Designing Molecular Functionality:
Challenges for Theoretical Approaches

Programme

of the

47th Symposium for Theoretical Chemistry

STC 2011

(18/08/2011)

Sunday, August 21, 2011

14:00–18:00	**Arrival**	Registration
18:00–18:15	**M. Reiher**	*Opening, Welcome, Information*
	Chair: M. Reiher	
18:15–18:50	**F. Diederich**	Opto-Electronic Organic Materials by Novel Acetylene Chemistry
18:50–19:25	**D. N. Beratan**	Theoretical Guidance For Chemical Synthesis
19:30–22:00	**Dinner**	

Monday, August 22, 2011

8:25–8:30	**M. Reiher**	*Information on Posters, Excursion, etc.*
	Chair: M. Reiher	
8:30–9:05	**A. Aspuru-Guzik**	Towards Simulation of Molecular Properties in Nanoscale Dissipative environments: Open Quantum Systems Density Functional Theory and Nano-enhanced spectroscopy
9:05–9:40	**L. Visscher**	A Subsystem Approach for the Quantum Mechanical Description of Large Biomolecules
9:40–10:05	**C. R. Jacob**	Unambiguous Optimization of Effective Potentials in Finite Basis Sets
Coffee break		
	Chair: J. Neugebauer	
10:35–11:10	**W. F. van Gunsteren**	Methodological Advances in the Computation of Relative Free Energies
11:10–11:45	**B. Kuhlman**	Computational Design of Protein Structures and Interfaces
11:45–12:10	**M. Oncak**	Modeling the UV Absorption and Photoelectron Spectra in Solution Using the Path Integral Molecular Dynamics
Lunch		
	Chair: C. Ochsenfeld	
14:00–14:35	**M. Parrinello**	The Well Tempered Ensemble
14:35–15:10	**P. Hünenberger**	The Representation of Ions, a Challenge for Classical Simulations
15:10–15:45	**O. A. von Lilienfeld**	From Electronic Structure Theory to Rational Compound Design
Coffee break		
	Chair: M. Hanrath	
16:15–16:50	**P. W. Ayers**	Two-Point Weighted Density Approximations for the Kinetic Energy and Exchange-Correlation Energy
16:50–17:25	**A. Dreuw**	Quantum Chemical Methods for Electronic Excited States of Large Molecules: From TDDFT to ADC
17:25–17:50	**M. Nest**	TDDFT as a Tool for Coherent Control of Valence Electrons
17:50–18:15	**T. Schwabe**	Environmental Effects on Electronic Excitations: Recent Advances for the Polarizable Embedding Method
Dinner		
20:00–22:00	**Poster session**	(even numbers)

Tuesday, August 23, 2011

	Chair: M. Kaupp	
8:30–9:05	**P. Geerlings**	Conceptual Density Functional Theory
9:05–9:40	**G. Frenking**	Donor-Acceptor Complexes of Main-Group Elements With Unusual Bonds
9:40–10:05	**S. Knecht**	The Nature of Chemical Bonding in f-Elements: U_2 Revisited with full Treatment of Spin–Orbit Coupling
Coffee break		
	Chair: M. Holthausen	
10:35–11:10	**S. Shaik**	Reactivity Patterns in Bond Activation by Metal Oxo Complexes
11:10–11:45	**F. Schoenebeck**	Catalysis from a Computational Perspective
11:45–12:10	**H. Bolvin**	Magnetic Properties of Sandwich Complexes of Lanthanides and Actinides
Lunch		take-away
Afternoon		Excursion to mount Pilatus (for registered participants)
Evening		Conference dinner (for registered participants)

Wednesday, August 24, 2011

	Chair: J. Gauss	
8:30–9:05	**N.N.**	*Hellmann Award Lecture*
9:05–9:40	**T. Saue**	4-Component Relativistic Calculations of the Magnetically Induced Current Density in Aromatic Systems
9:40–10:05	**D. Sundholm**	Calculation of Magnetically Induced Current Densities for Designing Molecular Functionality
Coffee break		
	Chair: R. Berger	
10:35–11:10	**J. Autschbach**	Calculation and Analysis of Molecular Optical and Spectroscopic Parameters Across the Periodic Table
11:10–11:45	**K. Ruud**	Calculating Molecular Properties in the Relativistic Domain
11:45–12:10	**C. van Wüllen**	Density Functional Calculations of Zero Field Splittings — Towards a Consistent Theory
Lunch		
	Chair: P. Botschwina	
14:00–14:35	**H.–J. Werner**	Explicitly Correlated Local Coupled-Cluster Methods for Large Molecules
14:35–15:10	**A. Rizzo**	Nonlinear Spectroscopies and Chirality
15:10–15:45	**T. D. Crawford**	Through the Looking Glass, and What the Quantum Chemist Found There
Coffee break		
	Chair: I. Frank	
16:15–16:50	**H. Su**	Versatile Character of Carbon
16:50–17:25	**G. C. Solomon**	Describing Local Currents in Molecular Electron Transport
17:25–17:50	**C. Herrmann**	Designing Molecular Spintronics Devices in the Coherent Tunneling Regime
17:50–18:30	**AGTC Meeting**	General Assembly
Dinner		
20:00–22:00	**Poster session**	(odd numbers)

Thursday, August 25, 2011

	Chair: C. Marian	
8:30–9:05	**S. Grimme**	Importance of London Dispersion Interactions for Chemical Functions
9:05–9:40	**R. Lindh**	Analytic CD Gradients for HF, DFT, MP2 and CASSCF
9:40–10:05	**M. Korth**	Third-Generation Hydrogen-Bonding Corrections for Semiempirical QM Methods and Force Fields

Coffee break

	Chair: H. M. Senn	
10:35–11:10	**W. Thiel**	Theoretical Studies of Enzymatic Reactions
11:10–11:45	**C. Greco**	New Perspectives for the Computation of Electronic and Vibrational Properties in Metalloproteins: The Case of [FeFe]-Hydrogenase
11:45–12:10	**M. Stein**	Structural and Functional Mimics of Hydrogenase
12:10–12:30	**M. Reiher**	*Award of Poster Prizes, Closing Remarks*

Lunch

14:00	**Departure**	