Programme

Friday, September 2, 2011

11:00 -	**Registration Desk Open** (Okuma Auditorium)
Opening Session (Okuma Auditorium)	
15:30 - 16:30	**Opening Ceremony**
16:30 - 17:30	**2CL. Congress Lecture:** *Yuan T. Lee* Interplay Between Experiment and Theory
17:30 - 18:10	**2PL. Plenary Lecture:** *Keiji Morokuma* Theoretical Studies of Chemical Reactions - Gas Phase Reactions to Nano Structures, Catalyses, and Enzymatic Reactions in Ground and Excited Electronic States
19:00 - 21:00	**Welcome Reception** (Rihga Royal Hotel)

Saturday, September 3, 2011

08:15 -	**Registration Desk Open** (Bldg. 14)				
3A1. Frontier in DFT (101/Room A) Chair: *Viktor N. Staroverov*		**3B1. Electronic Property** (102/Room B) Chair: *Péter R. Surján*		**3D1. Biological Structure** (403/Room D) Chair: *Ryo Akiyama*	
08:45-09:15	**3A1-1I**: *Evert Jan Baerends* From Density Functional Theory to Density Matrix Functional Theory	08:45-09:15	**3B1-1I**: *Daniel Crawford* Chiral Spectroscopy: Towards a Reliable Comparison between Theory and Experiment	08:45-09:15	**3D1-1I**: *Hiroshi Noguchi* Dynamics of Biomembranes in Nano- to Micro-Meter Scales
09:15-09:45	**3A1-3I**: *Paul W. Ayers* Two-Point Weighted Density Approximations for the Kinetic Energy and Exchange-Correlation Energy	09:15-09:45	**3B1-3I**: *Trygve Helgaker* Molecules in Strong Magnetic Fields	09:15-09:45	**3D1-3I**: *Masahiro Kinoshita* Roles of Water and ATP in Functioning of ATP-Driven Proteins
09:45-10:00	**3A1-5C**: *Yutaka Imamura* Linearity Condition for Orbital Energy in Density Functional Theory: Construction of Orbital-Specific Hybrid Functionals	09:45-10:00	**3B1-5C**: *Sonia Coriani* Near-Edge X-Ray Absorption Fine Structure from Coupled Cluster Damped Response Theory Using an Asymmetric Lanczos-Chain Driven Algorithm	09:45-10:00	**3D1-5C**: *Damien Hall* Resolving Mixed Protein Amyloid-Aggregate Distributions
10:00-10:15	**3A1-6C**: *Jeng-Da Chai* Density Functional Theory with Fractional Occupations	10:00-10:15	**3B1-6C**: *Stefan Knippenberg* A Study into the Low-Lying Excited States of Small and Medium-Sized Molecules Using the (Unrestricted) ADC(2) Scheme: A Close Comparison with Experiment	10:00-10:15	**3D1-6C**: *Osamu Miyashita* Adding Dynamical Insight to Protein X-Ray Images by Solution and Crystal Molecular Dynamics Simulation
10:15-10:45 Coffee Break					
3A2. Method for Large System (101/Room A) Chair: *Dmitri G. Fedorov*		**3B2. Condensed Phase** (102/Room B) Chair: *Gren Patey*		**3D2. Non-linear Optics** (403/Room D) Chair: *Bernard Kirtman*	
10:45-11:15	**3A2-1I**: *Roland Lindh* Cholesky Decomposition in Quantum Chemistry: A Summary of the Current Status	10:45-11:15	**3B2-1I**: *Eran Rabani* Quantum Fluctuations Can Promote or Inhibit Glass Formation		
11:15-11:45	**3A2-3I**: *Christian Ochsenfeld* Linear- and Sub-Linear Scaling Quantum-Chemical Methods	11:15-11:45	**3B2-3I**: *Nobuyuki Matubayasi* Extended Concept of Solvation toward Unified Analysis of Molecular Binding in Weakly Ordered Systems	11:15-11:45	**3D2-3I**: *Masayoshi Nakano* Giant Enhancement of the Second Hyperpolarizabilities of Open-Shell Singlet Molecular Systems by an External Electric Field and Donor-Acceptor Substitution
11:45-12:15	**3A2-5I**: *Shuhua Li* New Developments and Applications of the Generalized Energy-Based Fragmentation Approach	11:45-12:00	**3B2-5C**: *Hideaki Takahashi* Computation of Reaction Free Energies by the QM/MM-ER Approach - Exact Treatment of the Many-Body Interactions	11:45-12:15	**3D2-5I**: *Antonio Rizzo* Nonlinear Chiroptical Properties and Spectroscopies
		12:00-12:15	**3B2-6C**: *Yasuteru Shigeta* Classical Cumulant Dynamics		
12:15-13:45 Lunch Break					

