International Workshop
"Theory and Computer Simulation of Polymers: New Developments"
(May 31 -- June 6, 2010, Moscow, Russia)
Preliminary scientific programme

The titles of sessions should not be considered as strongly restricting, they only serve for a rough orientation, and speakers should not feel themselves somehow constrained by the titles of their sessions. The time of a talk is indicated for talk and questions/discussion, and all contributors are asked to leave at least 5 minutes for questions/discussion.

Monday, May 31

19:00	**Come-together, registration**	

Tuesday, June 1

8:30-19:00	**Registration**	
8:45	**Opening**	
Session 1		
9:00-10:30	**Nanocomposites**	
30 min.	A.Khokhlov	Research on computer simulations of nanostructured systems in Moscow State University
20 min.	E.Allahyarov	Nanocomposite ionomer membranes with directed proton conductivity
20 min.	P.Komarov	Structure and temperature properties of nanocomposites based on PI/SiO2: Atomistic modeling
20 min.	S.Egorov	Adsorption/Expulsion of oligomers and linear macromolecules in polymer brush
10:30-11:00	Coffee	
11:00-12:30	**Confinements**	
30 min.	S.Nechaev	Beneath the KPZ growth: From crevices in ballistic deposition patterns to discrete shocks in Burgers turbulence
20 min.	R.Messina	Statistics of adsorbed polymers under shear flow
20 min.	A.Skvortsov	Analytical theory of finite-size effects in mechanical desorption of a single chain
20 min.	V.Rostiashvili	Adsorption and detachment of a single polymer under tension: some exotic phase transition
12:30-14:00	Lunch	
Session 2		
14:00-15:10	**Simulation Strategies**	
30 min.	D.Theodorou	Simulation strategies for addressing the long-time properties of polymer melts and glasses
20 min.	A.Likhtman	Microscopic definition of entanglement
20 min.	D.Andrienko	Multiscale description of charge transport in conjugated polymers

15:10-15:40	Coffee	
15:40-17:20	**Methodic Developments**	
30 min.	W.Briels	Can single particle models describe the dynamics of polymer melts and solutions?
30 min.	M.Müller	Measuring free energies of self-assembled structures by computer simulation
20 min.	M.Oettel	Density Functional Theory for hard colloids: Some aspects of freezing and depletion effects
20 min.	M.Villet	Beyond mean field: New tools for field-theoretic simulation
18:00	Culture programme	

Wednesday, June 2

Session 3

9:00-10:30	**Single Chain Properties and Different Related Topics**	
30 min.	K.Binder	Standart definitions of persistence length do not describe the local “intrinsic” stiffness of real polymer chains
20 min.	M.Tamm	Zigzag model and the KPZ equation in (2+1)D
20 min.	A.Subbotin	Bending elasticity of 2D molecular bottle-brush
20 min.	V.Avetisov	Ultrametric diffusion approach to multi-scale modeling of fluctuation-induced protein mobility
10:30-11:00	Coffee	
11:00-12:30	**Copolymers**	
30 min.	S.Kuchanov	New trends in the Weak Segregation Limit (WSL) theory of loopless copolymers
20 min.	U.Nagpal	Predictions of block copolymer morphology for lithographic application using Monte Carlo simulations
20 min.	I.Potemkin	Designed AB copolymers as efficient stabilizers of colloidal particles
20 min.	A.Chertovich	DPD simulations of copolymer melts
12:30-14:00	Lunch	

Session 4

14:00-15:30	**Semiflexible Polymers**	
30 min.	E.Frey	Conformation and dynamics of semiflexible polymers
20 min.	M.Bachmann	Statistical analyses of conformational transitions for small polymers
20 min.	S.Stepanow	Short chain expansion, distribution function with fixed orientation of one end, and adsorption onto an interface of a wormlike chain
20 min.	V.Ivanov	Computer simulations of phase behavior of solutions of semiflexible macromolecules in a thin film confinement
15:30-16:00	Coffee	
16:00-19:00	**Poster Session**	
19:00	**Conference Dinner**	

Thursday, June 3

Session 5

9:00-10:30	**Polymer Melts and Biopolymers**	
30 min.	H.Meyer	Static and dynamic bond-correlations in entangled bead-spring melts
20 min.	A.Arnold	Flexible polymers in confinement: how can bacteria segregate their DNA?
20 min.	N.Severin	Rupture of DNA molecules under tensile stress
20 min.	Yu.Krupyanskii	Folding of lysozyme-like copolymer at the presence of chemical chaperone TMAO
10:30-11:00	Coffee	
11:00-12:30	**Networks, Stars, Brushes**	
30 min.	J.-U.Sommer	Theory and simulation studies of order parameters in dry and swollen polymer networks
20 min.	Yu.Gotlib	The theory of the relaxation spectrum in polymer networks: Intra- and interchain network motions at different cross-link densities
20 min.	A.Merkurieva	Conformations of polymer stars combining hydrophobic and hydrophilic features
20 min.	P.Theodorakis	Molecular Dynamics Simulations of Bottlebrush Polymers under Poor Solvent Conditions
12:30-14:00	Lunch	

