

Workshop „Computer Simulations of Soft Matter and Biosystems“ (March 14 – 16 2007)
Kirchhoff-Institute for Physics, Heidelberg University

	Wednesday, March 14th	Thursday, March 15th	Friday, March 16th
09.00-10.00		KL 2: Prof. Wilfred van Gunsteren Methods to simulate biomolecular systems	KL 4: Prof. Jeremy Smith Dynamics of Protein Binding, Reaction, and Structural Change
10.00-10.30		Prof. Walter Thiel Correlated ab initio QM/MM studies of enzymes	Dr. Francois Nedelec Modelling Microtubules Structures
10.30-11.00		Prof. Reinhold Fink New ab initio multi configuration approaches designed for QM/MM applications	Dr. Alexey Zaikin Proteomalg: a new tool for in vitro digestion assay performed by 20S immunoproteasome and PA28
11.00-11.30		Coffee	Coffee
11.30-12.00		PD Nikos Doltsinis Photoisomerisation in liquid azobenzene studied by nonadiabatic QM/MM simulations	Dr. Esa Kuusela Cytoplasm and integrin dynamics in a 2D continuum model for cell migration
12.00-12.30	Arrival meal	Dr. Christine Peter Classical simulations from the atomistic to the mesoscale: coarse-graining an azobenzene containing liquid crystal	Dr. Björn Nadrowski The physics of an ear
12.30-13.00		Lunch Conference Photo at 13.45	Dr. Ulrike Bischler, PD Ulrich Schwarz Closing Remarks
13.30-14.00			
	PD Ulrich Schwarz, Dr. Indra Willms-Hoff, Prof. Willi Jäger Welcome		
14.00-15.00	KL 1: Prof. Alan Mark Self-assembly of Peptides and Membranes	KL 3: Prof. Gerhard Gompper Soft Matter Hydrodynamics	
15.00-15.30	Prof. Helmut Grubmüller Collective motions of biological macromolecules	Jens Smiatek and Ulf D. Schiller A new way of implementing partial slip boundary conditions	
15.30-16.00	Dr. Kei Moritsugu Langevin Model of Protein Dynamics	Kai Grass Electrohydrodynamics in bulk and in confined geometries	
16.00-16.30	Coffee	Coffee	
16.30-17.00	Prof. Martin Zacharias Nucleic acid and peptide conformation studied by molecular dynamics and advanced sampling methods	Dr. Anthony Maggs Aspects of fluctuation potentials in dielectrics	
17.00-17.30	Dr. Nick Kepper Modeling Chromatin Fibers I: Effect of Nucleosome Geometry	PD Dirk Hennig Cooperative escape dynamics of nonlinear oscillator chains	
17.30-18.00	Prof. Gero Wedemann Modeling chromatin fibers 2: effects of interactions between nucleosomes	Dr. Ilona D. Kosinska Transport in nanopores	
18.00-18.30	Jakob Schlüttig Modelling large protein clusters		
18.30-19.00	Poster Introductions		
19.00	Postersession + Dinner	Dinner Heidelberg Altstadt (Kulturbrauerei)	
21.00	Visit to BIOQUANT-building		