3A3. Relativistic Quantum Chemistry (101/Room A) Chair: *Trond Saue*		**3B3. Exciton Dynamics and Spectroscopy** (102/Room B) Chair: *Craig C. Martens*		**3D3. Catalytic Activity** (403/Room D) Chair: *Gernot Frenking*	
13:45-14:15	**3A3-1I**: *Jürgen Gauss* Cost-Effective Treatment of Relativistic Effects	13:45-14:15	**3B3-1I**: *Eitan Geva* Molecular Modeling of the Dynamics and Structure of Molecular Aggregates in Liquid Solution and Their Spectroscopic Signature	13:45-14:15	**3D3-1I**: *Shigeyoshi Sakaki* Theoretical Study of Gas-Adsorption to Metal-Organic-Framework (MOF)
14:15-14:45	**3A3-3I**: *Haruyuki Nakano* Four-Component Relativistic Multireference Perturbation Theory	14:15-14:45	**3B3-3I**: *Oliver Kühn* Multi-Exciton Dynamics in Molecular Aggregates	14:15-14:45	**3D3-3I**: *Ming Wah Wong* Dehydrogenation Mechanism of Chemical Hydrogen Storage Materials: Catalytic Role of Metal
14:45-15:15	**3A3-5I**: *Wenjian Liu* Ideas of Relativistic Quantum Chemistry	14:45-15:00	**3B3-5C**: *Aaron Kelly* Mixed Quantum-Classical Description of Excitation Energy Transfer in a Model Fenna-Matthews-Olsen Complex	14:45-15:15	**3D3-5I**: *Michel Dupuis* Computational Molecular Electrocatalysis: The Role of Proton Relays in H_2 Oxidation and Evolution Catalysts
		15:00-15:30	**3B3-6I**: *Yoshitaka Tanimura* Reduced Hierarchy Equations of Motion Approach to Multidimensional Spectroscopies of Biological Systems		
				15:15-15:30	**3D3-7C**: *Zygmunt Flisak* Theoretical Study of Counter Anion Displacement in Phenoxyimine-Based Catalysts of Ethylene Polymerization Activated with Perfluorophenylborate
		15:30-15:45	**3B3-8C**: *Tsutomu Kawatsu* Bridge-Mediated Electronic Coupling between Two Excited States, Calculating Based on the Localized Slater Determinant	15:30-15:45	**3D3-8C**: *Mia Ledyastuti* Why the Silica Surface Is Negatively Charged at pH=7?
15:45-16:15 Coffee Break					
3A4. Accelerated Method and DFT (101/Room A) Chair: *Michael W. Schmidt*		**3B4. Non-adiabatic Dynamics** (102/Room B) Chair: *Oliver Kühn*		**3D4. Molecular Device** (403/Room D) Chair: *Koichi Yamashita*	
16:15-16:45	**3A4-1I**: *Dmitri G. Fedorov* Recent Development of the Fragment Molecular Orbital Method	16:15-16:45	**3B4-1I**: *Kazuo Takatsuka* Nonadiabatic Theory in Electron Wavepacket Dynamics	16:15-16:45	**3D4-1I**: *Tamar Seideman* Toward Coherent Control in the Nanoscale
16:45-17:15	**3A4-3I**: *Yuji Mochizuki* Fragment Molecular Orbital Calculations with ABINIT-MP(X)	16:45-17:15	**3B4-3I**: *Massimiliano Di Ventra* Stochastic Time-Dependent Current-DFT: A Functional Theory of Open Quantum Systems	16:45-17:15	**3D4-3I**: *YiJing Yan* Hierarchical Equations of Motion for Quantum Dissipation and Quantum Transport
17:15-17:45	**3A4-5I**: *Yan Alexander Wang* Linear-Expansion Shooting Techniques for Accelerating Self-Consistent Field Convergence	17:15-17:30	**3B4-5C**: *Jiří Vaníček* On the Nonadiabaticity of Molecular Quantum Dynamics	17:15-17:30	**3D4-5C**: *Mitsutaka Okumura* Theoretical Study for Pseudo Degenerated Multi-Electron Systems and Applications for Real Systems
		17:30-17:45	**3B4-6C**: *Hyeon-Deuk Kim* Photo-Excited Non-Adiabatic Dynamics in Nano Materials	17:30-17:45	**3D4-6C**: *Kenji Sugisaki* Zero-Field Splitting Tensors of Arylnitrenes: A Theoretical Study
		17:45-18:15	**3B4-7I**: *Koji Ando* Simple Wavepacket Modeling of Electron and Nuclear Dynamics	17:45-18:00	**3D4-7C**: *Marco Anelli* Interactions with Electromagnetic Fields: Frequency-Dependent Magnetizability and Electric Permittivity
				18:00-18:15	**3D4-8C**: *Kresimir Rupnik* Novel Polarization-Phase Selective (PPS) Models: Probing and Imaging Unusual Electronic Behavior
18:30-20:30	**3PP.** Poster Presentation I (404, 405, 410)				

