

**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	<i>Opening, Welcome, Information</i>
	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	<i>Information on Posters, Excursion, etc.</i>
	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)
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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:
U₂ 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**