DVR 0065528

ESI/CECAM Workshop on

"Challenges across Large-Scale Biomolecular and Polymer Simulations"

February 21 – 24, 2017

organized by

Ivan Coluzza (U Vienna), Barbara Capone (U Vienna), Christoph Dellago (ESI, U Vienna), Samuela Pasquali (IBPC & U Paris), Tamar Schlick (New York U)

- **Tuesday, February 21, 2017**
  Session 1

  13:00 – 14:30 *Registration*

  14:30 – 15:00 **Tamar Schlick**
  In Memoriam: Klaus Schulten

  15:00 – 15:30 **Gerhard Hummer**
  Modeling Membrane Sensing and Remodeling Dynamics

  15:30 – 16:00 **Angel Garcia**
  Free-energy landscape of a hyperstable RNA tetraloop

  16:00 – 16:30 *Coffee Break*

  16:30 – 17:00 **Samuela Pasquali**
  Predicting and Exploring Complex Nucleic Acids Architectures through a Coarse-Grained Model

  17:00 – 17:30 **Angelo Rosa**
  Chromosome organization and the Physics of crumpled polymers

  17:30 – 18:00 **Jonathan Doye**
  Large-scale DNA simulations with oxDNA

- **Wednesday, February 22, 2017**
  Session 2

  09:00 – 09:30 **Doros Theodorou**
  Multiscale Molecular Simulations of Polymer-Matrix Nanocomposites

  09:30 – 10:00 **Barbara Capone**
  Multiscale Coarse Graining of Polymer Solutions

  10:00 – 10:30 **Pietro Faccioli**
  Self-Consistent Atomistic Calculation of Protein Folding Pathways

  10:30 – 11:00 *Coffee Break*

11:00 – 11:30 **Raffaello Potestio**
Multi-resolution modelling for biomolecular simulations

11:30 – 12:00 **Cristian Micheletti**
Pore translocation of knotted polymer chains: how friction depends on knot complexity

12:00 – 12:30 **Karissa Sanbonmatsu**
Simulating movement of the 30S head during translocation

12:30 – 14:30 *Lunch Break*

Session 3

14:30 – 15:00 **Peter Bolhuis**
Multiscale Simulations of Patchy Particle Systems Combining Molecular Dynamics, Path Sampling and Greens Function Reaction Dynamics

15:00 – 15:30 **Dave Thirumalai**
Understanding RNA folding

15:30 – 16:00 **Marc Baaden**
Large-scale Data Exploration and Analysis across Biomolecular Simulations

16:00 – 16:30 *Coffee Break*

16:30 – 17:00 **Bert de Groot**
Challenges and opportunities in large scale alchemical free energy simulations.

17:00 – 17:30 **Wonpil Im**
CHARMM-GUI Toward Large-Scale Biomolecular and Polymer Simulations

19:30 *Social Dinner*

- **Thursday, February 23, 2017**
  Session 4

  09:00 – 09:30 **Gianluca Lattanzi**
  Challenges in computational biophysics: from membrane proteins to biosensors

  09:30 – 10:00 **Peter Freddolino**
  Modeling Protein-Nucleic Acid Interactions from Atomistic to Cellular Scales

  10:00 – 10:30 **Modesto Orozco**
  Advances and challenges in the simulation of DNA

  10:30 – 11:00 *Coffee Break*

  11:00 – 11:30 **Michele Vendruscolo**
  Structural basis for the different aggregation propensities of Abeta40 and Abeta42

  11:30 – 12:00 **Chris Oostenbrink**
  Reversible guest-host interactions from extensive simulations

  12:00 – 12:30 **Ron Elber**
  Electric Fields Across Heterogeneous Membranes

  12:30 – 14:30 *Lunch Break*

Session 5

14:30 – 15:00 **Ivan Coluzza**
Artificial Chaperonins

15:00 – 15:15 **Ewa Anna Oprzeska-Zingrebe**
Interactions Between a Short DNA Oligonucleotide and Urea in the Light of Kirkwood-Buff Theory: a Molecular Dynamics Simulation Study

15:15 – 15:30 **Martin Goethe**
Prediction of Protein Configurational Entropy (Popcoen)

15:30 – 16:00 **Lennart Nilsson**
Codon Recognition on the Ribosome - Free Energy and QM/M Calculations

16:00 – 16:30 *Coffee Break*

16:30 – 17:00 **Helmut Grubmüller**
Atomistic Simulation of Single Molecule Experiments: Molecular Machines and a Dynasome Perspective

17:00 – 17:30 **Jeremy C. Smith**
Proteins: Forever Aging

- **Friday, February 24, 2017**
  Session 6

09:00 – 09:30 **Simone Melchionna**
Macromolecules and hydrodynamics: a simulation approach

09:30 – 10:00 **Yassmine Chebaro**
Role of intrinsically disordered regions in the nuclear receptors architecture

10:00 – 10:30 **Sarah Harris**
Multiscale Modelling of Biomolecules: From atomistic Molecular Dynamics to the continuum limit with Fluctuating Finite Element Analysis

10:30 – 11:00 *Coffee Break*

11:00 – 11:30 **Amir Lohrasebi**
The influence of a 2450 MHz electric field on the microtubule mechanical properties: a multi scale modeling approach

11:30 – 12:00 **Othmar Steinhauser**
Protein in Reverse Micelles - The Dielectric Approach

12:00 – 12:30 **Stefan Boresch**
Playing the Devil's Advocate: Some Challenges with Respect to Large-scale Biomolecular Simulations

12:30 – 13:00 **Summary & Conclusions**

The workshop will take place in the Joseph Loschmidt Hörsaal at the Faculty of Chemistry, University of Vienna, Währinger Str. 42, 1090 Vienna!