Sunday, September 4, 2011

08:15-	**Registration Desk Open** (Bldg.14)				
4A1. Biochemical Simulation (101/Room A) Chair: *Ulf Ryde*		**4B1. Solvation and Basic Theory** (102/Room B) Chair: *Nobuyuki Matubayasi*		**4C1. Fundamental Method** (201/Room C) Chair: *Frederick R. Manby*	
08:45- 09:15	**4A1-1I**: *Pawel Michal Kozlowski* Computational Modeling of Methyl Transfer Reactions Catalyzed by Cobalamin-Dependent Methionine Synthase Enzyme	08:45- 09:15	**4B1-1I**: *Kenichiro Koga* A General View on Hydrophobicity	08:45- 09:15	**4C1-1I**: *Garnet Kin-Lic Chan* Strong Correlation of Electrons in Molecules and Solids
09:15- 09:30	**4A1-3C**: *Linus Oscar Johannissen* Good Vibrations in Enzymatic H-Tunnelling: The Effect of Pressure on Barrier Compression and Isotope Effects	09:15- 09:45	**4B1-3I**: *Gren Patey* Computational Investigations of Complex Aqueous Solutions and Heterogeneous Ice Nucleation	09:15- 09:45	**4C1-3I**: *So Hirata* The Existence of Thermodynamic Limit and Size-Consistent Design
09:30- 10:00	**4A1-4I**: *Alia Tadjer* MD Simulations of Micelles Formation in $C_{12}E_x$ Solutions				
		09:45- 10:00	**4B1-5C**: *Tokuei Sako* Hund's Rule and Conjugate Fermi Hole in Two-Electron Atomic Systems	09:45- 10:00	**4C1-5C**: *Takashi Tsuchimochi* Generalization of Constrained Unrestricted Mean-Field Methods for Controlling Spin-Contamination: Application to Singlet-Triplet Splittings
10:00- 10:15	**4A1-6C**: *Poonsiri Thipnate* 4D-QSAR Analysis for the Cytotoxicity of Lamellarins against Human Hormone-Dependent T47D Breast Cancer Cells			10:00- 10:15	**4C1-6C**: *James S. M. Anderson* Novel Basis-Set Free Approaches to Solving the Electronic Schrödinger Equation
10:15-10:45 Coffee Break					
Plenary Lecture (201/Room C) Chair: *Shinji Saito*					
10:45- 11:25	**4PL-1**: *Biman Bagchi* Understanding Nucleation Phenomena at Large Metastability: From Gas-Liquid Transition to Metastable Solids and Polymers				
4A2. Solid Surface (101/Room A) Chair: *Mitsutaka Okumura*		**4B2. Molecular Function** (102/Room B) Chair: *Antonio Rizzo*		**4C2. Frontier in DFT** (201/Room C) Chair: *Peter James Knowles*	
11:30- 11:45	**4A2-1C**: *Tomokazu Yasuike* Open-Boundary Cluster Model for Electronic Excited States of Adsorbate-Surface Systems	11:30- 11:45	**4B2-1C**: *Philippe Baranek* First-Principles Modelling of Dynamic, Dielectric and Catalytic Properties of Various Materials for the Production and Storage of Energy	11:30- 12:00	**4C2-1I**: *Viktor N. Staroverov* Orbital-Dependent Energy Expressions for Kohn-Sham Potentials
11:45- 12:00	**4A2-2C**: *Jun Haruyama* Excited-State Nuclear Forces on the Adiabatic Potential Energy Surfaces by Time-Dependent Density Functional Theory	11:45- 12:00	**4B2-2C**: *Takuya Minami* Density Functional Theory Study on Charge-Transfer and Local Excitation States of Pentacene/C_{60} Model Complex		
12:00- 12:15	**4A2-3C**: *Jaehoon Jung* Role of the Interface in the Chemical Reactivity of Ultrathin Oxide Film	12:00- 12:15	**4B2-3C**: *Hitoshi Fukui* Second Hyperpolarizabilities of Open-Shell Singlet Metal-Metal Multiple Bonded Systems	12:00- 12:15	**4C2-3C**: *Chunping Hu* TDDFT Study on Quantization Behaviors of Nonadiabatic Couplings in Polyatomic Systems
12:15-13:45 Lunch Break					
Plenary Lecture (201/Room C) Chair: *Kazuo Takatsuka*					
13:45- 14:25	**4PL-2**: *James Thomas Hynes* Short-Time Frictional Solvent Effects on Conical Intersection Dynamics for a Model Photoisomerization				

