimring (University of California, San Diego)

Ordering and instabilities in dense bacterial populations

9:45 – 10:05 Johannes Baumgart (Max-Planck-Institute for the Physics of Complex Systems, Dresden)

Modeling the Fluid-Structure Interaction of the Hair Bundle

10:05 – 10:25 Wolfgang Alt (Universität Bonn)

Coupling of cytoplasm flow dynamics and membrane protein kinetics drives adhesive cell locomotion and interaction

Coffee break

Session 4 (11:00 am – 12:45 pm): Modeling of active systems II

11:00 – 11:45 Martin Falcke (Max-Delbrück-Center for Molecular Medicine, Berlin)

Actin filament elasticity and retrograde flow shape the force-velocity relation of motile cells

11:45 – 12:05 Roland G. Winkler (Forschungszentrum Jülich)

Swimming of Bacteria: Synchronization and Bundling of Flagella

12:05 – 12:25 Holger Stark, Reinhard Vogel (Technische Universität Berlin)

Modeling the Motor-Driven Bacterial Flagellum

Lunch

Thursday afternoon, February 23

Lunch

Session 5 (2:00 pm – 3:25 pm): Transport through nanopores and in confined geometries

2:00 – 2:45 Murugappan Muthukumar (University of Massachusetts, Amherst)

How DNA worms through protein channels and nanopores

2:45 – 3:05 Steffen Martens (Humboldt-Universität Berlin)

Biased and flow driven Brownian motion in periodic channels

3:05 – 3:25 Gerhard Schmid (Universität Augsburg)

Entropic Splitter

Coffee break

Session 6 (3:55 pm – 6:15 pm): Modeling of enzymatic reactions and QM/MM

3:55 – 4:40 Rich A. Friesner (Columbia University, New York)

DFT-LOC methods applied to metal-containing system

4:40 – 5:00 Biswaroop Mukherjee / Nikos Doltsinis

(Max Planck Institut für Polymerforschung, Mainz / Universität Münster)

Multiscale modelling of photoactive liquid crystals: from quantum to coarse grained

5:00 – 5:20 Bernd Engels (Universität Würzburg)

New approaches for efficient simulation of complex soft matter

Coffee break

5:35 – 5:55 Christian Ochsenfeld (Ludwig-Maximilians-Universität München)

Efficient Quantum-Chemical Schemes for Scanning Potential Energy Landscapes in Complex Systems

5:55 – 6:15 Walter Thiel (Max-Planck-Institut für Kohlenforschung, Mülheim)

Semiempirical QM/MM excited-state dynamics

6:20 pm: Bus departure to Krongut Bornstedt, Conference Dinner

Friday, February 24

Breakfast

Session 7 (9:00 am – 10:45 am): Simulations of soft matter II

9:00 – 9:45 Sabine Klapp (Technische Universität Berlin)

Dynamics of ferrofluids in external fields: Chaining, layering, and anomalous diffusion

9:45 – 10:05 Ulf D. Schiller (Forschungszentrum Jülich)

Modeling red blood cells as a liquid crystalline elastic membrane: insights into equilibrium shape and remaining elastic strains

10:05 – 10:25 Jasna Zelko (Max Planck Institut fuer Polymerforschung, Mainz)

Towards a New Algorithm for Multiphase Lattice Boltzmann Simulations

10:25 – 10:45 Owen A. Hickey (Universität Stuttgart)

Implicit method for the electrohydrodynamics of polyelectrolytes using Lattice-Boltzmann

Coffee break

Session 8 (11:15 am – 13:00 pm): Biomatter in nonequilibrium

11:15 – 12:00 Stefan Klumpp (Max Planck Institut für Kolloid und Grenzflächenforschung, Potsdam)

Tug-of-war: Mechanical coordination of biomolecular motors

12:00 – 12:45 Roland Netz (Freie Universität Berlin)

Simulation approaches to friction in biomatter

12:45 – 13:00 Closing remarks

Lunch (Lunch packages are available) and Departure

Poster Session

Please put up your poster before the poster session.

