Winter School 2009
Multiscale Simulation Methods in Molecular Sciences

	Monday 2 March	Tuesday 3 March	Wednesday 4 March	Thursday 5 March	Friday 6 March
9:00-10:00	9:45-10:00 Opening *Thomas Lippert*	Density Functional Theory and Linear Scaling *Rudolf Zeller*	DFT Embedding and Coarse Graining Techniques *Mike Payne*	Two Topics in Ab Initio Molecular Dynamics: Multiple Length Scales and Exploration of Free-Energy Surfaces *Mark E. Tuckerman*	Coarse Grained Electronic Structure Using Neural Networks *Jörg Behler*
10:00-11:00	Large Spatiotemporal-Scale Material Simulations on Petaflops Computers *Aiichiro Nakano*	QM/MM Methodology: Fundamentals, Scope, and Limitations *Walter Thiel*	De Novo Protein Folding with Distributed Computational Resources *Wolfgang Wenzel*	Multiscale Methods for the Description of Chemical Events in Biological Systems *Marcus Elstner*	Computer Simulations of Systems with Hydrodynamic Interactions: The Coupled Molecular Dynamics – Lattice Boltzmann Approach *Burkhard Dünweg*
11:00-11:30	**Coffee Break**				
11:30-12:30	Molecular Dynamics - Extending the Scale from Microscopic to Mesoscopic *Godehard Sutmann*	Soft Matter, Fundamentals and Coarse Graining Strategies *Kurt Kremer*	An Introduction to the Tight Binding Approximation – Implementation by Diagonalisation *Anthony T. Paxton*	Wavelets and Their Application for the Solution of Poisson's and Schrödinger's Equation *Stefan Goedecker*	Application of Residue-Based and Shape-Based Coarse Graining to Biomolecular Simulations *Klaus Schulten*
12:30-14:30	**Lunch Break**				
14:30-15:30	Introduction to Multigrid Methods for Elliptic Boundary Value Problems *Arnold Reusken*	Introduction to Parallel Computing *Bernd Mohr*	Strategies for Implementing Scientific Applications on Parallel Computers *Bernd Körfgen*	Bond-Order Potentials for Bridging the Electronic to Atomistic Modelling Hierarchies *Ralf Drautz*	
15:30-16:30	Eletronic Structure: Hartree -Fock and Correlation Methods *Christof Hättig*	Adaptive Resolution Schemes *Luigi Delle Site*	Practical Session	First-Principles Statistical Mechanics Approaches to Surface Physics and Catalysis *Karsten Reuter*	
16:30-17:00	**Coffee Break**				
17:00-18:00	Monte Carlo and Kinetic Monte Carlo Methods – A Tutorial *Peter Kratzer*	Multiscale Modelling of Magnetic Materials: From the Total Energy of the Homogeneous Electron Gas to the Curie Temperature of Ferromagnets *Phivos Mavropoulos*	Practical Session	First-Principles Based Multiscale Modelling of Alloys *Stefan Müller*	
Evening	**Reception and Get-Together**	**Poster-Session I**	**Poster-Session II**	**Conference Dinner**	