4A3. Biological Reaction (101/Room A) Chair: *Pawel Michal Kozlowski*		**4B3. Reaction Dynamics** (102/Room B) Chair: *Irene Burghardt*		**4C3. Embedded Theory and Large System** (201/Room C) Chair: *Takahito Nakajima*	
14:30-15:00	**4A3-1I**: *Ulf Ryde* Comparison of QM Cluster Calculations and QM/MM Calculations for Reactions in Proteins	14:30-15:00	**4B3-1I**: *Oleg S. Vasyutinskii* Universal Product Angular-Momentum Distributions in Photodissociation and Reaction Collisions	14:30-15:00	**4C3-1I**: *Frederick R. Manby* Embedding as a New Perspective on Electronic Structure Theory
15:00-15:15	**4A3-3C**: *Lung Wa Chung* Reaction Mechanisms of Novel Fluorescent Proteins	15:00-15:30	**4B3-3I**: *Anne B. McCoy* Studies of Solvent Mediated Long-Range Electron Transfer $IBr^{-*}...CO_2$ and Excited State Dynamics of ICN^{-*}	15:00-15:30	**4C3-3I**: *Lucas Visscher* Towards an Accurate WFT-in-DFT Subsystem Approach to Computational Chemistry
15:15-15:30	**4A3-4C**: *Pornthip Boonsri* Structural and Energetic Analysis of Mutant K103N HIV-1 Reverse Transcriptase/Efavirenz Complex Using ONIOM Calculations				
				15:30-15:45	**4C3-5C**: *Takeo Hoshi* Large-Scale Electronic Structure Calculation with ELSES and Its Application to Conjugated Polymer
15:45-16:15 Coffee Break					
4A4. DNA and Molecular Recognition (101/Room A) Chair: *Yasuteru Shigeta*		**4B4. Solvation and Ab Initio Molecular Dynamics** (102/Room B) Chair: *Rossend Rey*		**4C4. Concept in Quantum Chemistry** (201/Room C) Chair: *Garnet Chan*	
16:15-16:45	**4A4-1I**: *Marcus Elstner* A Coarse Grained QM/MM Approach for the Description of Hole Transfer in DNA	16:15-16:45	**4B4-1I**: *Sotiris S. Xantheas* The Performance of Density Functional Theory for Hydrogen Bonded Systems: Shortcomings and Solutions	16:15-16:45	**4C4-1I**: *Michael W. Schmidt* Kinetic Energy and Chemical Binding
16:45-17:00	**4A4-3C**: *Prapasiri Pongprayoon* Biomimetic Design of Charged Brush-like Nanopores: Simulation Studies	16:45-17:00	**4B4-3C**: *Hirotoshi Mori* Ab Initio Fragment Molecular Orbital-Molecular Dynamics (FMO-MD) Study of Solvation Differences between Cis- and Trans-Platins in Water	16:45-17:15	**4C4-3I**: *Edward F. Valeev* Quantum Chemistry Beyond Atomic Orbitals and Slater Determinants
17:00-17:15	**4A4-4C**: *Yutaka Maruyama* Solvent and Salt Effects on Structural Stability of Human Telomere	17:00-17:15	**4B4-4C**: *Masanori Tachikawa* Multi Component Molecular Theory for Hydrogen Bonded Systems and Positronic Compounds		
17:15-17:30	**4A4-5C**: *Jörg Gruneberg* Complexity in Molecular Recognition	17:15-17:30	**4B4-5C**: *Himanshu Mishra* Anions Dramatically Enhance Proton Transfer across Water Interfaces	17:15-17:30	**4C4-5C**: *Elena F. Sheka* Why sp^2 Nanosilicons Should Not Form: Insight from Quantum Chemistry
Plenary Lecture (201/Room C) Chair: *Per E.M. Siegbahn*					
17:35-18:15	**4PL-3**: *Leo Radom* A Computational Approach to the Study of Free Radical Chemistry				
18:30-20:30	**4PP.** Poster Presentation II (404, 405, 410)				

Monday, September 5, 2011

08:15-	**Registration Desk Open** (Bldg.14)				
5A1. Water Spectroscopy and Structure (101/Room A) Chair: *Hideaki Takahashi*		**5B1. Quantum Dynamics** (102/Room B) Chair: *YiJing Yan*		**5C1. Electron Correlation Theory** (201/Room C) Chair: *Haruyuki Nakano*	
08:45-09:15	**5A1-1I**: *John M. Herbert* Structure and Spectroscopy of the Hydrated Electron: Polarizable QM/MM Simulations	08:45-09:15	**5B1-1I**: *Irene Burghardt* Quantum Dynamics of Photoprocesses in Extended Molecular Systems: Coherence and Correlations at the Nanoscale	08:45-09:15	**5C1-1I**: *Wim Klopper* The MP2-F12 Method in the Turbomole Program Package
09:15-09:30	**5A1-3C**: *Hajime Torii* Effects of Intermolecular Electron Density Modulations on the Terahertz Spectral Intensity of Liquid Water	09:15-09:45	**5B1-3I**: *Michael Thoss* Quantum Dynamical Treatment of Systems with Many Degrees of Freedom Using Time-Dependent Multiconfiguration Methods	09:15-09:45	**5C1-3I**: *David Peter Tew* Local Explicitly Correlated MP2 Theory Using Pair Natural Orbitals
09:30-09:45	**5A1-4C**: *Kaito Takahashi* Theoretical Analysis on the Effect of Intramolecular Hydrogen Bonding on the Overtone Spectra in Simple 1-n Alkanediols				
09:45-10:00	**5A1-5C**: *Urszula Góra* Revealing Mysteries of the Water Hexamer	09:45-10:00	**5B1-5C**: *Hideo Sekino* Quantum Dynamics Simulation in Balanced Resolution Representation in Time-Space	09:45-10:00	**5C1-5C**: *Taweetham Limpanuparb* Resolving Coulomb Operator - A New Approach toward Faster QM Methods
10:00-10:15	**5A1-6C**: *Jer-Lai Kuo* On the Development of a First-Principle Based Multi-Model Method to Study Aqueous Systems: From Clusters, Interfaces to Condensed Phases	10:00-10:15	**5B1-6C**: *Philipp Marquetand* Semiclassical Molecular Dynamics Including Spin-Orbit Coupling and Electric Fields	10:00-10:15	**5C1-6C**: *Philip E. Hoggan* New Three-Body Correlation Expression Applied to Solid Surface Quantum Monte Carlo Simulation
10:15-10:45 Coffee Break					
Plenary Lecture (201/Room C) Chair: *Piotr Piecuch*					
10:45-11:25	**5PL-1**: *Hiroshi Nakatsuji* Quantum Chemistry in Schrödinger Accuracy				
5A2. Meso/Nano Systems (101/Room A) Chair: *Leo Radom*		**5B2. GPGPU** (102/Room B) Chair: *Jiří Pittner*		**5C2. Strong Correlation** (201/Room C) Chair: *Willem Klopper*	
11:30-12:00	**5A2-1I**: *Julian D. Gale* Nucleation and Growth of Calcium Carbonate: How Non-Classical Is It?	11:30-12:00	**5B2-1I**: *Todd J. Martinez* Electronic Structure and First Principles Dynamics on Graphical Processing Units	11:30-12:00	**5C2-1I**: *Gustavo E. Scuseria* Strong Correlations from Constrained Mean-Field Approaches
12:00-12:15	**5A2-3C**: *Oraphan Saengsawang* Novel ZIFs Material as Molecular Separator Studied by Computer-Aided Modeling Approaches				
12:15-14:00 Lunch Break					
14:00- Excursion					

