

STC2005 Scientific Programme

	Monday, September 5	Tuesday, September 6	Wednesday, September 7
9:00	Session 1: Chairman RODE, Bernd Michael 09:00-09:30 Rode, Bernd Michael Welcome Address	Session 5: Chairman DOMCKE, Wolfgang 09:00-09:45 Richards, Graham Pattern Recognition and Grid Computing in Drug Discovery	Session 9: Chairman FRENKING, Gernot 09:00-09:45 Furche, Philipp Time-dependent density functional treatment of ultrafast phenomena
10:00	09:30-10:15 van Gunsteren, Wilfred F. Computer Simulation of Biomolecular Systems: (im)possibilities and perspectives.	09:45-10:30 Hellmann Award Ceremony and Lecture	09:45-10:15 Maroulis, George Interaction-induced electric dipole moment and dipole (hyper)polarizability in CO ₂ ...Rg, Rg = He, Ne, Ar, Kr and Xe.
	10:15-10:45 Coffee Break	10:30-11:05 Coffee Break	10:15-10:45 Coffee Break
	Session 2: Chairman THIEL, Walter 10:45-11:05 Scheurer, Christoph		Session 10: Chairman MAROULIS, George 10:45-11:05 Hofer, Thomas
11:00	Towards ab-initio simulation of multidimensional IR-spectra of peptides 11:05-11:25 Klamroth, Tillmann Time dependent configuration interaction calculations for ultrafast laser driven many electron dynamics in molecular systems 11:25-11:45 Stock, Gerhard Nonequilibrium Molecular Dynamics Simulations of Photoswitchable Peptides 11:45-12:05 Neugebauer, Johannes The Merits of the Frozen-Density Embedding to Model Solvatochromic Shifts	Session 6: Chairman MANZ, Jörn 11:05-11:25 Kast, Stefan M. Hybrid integral equation/simulation models 11:25-11:45 Lischka, Hans High-level multireference ab initio theory applied to on-the-fly dynamics: the photochemistry of the C=C bond. 11:45-12:05 Neufeld, Anatole Ab initio nonadiabatic dynamics of polyatomic molecules: beyond mean-field and surface hopping approaches	Ab initio Quantum Mechanical Charge Field (QMCF) Molecular Dynamics - A QM/MM - MD Procedure for Accurate Simulations of Ions and Complexes 11:05-11:25 Scherer, Philipp Simulation of large molecular ions in solution using effective fragment potentials. Application to molecular aggregation and photoinduced solvent to dye electron transfer
12:00	12:05-12:25 Heine, Thomas DFTxTB - a unified quantum-mechanical hybrid method 12:25-12:45 Eisfeld, Wolfgang Theoretical simulation of vibrationally resolved electronic spectra	12:05-12:25 Schmatz, Stefan State-selected quantum reaction dynamics of complex-forming ion-dipole systems 12:25-12:45 Moyano, Gloria Chemical Dynamics on Interpolated Potential Energy Surfaces	11:30-13:00 Poster Session II Posters P-200 to P-299
	Lunchtime		

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14:30	Session 3: Chairman LISCHKA, Hans 14:30-14:50 Sanchez Marcos, Enrique The Hydration Structure of Metal Aquaions Exhibiting Anisotropic Solvent Environments: The Pd ²⁺ , Pt ²⁺ and AnO ₇ ²⁺ cases. 14:50-15:10 Wedig, Ulrich	Session 7: Chairman BOTSCHWINA, Peter 14:30-14:50 Liedl, Klaus Dynamic Mechanisms of DNA Sequence Recognition 14:50-15:10 Hamacher, Kay Computing the amino acid specificity of fluctuations in biomolecular systems 15:10-15:30 Scholz, Reinhard Spectroscopic properties of alpha-PTCDA single crystals and PTCDA molecules adsorbed on metal substrates 15:30-15:50 van Mourik, Tanja The structure of the gas-phase tyrosine-glycine dipeptide 15:50-16:10 Lewerenz, Marius	Session 11: Chairman LIEDL, Klaus 14:30-14:50 Bühl, Michael Structure, Dynamics, and NMR Properties of Transition Metal Complexes in Aqueous Solution 14:50-15:10 Woywod, Clemens Exact and approximate wave packet dynamics with quantum trajectories 15:10-15:30 Wenzel, Wolfgang High Throughput in-silico screening against flexible protein receptors 15:30-15:50 Dong, Yi Structural and electronic properties of nanostructured HAIO and AIO 15:50-16:10 Fouqueau, Antony Structures and Dynamics of Protonated Water Clusters
15:00	Chemical Bonding in Intermetallic Phases 15:10-15:30 Usyvat, Denis Fast local-MP2 method for crystals using Density Fitting approximation 15:30-15:50 Kästner, Johannes Nitrogenase: DFT Calculations Provide Insight into Biological Nitrogen Fixation 15:50-16:10 Kühn, Oliver	Large amplitude coupled vibrations in the hydrogen bonded systems HF-H ₂ O, HF-H ₂ S, HCl-H ₂ O and HCl-H ₂ S	
16:00	Multidimensional Laser-Driven Quantum Dynamics of Heme CO Compounds		
16:10-16:40 Coffee Break			
	Session 4: Chairman SANCHEZ MARCOS, Enrique 16:40-17:00 Kroemer, Romano Quantum chemical investigation of biomolecules and their water clusters in the gas phase 17:00-17:20 Sternberg, Ulrich Extremely Fast Chemical Shift Calculations for Constrained Molecular Mechanics Simulations 17:20-17:40 Boese, Daniel A. Ab initio Calculations on Hydrogen Bonded Complexes 17:40-18:00 Kleinekathöfer, Ulrich Influence of ultra-fast laser pulses on the electron transfer in molecular wires	Session 8: Chairman SCHWARZ, W. H. Eugen 16:40-17:00 Klopper, Wim New correlation factors for explicitly correlated electronic wavefunctions 17:00-17:20 Ochsenfeld, Christian Rigorous Integral Screening for Electron Correlation Methods 17:20-17:40 Köhn, Andreas Coupled-cluster with arbitrary excitation levels: Implementation, and test of perturbative approximations and subspace-based truncations 17:40-18:00 Springborg, Michael Polarization and external fields for infinite chains	Session 12: Chairman RODE, Bernd Michael 16:40-17:00 Steinhauser, Othmar Simulation Studies of the Protein Water Interface 17:00-17:30 Schwarz, W. H. Eugen Paradoxa in Theoretical chemistry and Other Fields 17:30-18:00 STC 2006 Presentation of the forthcoming Symposium on Theoretical Chemistry 2006
17:00			
18:00	18:00-18:30 AGTC-Meeting 18:30-20:00 Poster Session I Posters P-100 to P-199	18:00-20:00 Reception	18:00-18:15 Rode, Bernd Michael Closing
19:00		20:00-22:00 Concert	

organised by:

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