

Moscow State University, Faculty of Physics

Theory and Computer Simulation of Polymers: New Developments

International Workshop

May 31 – June 6, 2010, Moscow, Russia

Second Announcement

1 Motivation and objectives

This workshop takes place within the framework of a long-standing collaboration between the groups of Prof. A. Khokhlov at the Faculty of Physics of Moscow State University and Prof. K. Binder at the Institute of Physics of Johannes-Gutenberg-University of Mainz which is supported by DFG and RFBR grants (at the present time it is the joint project DFG 436 RUS 113/791 and RFBR 09-03-91339-NNIO, and this meeting is a planned activity within this joint project).

The main goal of the meeting is the discussion of the current stage of this project which is dedicated to computer simulations of stiff-chain macromolecules and other liquid-crystalline systems at adsorbing surfaces and in confinements. However, this does not restrict the topics to be discussed during the workshop. The meeting will also offer a unique opportunity for the discussion of related research on macromolecular systems, like, for example, the properties of copolymer systems. It is also our aim that this conference provides a broad exchange of ideas and experience between scientists from different countries working in the field of theory and computer simulation of macromolecular systems. This meeting should be also beneficial from the educational viewpoint for the students and PhD students working in the area of polymers. The participation in the conference is not restricted to the members of the above mentioned research groups.

This workshop is already the third one initiated by the collaboration of groups in Mainz and Moscow. Two previous workshops took place in 2002 and 2006 - "Computer Simulations of Macromolecular Systems: Dense States of Semiflexible Macromolecules and Copolymers" (May 21-26, 2002, Moscow, Russia) and "Statistical Mechanics of Polymers: New Developments" (June 6-11, 2006, Moscow, Russia).

2 Organization

2.1 Organizers

- Faculty of Physics, Moscow State University (Moscow, Russia)
- Institute of Physics, Johannes Gutenberg-University (Mainz, Germany)

2.2 Organizing Committee

Alexei Khokhlov (Chairman), Kurt Binder (Co-Chairman), Victor Ivanov, Friederike Schmid, Wolfgang Paul, Julia Martemyanova (Scientific Secretary)

2.3 Language

English is the official language of the meeting.

2.4 Location and accommodation

The oral presentations of the meeting will be held in the conference hall at the Physics Department of Moscow State University. Posters will be placed in the corridor in front of this room.

The hotel in the main building of Moscow State University is planned for the accommodation of participants (or one of the hotels in the vicinity of MSU).

2.5 Schedule

The arrival of participants is planned for May 31, and the lectures will start on June 1 in the morning, and will end on June 5 at lunchtime.

The oral presentations are planned for 30 minutes (20 min. talk + 10 min. for questions and discussion) to provide a workshop atmosphere with sufficient time for a detailed discussion of the contributions. There are also shorter oral presentations planned for 20 min. each (15 min. talk + 5 min. discussion). The poster session is planned for the presentations of the results of PhD students and students.

2.6 Budget

To cover the administrative expenses (coffee breaks, consumable) a conference fee of EUR 120,- per person will be charged (reduced fee is possible for participants from Russia). Additionally, the flat sum of EUR 80,- per person will be charged for lunches.

The workshop is financially supported by:

- *Deutsche Forschungsgemeinschaft* within the project "Computer Simulation of Adsorption of Semiflexible Polymers" DFG 436 RUS 113/791 (travel expenses and accommodation of project participants, conference fee, lunches);
- *Russian Foundation for Basic Research* (travel expenses and accommodation of Russian participants from outside Moscow, conference fee, lunches; if we will succeed to get additional support from RFBR for organizing international workshops, which we will apply for, also travel expenses of more participants from abroad can be covered).

3 Tentative List of Participants

The preliminary titles of the talks and posters, which are already known, are also indicated.