Tuesday, September 6, 2011

08:15-	**Registration Desk Open** (Bldg.14)				
6A1. Exotic Bond (101/Room A) Chair: *Chin-Hui Yu*		**6B1. Simulation of Hydrogen Bonded System** (102/Room B) Chair: *Sotiris S. Xantheas*		**6C1. Coupled Cluster Method** (201/Room C) Chair: *So Hirata*	
08:45- 09:15	**6A1-1I**: *Shigeru Nagase* Interesting Bonds Formed by Heavier Main Group Elements	08:45- 09:15	**6B1-1I**: *Craig C. Martens* Coherent Quantum Processes in Thermal and Nonequilibrium Environments	08:45- 09:15	**6C1-1I**: *Peter James Knowles* Approximate Variational Coupled Cluster Theory
09:15- 09:45	**6A1-3I**: *Gernot Frenking* Donor-Acceptor Complexes of Main Group Elements with Unusual Bonds	09:15- 09:45	**6B1-3I**: *Rossend Rey* Energy Relaxation Pathways in Liquid Water	09:15- 09:45	**6C1-3I**: *Mihály Kállay* General Implementation of the Relativistic Coupled-Cluster Method
09:45- 10:00	**6A1-5C**: *Jen-Shiang K. Yu* Accurate Evaluation of Very-Low Ionization Potentials of Group VI Metal-Metal Coordination Compounds	09:45- 10:00	**6B1-5C**: *Motoyuki Shiga* Ab Initio Path Integral Simulations of Hydrogen Bonded Systems	09:45- 10:00	**6C1-5C**: *Ágnes Szabados* Unitary Perturbation Theory for the Electron Correlation Problem
10:00- 10:15	**6A1-6C**: *Ulises Miranda* State-of-the-Art Calculation of the Ground State of the Sc_2 Dimer	10:00- 10:15	**6B1-6C**: *Young Min Rhee* Interpolated Potential Energy Surfaces for Condensed Phase Molecular Dynamics	10:00- 10:15	**6C1-6C**: *Monika Agnieszka Musiał* Coupled Cluster Method in Application to the Double Ionized and Double Electron Attached States
10:15-10:45 Coffee Break					
Plenary Lecture (201/Room C) Chair: *Jürgen Gauss*					
10:45- 11:25	**6PL-1**: *Rodney J. Bartlett* Looking at the World from a Coupled-Cluster Perspective				
6A2. Fullerene and Carbon Nanotube (101/Room A) Chair: *Shigeru Nagase*		**6B2. Non-adiabatic Ab Initio Molecular Dynamics** (102/Room B) Chair: *Koji Ando*		**6C2. Multireference Explicitly-correlated Theory** (201/Room C) Chair: *David Peter Tew*	
11:30- 11:45	**6A2-1C**: *Matthew Andrew Addicoat* An Optimized Genetic Algorithm for the Functionalization of Fullerenes	11:30- 12:00	**6B2-1I**: *Tetsuya Taketsugu* Incorporation of Nuclear Quantum Effects to Ab Initio Molecular Dynamics Approach	11:30- 12:00	**6C2-1I**: *Jozef Noga* Multireference F12 Coupled Cluster Theory
11:45- 12:00	**6A2-2C**: *Alister James Page* Mechanisms of Carbon-Based Nanostructure Self-Assembly: Insights from Density-Functional Tight-Binding Molecular Dynamics				
12:00- 12:15	**6A2-3C**: *Stephan Irle* New Insights from Quantum Chemical Molecular Dynamics Simulations on the Formation Mechanism of Metallofullerenes	12:00- 12:15	**6B2-3C**: *Toshifumi Mori* The Role of Rydberg State in the Photochemistry of Ethylene	12:00- 12:15	**6C2-3C**: *Toru Shiozaki* Multireference Explicitly Correlated F12 Theories
12:15-13:45 Lunch Break					
Plenary Lecture (201/Room C) Chair: *Suryanarayana S. Ramasesha*					
13:45- 14:25	**6PL-2**: *Kizashi Yamaguchi* Developments of Broken Symmetry Methods - Application to the $CaMn_4O_5$ Cluster at OEC of PSII Refined to 1.9 Å X-Ray Resolution				