Session 6

14:00-15:30	**Polyelectrolytes and Related Topics**	
30 min.	T.Birshtein	Core - crown conformations in polyelectrolyte stars
20 min.	S.Lyulin	Simulation of hyperbranched polymers in complexes with linear polyelectrolytes
20 min.	A.Rabinovich	Structure and properties of polyunsaturated phosphatidylcholine bilayers: Molecular dynamics simulation
20 min.	E.Zheligovskaya	The role of the surface layer of water in self-organization of polymer systems
15:30-16:00	Coffee	
16:00-17:30	**Copolymers and Single Chains**	
30 min.	I.Erukhimovich	On the microscopic theory of microphase separation in two-component bottle brushes
20 min.	H.-P.Hsu	Structure analysis of molecular bottle-brushes in a good solvent: Simulation and experiment
20 min.	K.Daoulas	Structure formation in supramolecular copolymers: a DFT based Monte Carlo approach
20 min.	V.Vasilevskaya	Self-organization of amphiphilic macromolecules.
18:00	Culture Programme	

Friday, June 4

Session 7

9:00-10:30	**Hydrodynamics and Transport**	
30 min.	M.Müser	The role of geometry and chemical detail for slip boundary condition of polymers near adhesive walls
30 min.	V.Mavrantzas	Quantifying chain reptation in entangled polymer melts: Topological and dynamical mapping of atomistic simulation results onto the tube model
30 min.	R.Winkler	Mesoscale hydrodynamic simulations of polymers in external fields

10:30-11:00	Coffee	
11:00-12:30	**Single Chains**	
30 min.	A.Milchev	DNA ejection from a Nanopore: Theory and Experiment
20 min.	A.Polotsky	Mechanical unfolding of a homopolymer globule: Theory and self-consistent field modeling
20 min.	W.Paul	Protein thermodynamics of a homopolymer chain
20 min.	P.Virnau	Entanglements in globular polymer phases
12:30-14:00	Lunch	
Session 8		
14:00-15:30	**Dynamics of Polymer Systems**	
30 min.	V.Lobaskin	Modelling of polymer dynamics under shear
20 min.	J.Farago	Mode-coupling approach to the subdiffusive early stage of polymer diffusion in a melt
20 min.	E.Govorun	Slow mode in the dynamics of polymer solutions
20 min.	Ya.Kudryavtsev	Interdiffusion in polymer blends with polydisperse components
15:30-16:00	Coffee	
16:00-17:30	**Polyelectrolytes**	
30 min.	A.Darinskii	Microstructure of complexes formed by charged bottle-brushes and linear polyelectrolytes: Computer simulation
20 min.	F.Schmid	Coarse-grained simulations of molecular transport in microchannels
20 min.	I.Neelov	Mechanical stretching of coiled –coil proteins.Computer simulation
20 min.	G.Freeman	Exploring DNA confinement via coarse-grain molecular simulation
18:00	Culture Programme	

Saturday, June 5

Session 9		
9:00-10:10	**Polymer Melts and Solutions**	
30 min.	A.Semenov	Theory of long-range correlations in glass-forming polymer liquids
20 min.	L.Spirin	MD simulations of brush-like systems with soft colloids
20 min.	C.-C.Huang	Mesoscale simulation of semidilute polymer solutions
10:10-10:40	Coffee	
10:40-11:30	**Methodic Development**	
30 min.	T.Schilling	Computing absolute free energies of disordered structures
20 min.	L.Manevich	The concept of limiting phase trajectories and transition “delocalization – localization” in oligomer chains
11:30	**Closing**	
11:45-13:00	Lunch	
13:00	Culture Programme	

Sunday, June 6

9:00 Culture Programme

Preliminary list of poster presentations (more posters from Russian PhD students and students are expected):

1) He S. Polyelectrolyte brushes: MD simulations and SCF theory
2) Berezovska G. Monte Carlo Study of Semiflexible Star-Branched Polymers in Good Solvents
3) Bezkorovaynaya O. Conformational Sampling with Coarse-Grained Peptide Models
4) Dolgushev M. Dynamics of semiflexible tree-like networks
5) Gribova N. Colloids confined in a slit pore: from 2D to 3D behaviour
6) Lyubimov I. Rescaling the accelerated dynamics from MD simulation of coarse-grained polymer melts
7) Komarov P. Simulations of Morphology Development forWater-Containing Sulfonated Poly(Ether Ether Ketone) Membranes
8) Lukyanov A. Influence of system size on simulated charge mobility in amorphous films of tris(8-hydroxyquinolinato)aluminium (Alq3)
9) Severin N. Graphenes on mica
10) Naumenkova T. Molecular Dynamics of Natural Biologically Active Short Peptides: Investigating Crusial Features of Secondary Structure in Different Environments
11) Neratova I. Solvent-regulated morphologies of block copolymer films
12) Popova H. Phase transitions of folding, anomalous diffusion and adsorption kinetics of polymerized membranes
13) Tretyakov N. Statistical properties of polymer films on a substrate
14) Trukhina Yu. Monte Carlo simulation of hard spherocylinders under confinement
15) Winkler A. Monte Carlo simulations of colloid-polymer mixtures in cylindrical confinement
16) Bayani B. Influence of location and interaction on quantumtunneling
17) Vogel T. Conformational phase diagram for polymers adsorbed at ultrathin nanowires
18) Larin S. Interpolyelectrolyte complexes formed by two stars and linear polyelectrolyte: effects of polyelectrolyte chain length and star topology
19) Glagolev M. Physical gels composed of macromolecules with helix secondary structure
20) Glagoleva A. Adsorption of amphiphilic macromolecules
21) Ermilov V. Self-organization of chiralic amphphilic macromolecules
22) Krotova M. Interpolymer polyelectrolyte complexes: theory and computer modelling
23) Gavrilov A. DPD simulation of multiblockcopolymers microphase separation
24) Kikot I. New coarse-grain model for analysis of localized nonlinear excitations in DNA
25) Guseva D. Macromolecular reactions in incompatible blends: computer simulation
26) Polynsky M. Reversible polycondensation of inhomogeneous system: DPD computer simulation