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Oral presentations

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1) Allahyarov E. (Cleveland, Duesseldorf, Moscow), "Nanocomposite ionomer membranes with directed proton conductivity"

- 2) Andrienko D. (Mainz, Germany), the title will be either "Versatile Object-Oriented Toolkit for Coarse-graining Applications: theory and implementation" or "Multiscale description of charge transport in conjugated polymers"
- 3) Arnold A. (Stuttgart, Germany), "Flexible polymers in confinement: how can bacteria segregate their DNA?"
- 4) Avetisov V. (Moscow, Russia), "Ultrametric diffusion approach to multi-scale modeling of fluctuation-induced protein mobility"
- 5) Bachmann M. (Juelich, Germany), "Statistical analyses of conformational transitions for small polymers"
- 6) Binder K. (Mainz, Germany), "Local intrinsic stiffness of real polymer chains - how can meaningful estimates of a persistence length be extracted from simulations or experiments"
- 7) Birshstein T. (St.Petersburg, Russia), "Core - crown conformations in polyelectrolyte stars"
- 8) Borisov O. (Pau, France), "Poisson-Boltzmann theory of weak polyelectrolyte brushes"
- 9) Briels W.J. (Twente, The Netherlands), "Can single particle models describe the dynamics of polymer melts and solutions?"
- 10) Chertovich A. (Moscow, Russia), "DPD simulations of copolymer melts"
- 11) Daoulas K. (Goettingen, Germany), "Structure formation in supramolecular copolymers: a DFT-based Monte Carlo approach"
- 12) Darinskii A. (St.Petersburg, Russia), "Microstructure of complexes formed by charged bottle-brushes and linear polyelectrolytes: Computer simulation"
- 13) Egorov S. (Virginia, USA; Mainz, Germany), "Simulation and Density Functional Theory Study of Adsorption/Expulsion of Short Chain Oligomers to/from a Polymer Brush"
- 14) Erukhimovich I. (Moscow, Russia), "On the microscopic theory of microphase separation in two-component bottle brushes"
- 15) Everaers R. (Lyon, France), "A semi-quantitative lattice model for RNA and DNA association, folding and melting"
- 16) Frey E. (Muenchen, Germany), "Conformation and Dynamics of Semiflexible Polymers"
- 17) Govorun E. (Moscow, Russia), "Slow mode in the dynamics of polymer solutions"
- 18) Grosberg A. (New York, USA), "Large scale structure of chromatin" or "DNA capture into a nanopore"
- 19) Hsu H.-P. (Mainz, Germany), "Structure Analysis of Molecular Bottle-brushes in a good solvent: Simulation and Experiment"
- 20) Huang C.-C. (Juelich, Germany), "Mesoscale Simulation of Semidilute Polymer Solutions"
- 21) Ivanov V. (Moscow, Russia), "Computer simulations of phase behavior of solutions of semiflexible macromolecules in a thin film confinement"
- 22) Johner A. (Strasbourg, France), "Dense polymer solutions confined to capillaries"
- 23) Khalatur P. (Tver, Russia), "Large-scale atomistic simulation of a nanosized fibril formed by thiophene-peptide "molecular chimeras"
- 24) Khokhlov A. (Moscow, Russia), "Polymer Nanocomposites: Theory and Computer Simulations"
- 25) Komarov P. (Tver, Russia), "Structure and Temperature Properties of Nanocomposites Based on PI/SiO₂: Atomistic modeling"
- 26) Kramarenko E. (Moscow, Russia), "Micelles with ion-containing cores"
- 27) Krupyanskii Yu. (Moscow, Russia), "Folding of Lysozyme-Like Copolymer at the Presence of Chemical Chaperone TMAO"
- 28) Kuchanov S. (Moscow, Russia), "New trends in the Weak Segregation Limit (WSL) theory of loopless copolymers"
- 29) Kudryavtsev Ya. (Moscow, Russia), "Effects of polydispersity in the dynamics of polymer blends"