Wednesday, February 22, starts 6:15 pm – late

Poster 1

C. Seitz, K. Kopp, I. Antes (Technische Universität München)

Efficient sampling of conformational changes in proteins induced by peptide binding

Poster 2

Michele Campisi (Universität Augsburg)

Quantum Fluctuation Relations

Poster 3

Cristiano L. Dias, Hue Sun Chan (University of Toronto)

Pressure dependence of hydrophobic interactions

Poster 4

Denis Flaig, Matthias Beer, Christian Ochsenfeld (Ludwig-Maximilians-Universität München)

Describing Dynamic Molecular Systems by Nuclei-Selected NMR Shieldings within Linear- and Sublinear-Scaling QM and M/MM Approaches

Poster 5

Nikos Doltsinis, Marcus Böckmann, Dominik Marx, Biswaroop Mukherjee, Luigi Delle Site, Christine Peter, Kurt Kremer (Universität Münster)

Multiscale modelling of photoactive liquid crystals I: from quantum to classical

Poster 6

Stephan Gekle (Technische Universität München)

Dielectric spectrum of interfacial water

Poster 7

Jan Philipp Götze, Mario Silva-Junior, Walter Thiel (MPI für Kohlenforschung, Mülheim an der Ruhr)

The N5•••H excited state decay channel of 1-deaza-flavin depends on rotational orientation of the donor water molecule

Poster 8

Z. Jurek, R. Thiele, B. Ziaja, R. Santra (Deutsches Elektronen-Synchrotron, Hamburg)

Effect of two-particle correlations on x-ray coherent diffractive imaging studies performed with continuum models

Poster 9

Stefan Kesselheim, Christian Holm (Universität Stuttgart)

Lattice Boltzmann Simulations of Electrokinetic Phenomena with explicit Ions

Poster 10

Rong-Zhen Liao, Walter Thiel (MPI für Kohlenforschung, Mülheim an der Ruhr)

Comparison of QM-only and QM/MM Models for the Mechanism of Tungsten-Dependent Acetylene hydratase



Poster 11

P. K. Ghosh, P. Hänggi, F. Marchesoni, Steffen Martens, F. Nori, L. Schimansky-Geier, G. Schmid (Humboldt Universität Berlin)

Driven Brownian transport through arrays of symmetric obstacles

Poster 12

Tim Meyer, Ernst Walter Knapp (Freie Universität Berlin)

Database of multivalent receptors (MVR-DB) deduced from the database of protein structures

Poster 13

Markus Miettinen, Volker Knecht, Luca Monticelli and Zoya Ignatova (Universität Potsdam)

Kinetic stabilities of suggested polyglutamine aggregation initiating conformers

Poster 14

Biswaroop Mukherjee, Luigi Delle Site, Christine Peter, Kurt Kremer, Marcus Böckmann, Dominik Marx, Nikos Doltsinis (Max Planck Institut für Polymerforschung, Mainz)

Multiscale modelling of photoactive liquid crystals II: from atomistic to coarse grained

Poster 15

Jorge Numata, Alok Juneja, Ernst-Walter Knapp (Freie Universität Berlin)

Balanced and bias-free computation of conformational entropy differences for molecular trajectories

Poster 16

Iakov Polyak, Manfred T. Reetz, Walter Thiel (MPI für Kohlenforschung, Mülheim an der Ruhr)

QM/MM Study on the Mechanism of the Enzymatic Baeyer-Villiger Reaction

Poster 17

Shervin Raafatnia (Universität Stuttgart)

Colloidal electrophoretic mobility in the presence of multivalent salt

Poster 18

Ilkay Sakalli, Elankumaran. K, Joachim-Schöberl, Ernst Walter Knapp (Freie Universität Berlin)

Calculation of pKa values and solving the Poisson equation using the Finite Element Method

Poster 19

Kakali Sen, Walter Thiel (MPI für Kohlenforschung, Mülheim an der Ruhr)

Investigation of Molecular Oxygen Activation in P450eryF using hybrid QM/MM methodology

Poster 20

Jiajia Zhou, Aleksey V. Belyaev, Olga I. Vinogradova, Friederike Schmid (Johannes Gutenberg-Universität Mainz)

Pressure-driven flow through a channel with symmetric striped-pattern

Poster 21

Manuela Mura, Andrei V Zvelindovsky (University of Central Lancashire, Preston)

Modelling of aurein 2.3 in a biomembrane