BuildMoNa

UNIVERSITÄT LEIPZIG

SCIENTIFIC AND METHOD MODULES

Module name	Multifunctional Scaffolds: Modeling and Simulating Macromolecules
Number	2013-T2
Aims	The basic background in modeling and simulating macromolecules will be taught to enable the students to use highly dynamic polymer scaffolds as an organising matrix for smart nanoelements and active devices. A particular focus will be on methods for bridging the many length and time scales which hamper efficient computer simulations of multifunctional polymer scaffolds.
Basics	Material covered in basic modules B3 and B2 (polymer physics [viscoelasticity, statistical physics and thermodynamics of polymer chains], properties and isolation of biopolymers [DNA, actin, intermediate filaments, microtubule], Brownian motion, cell motility).
Contents	General concepts of statistical and polymer physics, basic ideas and selected applications of multiscale modeling, polymer adsorption, experimental deposition techniques, polymers under external forces, force measurements by optical tweezers, bending stiffness effects of semiflexible polymers, chain-growth computer simulations (PERM), Monte Carlo simulations (generalized ensembles).
Methods	Theory and modeling concepts (polymers in confinements and under external forces, stiffness effects), computer simulation methodologies for (semi)flexible polymers (chain-growth algorithms, Monte Carlo methods, scaling theories, etc.), polymer deposition techniques, interaction measurements by optical tweezers.
Type	Two-day block course/ bi-yearly recurrence with modification
Date (month/year)	20–21 June 2013
Time	09:15-18:30 (room 113), 09:30-17:00 (room 210), ITP Brüderstr. 16
Work load	15 hours presence/ 45 hours self-study
Examination	Written exam
Credit points	2
Responsible scientists	Wolfhard Janke, Friedrich Kremer
International guest lecturers	Stefan Förster (Martin-Luther-Universität Halle-Wittenberg), Hsiao-Ping Hsu (Universität Mainz), Kurt Kremer (MPI für Polymerforschung, Mainz), Sanjay Kumar (Banaras Hindu University, Varanasi, India)
Industrial partners	
Recommendations for literature, e-learning	C. Holm, K. Kremer (eds.), Advanced Computer Simulation Approaches for Soft Matter Sciences I, II, III, Advances in Polymer Science **173**, **185**, **221** (Springer, 2005, 2005, 2008); H.-P. Hsu, P. Grassberger, *A review of Monte Carlo simulations of polymers with PERM*, J. Stat. Phys. **144** (2011) 597-637; S. Kumar, M.S. Li, *Biomolecules under mechanical force*, Phys. Rep. **486** (2010) 1-74: H. Arkin, W. Janke, *Polymer-attractive spherical cage system*, Eur. Phys. J. - Special Topics **216** (2013) 181-190.

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SCHEDULE for Module 2013-T2 (tentative)

Time	Lecturer	Programme	Location
Day 1 (20.06.2013)			
09:15-09:30	Wolfhard Janke	Introduction	Room 113
09:30-11:00	Sanjay Kumar	(Bio)polymers under mechanical force I	
11:00-12:30	Hsiao-Ping Hsu	Polymer simulations with PERM I	
LUNCH	Informal Discussions		
13:30-15:00	Hsiao-Ping Hsu	Polymer simulations with PERM II	
15:00-16:30	Wolfhard Janke	Computer simulations of polymer adsorption	
16:30-18:00	Stefan Förster	Single polymer deposition	
18:00-18:30	All participants	Plenary Discussion	
Day 2 (21.06.2013)			
09:30-11:00	Kurt Kremer	Multiscale modeling I	Room 210
11:00-12:30	Sanjay Kumar	(Bio)polymers under mechanical force II	
LUNCH	Informal Discussions		
13:30-15:00	Kurt Kremer	Multiscale modeling II	
15:00-16:30	Friedrich Kremer	Receptor/Ligand interactions as measured by Optical Tweezers	
16:30-17:00	All participants	Plenary Discussion	

Didactic elements:
Lectures, plenary discussion and exercises, etc.

Expected performance:
Active participation in discussions, exercises, and written examination