6A3. Nanotube and Extended Carbon System (101/Room A) Chair: *Frédéric Castet*		**6B3. Electronic Structure and Reaction** (102/Room B) Chair: *Kenneth Ruud*		**6C3. Linear-scaling Method in Quantum Chemistry** (201/Room C) Chair: *David Sherrill*	
14:30-15:00	**6A3-1I**: *Haibin Su* Multi-Paradigm Simulations at the Nanoscale: Methodology and Applications to Functional Carbon Materials	14:30-15:00	**6B3-1I**: *Péter R. Surján* Composite Particles in Quantum Chemistry: From Two-Electron Bonds to Cold Atoms	14:30-15:00	**6C3-1I**: *Poul Jørgensen* The Divide-Expand-Consolidate (DEC) Coupled Cluster Method. A Linear-Scaling Approach with Energy-Based Error Control
15:00-15:15	**6A3-3C**: *Kaoru Yamazaki* Stone-Wales Rearrangement in Pyrene via the S_1 State	15:00-15:30	**6B3-3I**: *Benoît Champagne* Theoretical Aspects on the Evaluation and Interpretation of the Third-Order Nonlinear Optical Properties of Diradical Compounds	15:00-15:30	**6C3-3I**: *Piotr Piecuch* Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems and Their Multi-Level Generalizations
15:15-15:30	**6A3-4C**: *Balázs Hajgató* Symmetry Broken Edge States of Linear Acenes: Artifact or Reality?				
15:30-15:45	**6A3-5C**: *Marco Antonio Chaer Nascimento* Alkali Halides Nanotubes: Structure and Stability	15:30-15:45	**6B3-5C**: *Vitaly G. Kiselev* Tautomeric Equilibria and Thermal Decomposition of Nitrogen-Rich Heterocycles: New Insights from High-Level Ab Initio Calculations	15:30-15:45	**6C3-5C**: *Yuriko Aoki* Highly Accurate Linear Scaling Method -Elongation Method- and Its Applications to Large Systems
15:45-16:00	**6A3-6C**: *Yousung Jung* Favorable Confinement of Water inside the Carbon Nanotubes Is Driven by Hydrogen Bond and Entropy	15:45-16:00	**6B3-6C**: *Tamás Veszprémi* Quantum Chemical Simulations of Chemical Vapor Deposition Reactions	15:45-16:00	**6C3-6C**: *Masato Kobayashi* Divide-and-Conquer Evaluation of Optical Response Properties
16:00-16:30 Coffee Break					
Plenary Lecture (201/Room C) Chair: *Wenjian Liu*					
16:30-17:10	**6PL-3**: *Werner Kutzelnigg* Rate of Convergence of Basis Expansions in Quantum Chemistry				
6A4. Photosynthesis (101/Room A) Chair: *Kazunari Yoshizawa*		**6B4. Bio/Cluster System** (102/Room B) Chair: *Michel Dupuis*		**6C4. Weak Interaction and Concept in DFT** (201/Room C) Chair: *Gustavo E. Scuseria*	
17:15-17:45	**6A4-1I**: *Per E.M. Siegbahn* The Structure of the Water Oxidizing Complex in Photosystem II	17:15-17:45	**6B4-1I**: *Spiridoula Matsika* Theoretical Studies of Photophysical Events in π-Stacked Dimers of Nucleobases	17:15-17:45	**6C4-1I**: *Andreas Savin* Correcting Model Energies by Numerically Integrating along the Adiabatic Connection and a Link to Density Functional Theory
17:45-18:15	**6A4-3I**: *Lyudmila V. Slipchenko* Exciton Coupling and Energy Transfer: From Prototypical Bichromophores to Photosynthetic Proteins	17:45-18:00	**6B4-3C**: *Gerardo Delgado-Barrio* Quantum Chemistry Calculations in Helium Clusters Doped with Diatomic Molecules	17:45-18:15	**6C4-3I**: *C. David Sherrill* Assessing the Performance of Density-Functional and Wavefunction Quantum Chemical Methods for Noncovalent Interactions
		18:00-18:15	**6B4-4C**: *Péter G. Szalay* Excited States of Nucleotide Bases and Nucleotides: Matrix Isolation Spectroscopic and Quantum Chemical Study		
18:15-18:45	**6A4-5I**: *Yuan-Chung Cheng* Electronic Coherence Effects in Photosynthetic Light Harvesting	18:15-18:30	**6B4-5C**: *Warabhorn Boonyarat* Distribution and Orientation of Retinol in Dipalmitoylphosphatidylcholine Bilayer	18:15-18:30	**6C4-5C**: *Rafał Podeszwa* Dispersionless Density Functional Theory with Physically Sound Dispersion Correction
				18:30-18:45	**6C4-6C**: *Yousung Jung* Cubic Scaling Doubly Hybrid Density Functional Method Close to Chemical Accuracy and Its Gradient Theory
18:45-19:30 Snack and Coffee Break					
Plenary Lecture (201/Room C) Chair: *Roi Baer*					
19:30-20:10	**6PL-4**: *Eberhard K.U. Gross* Analysis and Control of Electronic Motion in the Time Domain				

