Computational Nanoscience: Do It Yourself!
NIC Winter School 2006

	Tuesday 14 February	Wednesday 15 February	Thursday 16 February	Friday 17 February	Saturday 18 February
9:00-10:00		The Pseudopotential Plane Wave Approach Bernd Meyer	The Korringa-Kohn-Rostoker (KKR) Green Function Method I. Electronic Structure of Periodic Systems Phivos Mavropoulos	On Exchange-Correlations Functionals (LDA and GGA) Robert O. Jones	Practical Session 4: Pick Your Favored Problem and Work on It
10:00-11:00		The Full-Potential Linearized Augmented Plane Wave Method Stefan Blügel	Basis Sets, Accuracy, and Calibration in Quantum Chemistry Thomas Müller	Spin-Polarized DFT Calculations and Magnetism Rudolf Zeller	
11:00-11:30		Coffee Break			
11:30-12:30		Parallel Linear Algebra Methods Bernd Körfgen	Molecular Dynamics - Vision and Reality Godehard Sutmann	Surface Phase Diagrams from Ab Initio Thermodynamics Bernd Meyer	
12:30-14:00	Registration	Lunch Break			
14:00-15:00	14:00-14:15 Opening Remarks Thomas Lippert	14:00 - 15:30 Introduction to Parallel Computing Bernd Mohr	An Introduction to Ab Initio Molecular Dynamics Simulations Dominik Marx	Practical Session 3: Determining the Structure of Solids, Liquids, and Clusters	Practical Session 4: Pick Your Favored Problem and Work on It
	14:15-15:15 Ab Initio Electronic Structure Calculations: Status and Challenges Matthias Scheffler				
15:00-18:00	15:15-16:15 Introduction to Hartree-Fock and CI Methods Volker Staemmler	Practical Session 1: Parallel Linear Algebra	Practical Session 2: Getting Familiar with the Codes		
	Coffee Break				
	16:45-17:45 Introduction to Density Functional Theory Robert O. Jones				
Evening	Reception and Get-Together Thomas Lippert			Poster Session Contributions from Participants Catered Meal	

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	Sunday 19 February	Monday 20 February	Tuesday 21 February	Wednesday 22 February
9:00-10:00	Excursion to Cologne with City Tour by Bus, Guided Tour of the Cathedral, and Dinner	Beyond Hartree-Fock: MP2 and Coupled-Cluster Methods for Large Systems Christof Hättig	Free Energy and Rare Events in Molecular Dynamics Nikos L. Doltsinis	Molecular Dynamics Beyond the Born-Oppenheimer Approximation: Mixed Quantum-Classical Approaches Nikos L. Doltsinis
10:00-11:00		Non-Collinear Magnetism: Exchange Parameter and T_c Gustav Bihlmayer	Time-Dependent Density Functional Theory Nikos L. Doltsinis	Ab Initio Description of Electronic Transport Daniel Wortmann
11:00-11:30		Coffee Break 		
11:30-12:30		The Korringa-Kohn-Rostoker (KKR) Green Function Method II. Impurities and Clusters in the Bulk and on Surfaces Peter H. Dederichs	The Optimized Effective Potential Method and LDA+U Stefan Kurth	Many-Body Perturbation Theory: The GW Approximation Christoph Friedrich
12:30-14:00		Lunch Break 		12:30-12:45 Closing Remarks Lunch
14:00-18:00		Practical Session 5: Computing Properties of Solids, Liquids, and Clusters	Practical Session 6: Advanced Applications	