- 30) A. Likhtman (Reading, UK), "Microscopic definition of entanglement in polymer melts in equilibrium and in flow"
- 31) Lyulin S. (St.Petersburg, Russia), "Simulation of Hyperbranched polymers in complexes with linear polyelectrolytes"
- 32) Lobaskin V. (Dublin, Ireland), "Modelling of polymer dynamics under shear"
- 33) Mavrantzas V. (Patras, Greece), "Quantifying chain reptation in entangled polymer melts: Topological and dynamical mapping of atomistic simulation results onto the tube model"
- 34) Merkurieva A. (St.Petersburg, Russia), "Conformations of polymer stars combining hydrophobic and hydrophilic features"
- 35) Merlitz H. (Xiamen, China), "Surface modification through switchable polymer brushes: A Molecular dynamics study"
- 36) Messina R. (Duesseldorf, Germany), tba
- 37) Meyer H. (Strasbourg, France), "Static and Dynamic Bond-Correlations in Entangled Bead-Spring Melts"
- 38) Milchev A. (Sofia, Bulgaria), "Breaking and Healing of a Polymer Chain under Tension: Theory and Computer Experiment"
- 39) Mueller M. (Goettingen, Germany), "Measuring free energies of self-assembled structures by computer simulation"
- 40) Mueser M. (Saarbruecken, Germany), "The role of geometry and chemical detail for slip boundary condition of polymers near adhesive walls"
- 41) Neelov I. (St.Petersburg, Russia), "Computer simulation of dendrimer-peptide interactions"
- 42) Obukhov S. (Florida, USA), "Nanoscale two velocity hydrodynamics of polymer melt"
- 43) Oettel M. (Mainz, Germany), "Density Functional Theory for hard colloids: Some aspects of freezing and depletion effects"
- 44) Paul W. (Halle, Germany), "Protein Thermodynamics of a Homopolymer Chain"
- 45) Polotsky A. (St.Petersburg, Russia), "Mechanical unfolding of a homopolymer globule: theory and self-consistent field modeling"
- 46) Potemkin I. (Moscow, Russia), "Designed AB copolymers as efficient stabilizers of colloidal particles"
- 47) Rabinovich A. (Petrozavodsk, Russia), "Structure and properties of polyunsaturated phosphatidylcholine bilayers: molecular dynamics simulation"
- 48) Rostiashvili V. (Mainz, Germany), "Pulling an adsorbed polymer from a surface: Theory and Computer Simulation"
- 49) Schilling T. (Luxemburg), "Computing absolute free energies of disordered structures by molecular simulation"
- 50) Schmid F. (Mainz, Germany), "Coarse-grained simulations of molecular transport in microchannels"
- 51) Semenov A. (Strasbourg, France), "Theory of long-range correlations in glass-forming polymer liquids"
- 52) Severin N. (Berlin, Germany), "Rupture of DNA molecules under tensile stress"
- 53) Shchur L. (Moscow, Russia), "Fractal dimension of critical interfaces and Duplantier' duality"
- 54) Skvortsov A. (St.Petersburg, Russia), "Analytical Theory of Finite-Size Effects in Mechanical Desorption of a Single Chain"
- 55) Sommer J.-U. (Dresden, Germany), "Theory and simulation studies of order parameters in dry and swollen polymer networks"
- 56) Stepanow S. (Halle, Germany), "Dynamics of a Gaussian polymer with fixed end-to-end distance"
- 57) Subbotin A. (Moscow, Russia), "Bending elasticity of 2D molecular bottle-brush"

- 58) Theodorou D. (Athene, Greece), "Simulation strategies for addressing the long-time properties of polymer melts and glasses"
- 59) Timoshenko E. (Dublin, Ireland), "Structural transitions in self-assembly of rationally designed oligopeptides"
- 60) Vasilevskaya V. (Moscow, Russia), "Self-organization of amphiphilic macromolecules"
- 61) Villet M. (Santa Barbara, USA), "Beyond Mean Field: New Tools for Field-Theoretic Simulation"
- 62) Virnau P. (Mainz, Germany), "Entanglements in globular polymer phases"
- 63) Winkler R. (Juelich, Germany), "Mesoscale hydrodynamic simulations of polymers in external fields"
- 64) Zheligovskaya E. (Moscow, Russia), "The Role of the Surface Layer of Water in Self-Organization of Polymer Systems"