Wednesday, September 7, 2011

08:15-	**Registration Desk Open** (Bldg.14)				
7A1. Charge Separation (101/Room A) Chair: *Masayoshi Nakano*		**7B1. Spectroscopy** (102/Room B) Chair: *Lyudmila V.Slipchenko*		**7C1. Range-separated and Constrained DFT** (201/Room C) Chair: *Peter M.W. Gill*	
08:45- 09:15	**7A1-1I**: *Frédéric Castet* Interfacial Dipole and Geminate Pair Energetics at Pentacene/C60 Heterojunctions	08:45- 09:15	**7B1-1I**: *Peter Saalfrank* Real-Time Electron Dynamics with Correlated Wavefunction Methods	08:45- 09:15	**7C1-1I**: *Roi Baer* A First Principles Density Functional Approach for Charge Transfer & Transport
09:15- 09:45	**7A1-3I**: *Suryanarayana Sastry Ramasesha* Modeling Dynamic Electronic Processes in Organic Electronic Devices	09:15- 09:45	**7B1-3I**: *Trond Saue* Mössbauer Spectroscopy for Heavy Elements: A 4-Component Relativistic Study	09:15- 09:45	**7C1-3I**: *Troy Van Voorhis* Better Ways to Get Excited States and Reaction Barriers from DFT
09:45- 10:15	**7A1-5I**: *Chao-Ping Hsu* Theories and Applications for Electronic Coupling in Electronic Transfer and Excitation Energy Transfer	09:45- 10:00	**7B1-5C**: *Ryoichi Fukuda* Electronic Excited States of Large Conjugated Molecules	09:45- 10:15	**7C1-5I**: *Takao Tsuneda* Recent Progress in Long-Range Corrected Density Functional Theory
		10:00- 10:15	**7B1-6C**: *Malinee Promkatkaew* Absorption and Emission Properties of the F, OH and NO_2 Substituted Cinnamates: A TD-DFT Investigation		
10:15-10:45 Coffee Break					
Plenary Lecture (201/Room C) Chair: *Benoît Champagne*					
10:45- 11:25	**7PL-1**: *Bernard Kirtman* Treatment of Vibronic Properties in Infinite Periodic Systems				
Molecular Device (101/Room A) Chair: *Katsuyuki Nobusada*		**X-ray** (102/Room B) Chair: *Masahiro Ehara*		**Concept in Quantum Chemistry** (201/Room C) Chair: *Mark S. Gordon*	
11:30- 12:00	**7A2-1I**: *Oleg Prezhdo* Quantum Dots – Artificial Atoms, Large Molecules or Small Pieces of Bulk? Insights from Time-Domain Ab Initio Studies	11:30- 12:00	**7B2-1I**: *Pascal Lablanquie* Properties of Hollow Molecules Containing a Double Core Hole, Probed by Single-Photon Double Ionization	11:30- 12:00	**7C2-1I**: *Peter M.W. Gill* Improved DFT from Electrons on a Sphere
12:00- 12:15	**7A2-3C**: *Tomoyuki Hayashi* Electron Tunneling in Respiratory Complex I	12:00- 12:15	**7B2-3C**: *Petra Ruth Kaprálová-Žd'ánská* Ionization of Helium in Strong XUV Laser Pulses - A Theoretical Simulation	12:00- 12:15	**7C2-3C**: *Kalidas D. Sen* Electronic Structure Calculations of Spherically Confined $N \geq 1$ Electron Atoms
12:15-13:45 Lunch Break					
Plenary Lecture (201/Room C) Chair: *Hiroshi Nakatsuji*					
13:45- 14:25	**7PL-2**: *Josef Michl* Singlet Fission				

