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 **09:30-10:15 van Gunsteren, Wilfred F.** Computer Simulation of Biomolecular Systems: (im)possibilities and perspectives.	**Session 5: Chairman** DOMCKE, Wolfgang **09:00-09:45 Richards, Graham** Pattern Recognition and Grid Computing in Drug Discovery **09:45-10:30 Hellmann Award** Ceremony and Lecture	**Session 9: Chairman** FRENKING, Gernot **09:00-09:45 Furche, Filipp** Time-dependent density functional treatment of ultrafast phenomena **09:45-10:15 Maroulis, George** Interaction-induced electric dipole moment and dipole (hyper)polarizability in CO2…Rg, Rg = He, Ne, Ar, Kr and Xe.
10:00	**10:15-10:45 Coffee Break**	**10:30-11:05 Coffee Break**	**10:15-10:45 Coffee Break**
11:00	**Session 2: Chairman** THIEL, Walter **10:45-11:05 Scheurer, Christoph** 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	**Session 10: Chairman** MAROULIS, George **10:45-11:05 Hofer, Thomas** 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 **11:30-13:00 Poster Session II** Posters P-200 to P-299
12:00	**12:05-12:25 Heine, Thomas** DFT×TB - 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	
	Lunchtime		

	Monday, September 5	Tuesday, September 6	Wednesday, September 7
14:30	**Session 3: Chairman** LISCHKA, Hans	**Session 7: Chairman** BOTSCHWINA, Peter	**Session 11: Chairman** LIEDL, Klaus
	14:30-14:50 Sanchez Marcos, Enrique The Hydration Structure of Metal Aquaions Exhibiting Anisotropic Solvent Environments: The Pd^{2+}, Pt^{2+} and AnO_2^{2+} cases.	**14:30-14:50 Liedl, Klaus** Dynamic Mechanisms of DNA Sequence Recognition	**14:30-14:50 Bühl, Michael** Structure, Dynamics, and NMR Properties of Transition Metal Complexes in Aqueous Solution
	14:50-15:10 Wedig, Ulrich	**14:50-15:10 Hamacher, Kay**	**14:50-15:10 Woywod, Clemens**
15:00	Chemical Bonding in Intermetallic Phases	Computing the amino acid specificity of fluctuations in biomolecular systems	Exact and approximate wave packet dynamics with quantum trajectories
	15:10-15:30 Usyvat, Denis	**15:10-15:30 Scholz, Reinhard**	**15:10-15:30 Wenzel, Wolfgang**
	Fast local-MP2 method for crystals using Density Fitting approximation	Spectroscopic properties of alpha-PTCDA single crystals and PTCDA molecules adsorbed on metal substrates	High Throughput in-silico screening against flexible protein receptors
	15:30-15:50 Kästner, Johannes	**15:30-15:50 van Mourik, Tanja**	**15:30-15:50 Dong, Yi**
	Nitrogenase: DFT Calculations Provide Insight into Biological Nitrogen Fixation	The structure of the gas-phase tyrosine-glycine dipeptide	Structural and electronic properties of nanostructured HAlO and AlO
	15:50-16:10 Kühn, Oliver	**15:50-16:10 Lewerenz, Marius**	**15:50-16:10 Fouqueau, Antony**
16:00	Multidimensional Laser-Driven Quantum Dynamics of Heme-CO Compounds	Large amplitude coupled vibrations in the hydrogen bonded systems HF-H_2O, HF-H_2S, HCl-H_2O and HCl-H_2S	Structures and Dynamics of Protonated Water Clusters
	16:10-16:40 Coffee Break		
	Session 4: Chairman SANCHEZ MARCOS, Enrique	**Session 8: Chairman** SCHWARZ, W. H. Eugen	**Session 12: Chairman** RODE, Bernd Michael
	16:40-17:00 Kroemer, Romano Quantum chemical investigation of biomolecules and their water clusters in the gas phase	**16:40-17:00 Klopper, Wim** New correlation factors for explicitly correlated electronic wavefunctions	**16:40-17:00 Steinhauser, Othmar** Simulation Studies of the Protein Water Interface
17:00	**17:00-17:20 Sternberg, Ulrich** Extremely Fast Chemical Shift Calculations for Constrained Molecular Mechanics Simulations	**17:00-17:20 Ochsenfeld, Christian** Rigorous Integral Screening for Electron Correlation Methods	**17:00-17:30 Schwarz, W. H. Eugen** Paradoxa in Theoretical chemistry and Other Fields
	17:20-17:40 Boese, Daniel A. Ab initio Calculations on Hydrogen Bonded Complexes	**17:20-17:40 Köhn, Andreas** Coupled-cluster with arbitrary excitation levels: Implementation, and test of perturbative approximations and subspace-based truncations	**17:30-18:00 STC 2006** Presentation of the forthcoming Symposium on Theoretical Chemistry 2006
	17:40-18:00 Kleinekathöfer, Ulrich Influence of ultra-fast laser pulses on the electron transfer in molecular wires	**17:40-18:00 Springborg, Michael** Polarization and external fields for infinite chains	
18:00	**18:00-18:30 AGTC-Meeting**	**18:00-20:00 Reception**	**18:00-18:15 Rode, Bernd Michael** Closing
	18:30-20:00 Poster Session I Posters P-100 to P-199		
19:00		**20:00-22:00 Concert**	

organised by:

Theoretical Chemistry Division
University of Innsbruck
A-6020 Innsbruck, Innrain 52a
Austria

http://www.stc2005.at
http://www-c724.uibk.ac.at/theochem

sponsored by:

The Austrian Federal Ministry for Education, Science and Culture (bm:bwk)
The Government of Tyrol
The City of Innsbruck
Sun Microsystems
IPS Vienna
University of Innsbruck
Sandoz Austria
Tourismusverband Innsbruck

Organising Comittee

Bernd Michael **RODE**

Daniel **FITZ**
Thomas **HOFER**
Margaret **OSTERMANN**
Kristof **PLANKENSTEINER**
Bernhard **RANDOLF**
Hannes **REINER**