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Posters (short list; more posters will be presented by Russian students and PhD students)
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- 1) Nagpal U. (Madison, USA), "Coarse grained Monte Carlo simulations for directed assembly for block copolymers"
- 2) Berezovska G. (Freiburg, Germany), "Monte Carlo Study of Semiflexible Star-Branched Polymers in Good Solvents"
- 3) Beskorovaynaya O. (Mainz, Germany), "Conformational Sampling with Coarse-Grained Peptide Models"
- 4) Dolgushev M. (Freiburg, Germany), "Dynamics of semiflexible tree-like networks"
- 5) Gribova N. (Stuttgart, Germany), "Colloids confined in a slit pore: from 2D to 3D behaviour"
- 6) Lyubimov I. (Oregon, USA), "Rescaling the accelerated dynamics from MD simulation of coarse-grained polymer melts"
- 7) Komarov P. (Tver, Russia), "Simulations of Morphology Development for Water-Containing Sulfonated Poly(Ether Ether Ketone) Membranes"
- 8) Lukyanov A. (Mainz, Germany), "Influence of system size on simulated charge mobility in amorphous films of tris(8-hydroxyquinolino)aluminium (Alq3)"
- 9) Severin N. (Berlin, Germany), "Graphenes on mica"
- 10) Naumenkova T. (Moscow, Russia), "Molecular Dynamics of Natural Biologically Active Short Peptides: Investigating Crucial Features of Secondary Structure in Different Environments"
- 11) Neratova I. (Tver, Russia), "Solvent-regulated morphologies of block copolymer films"
- 12) Popova H. (Sofia, Bulgaria), "Phase transitions of folding, anomalous diffusion and adsorption kinetics of polymerized membranes"
- 13) Radu M. (Mainz, Germany), "MC simulations regarding the melting transition in a 2d hard disk fluid"
- 14) Spirin L. (Mainz, Germany), "MD Simulations of Brush-like Systems with Soft Colloids"
- 15) Theodorakis P. (Mainz, Germany), "Molecular Dynamics Simulations of Bottlebrush Polymers under Poor Solvent Conditions"
- 16) Tretyakov N. (Goettingen, Germany), "Statistical properties of polymer films on a substrate"
- 17) Trukhina Yu. (Saarbruecken, Germany), "Monte Carlo simulation of hard spherocylinders under confinement"
- 18) Winkler A. (Mainz, Germany), "Monte Carlo simulations of colloid-polymer mixtures in cylindrical confinement"
- 19) Yaneva-Panayotova J. (Sofia, Bulgaria), "Polymer melt films and droplets on decorated substrates: equilibrium morphology and dynamic properties"

- 20) Bayani B. (Mainz, Germany), "Influence of location and interaction on quantum-tunneling"
- 21) Vogel T. (Juelich, Germany), "Conformational phase diagram for polymers adsorbed at ultrathin nanowires"
- 22) Larin S. (St.Petersburg, Russia), "Interpolyelectrolyte complexes formed by two stars and linear polyelectrolyte: effects of polyelectrolyte chain length and star topology"
- 23) Glagolev M. (Moscow, Russia), "Physical gels composed of macromolecules with helix secondary structure"
- 24) Glagoleva A. (Moscow, Russia), "Adsorption of amphiphilic macromolecules"
- 25) Ermilov V. (Moscow, Russia), "Self-organization of chiral amphiphilic macromolecules"
- 26) Krotova M. (Moscow, Russia), "Interpolymer polyelectrolyte complexes: theory and computer modelling"
- 27) Lazutin A. (Moscow, Russia), tba
- 28) Bogdanov A. (Moscow, Russia), tba