7A3. Water and Titanium Oxide (101/Room A) Chair: *John M. Herbert*		**7B3. Potential Energy Surface** (102/Room B) Chair: *Tetsuya Taketsugu*		**7C3. QM/MM and Large System** (201/Room C) Chair: *Troy Van Voorhis*	
14:30-14:45	**7A3-1C**: *Haibo Ma* Theoretical Study of the Structure Order in Supercritical Water	14:30-15:00	**7B3-1I**: *Koichi Ohno* Automated Exploration of Global Reaction Route Maps on the Potential Energy Surface	14:30-14:45	**7C3-1C**: *Glenn John Martyna* Towards an Order N Scaling Force Field with an Accurate Treatment of Many-Body Dispersion and Polarization
14:45-15:00	**7A3-2C**: *Samantha Jenkins* Spanning QTAIM Topology Phase Diagrams of Isomer Sets			14:45-15:00	**7C3-2C**: *Eirik F. da Silva* Development of the Explicit Solvation Shell Model
15:00-15:15	**7A3-3C**: *Kaito Takahashi* Water Catalyzed Overtone Induced Reaction for Hydrate Fluoromethanol: Fact of Fiction?	15:00-15:15	**7B3-3C**: *Satoshi Maeda* Nonadiabatic Reactions Studied by Automated Reaction Path Search Methods	15:00-15:30	**7C3-3I**: *Angela K. Wilson* Ab Initio Composite Methods: Beyond Ground State Main Group Species
15:15-15:30	**7A3-4C**: *Suehiro Iwata* Low Energy Structures of $(H_2O)_{25}$ Studied with Basin Paving Monte Carlo Simulation and with Perturbation Theory Based on Locally Projected Molecular Orbitals	15:15-15:45	**7B3-4I**: *Chin-Hui Yu* Strong and Weak Coordinates within the Context of the Multi-Coordinate Driven Algorithm		
15:30-15:45	**7A3-5C**: *Nurbosyn U. Zhanpeisov* Structure and Chemical Activity of Transition Metal Oxides and New Carbon K4 Structures: A Theoretical DFT Study			15:30-16:00	**7C3-5I**: *Mark S. Gordon* Solvent Effects on Electronic Excited States
15:45-16:00	**7A3-6C**: *Masato Sumita* Interface Water on TiO_2 Anatase (101) and (001) Surfaces: First-Principles Study with TiO_2 Slabs Dipped in Bulk Water	15:45-16:00	**7B3-6C**: *Pietro Faccioli* Dominant Reaction Pathways of Macromolecules: From Classical to Quantum Mechanical Calculations		
16:00-16:30 Coffee Break					
Plenary Lecture (201/Room C) Chair: *Trygve Helgaker*					
16:30-17:10	**7PL-3**: *Debashis Mukherjee* State-Specific Multi-Reference Coupled Cluster Formalisms: An Overview of a Suite of Recent Developments				
19:00- Banquet (Chinzan-so)					

Thursday, September 8, 2011

08:15-	**Registration Desk Open** (Bldg.14)				
8A1. Conductivity (101/Room A) Chair: *Michiel Sprik*		**8B1. TDDFT** (102/Room B) Chair: *Peter Saalfrank*		**8C1. Strong Correlation** (201/Room C) Chair: *Jozef Noga*	
08:45- 09:15	**8A1-1I**: *Koichi Yamashita* Theoretical Studies on Photoinduced Charge Separation of Molecular Hetero-Junction and Dye-Sensitized Solar Cells	08:45- 09:15	**8B1-1I**: *Kazuhiro Yabana* Real-Time TDDFT Calculation in Molecules and Solids	08:45- 09:15	**8C1-1I**: *Jiří Pittner* Towards Quantum Chemistry on Quantum Computers
09:15- 09:45	**8A1-3I**: *Matthias Ernzerhof* Orbital Theories for Molecular Electronic Devices	09:15- 09:45	**8B1-3I**: *Katsuyuki Nobusada* Photoinduced Electron Dynamics in Nanostructures: Nonuniform and Self-Consistent Light-Matter Interactions	09:15- 09:45	**8C1-3I**: *Wesley D. Allen* Advances in Multireference Coupled Cluster Theory
09:45- 10:15	**8A1-5I**: *Kwang S. Kim* Molecular Electronics and Ultrafast DNA Sequencing	09:45- 10:15	**8B1-5I**: *John F. Dobson* An Efficient Non-Pairwise-Additive Correlation Energy Functional for Dispersion Forces	09:45- 10:15	**8C1-5I**: *Takeshi Yanai* Advanced Multireference Quantum Chemistry with Large Active Space
10:15-10:45 Coffee Break					
8A2. Titanium Oxide (101/Room A) Chair: *Yutaka Imamura*		**8B2. Molecular Vibration** (102/Room B) Chair: *Suehiro Iwata*		**8C2. Fundamental Method** (201/Room C) Chair: *Takeshi Yanai*	
10:45- 11:15	**8A2-1I**: *Michiel Sprik* Oxidative Dehydrogenation of a Terminal Water at the Rutile TiO_2 (110)-Water Interface	10:45- 11:15	**8B2-1I**: *Kenneth Ruud* Analytic Calculations of Anharmonic Effects in Vibrational Spectra	10:45- 11:00	**8C2-1C**: *Kazuhide Ichikawa* Study of Simulation Method of Time Evolution in Rigged QED
				11:00- 11:30	**8C2-2I**: *Erkki J. Brändas* Analytical Principles and the Evolution of Physical Laws
11:15- 11:30	**8A2-3C**: *Keitaro Sodeyama* Adsorption and Excitation of Black-Dye on TiO_2 Anatase (101) Surface for Dye-Sensitized Solar Cells	11:15- 11:30	**8B2-3C**: *Kiyoshi Yagi* Anharmonic Vibrational Theory for Large Polyatomic Molecules		
Plenary Lecture (201/Room C) Chair: *Hiromi Nakai*					
11:35- 12:15	**8PL-1**: *Kimihiko Hirao* The K Supercomputer and Recent Advances in LC-DFT				
12:15- 12:45	**Closing Ceremony** (201/Room C)				