Sunday — Provisional Scientific Programme. Disclaimer: Neither the time table, nor the order of speakers is final, and may change until 30 November. — **Sunday**

Provisional

Sunday

Time	Sunday
13:30-14:00	OPENING
14:00-14:50	Schrödinger Medallist (2005) Plenary Lecture: Michele Parrinello "Pushing Back the Frontiers of Molecular Dynamics Simulations"
14:50-15:30	Dirac Medallist (2005) Plenary Lecture: Ursula Röthlisberger "From Enzymatic Reactions to Photoexcited Proteins: QM/MM Car-Parinello Simulations of Biological Systems"
15:30-16:00	Break
16:00-16:50	Schrödinger Medallist (2002) Plenary Lecture: Walter Thiel "Computational Methods for Large Molecules"
16:50-17:30	Dirac Medallist (2003) Plenary Lecture: Peter Schreiner "When can Organic Biradicals be "Stable"?"
18:00-20:00	Drinks and Light Meal

Provisional

Monday

Time	Informatics	Enzyme Catalysis	Molecular Structure	Electronic Structure	Industrial Catalysis	Reaction Mechanisms
08:00-08:50	Plenary Lecture: Jill Gready "Elusive Players in Enzyme Catalysis: Defining Protonation States and Proton Shuttles"					
	Protein Evolution and Protein Design		**The Theory and Modelling of Complex Systems**	**Interesting Properties of Large Molecular Systems**	**Metal and Oxide-Supported Metal Catalysis: Materials and Reactivity Aspects**	**Chemical Reaction Mechanisms**
09:00-09:30	SL Richard Goldstein **Deciphering patterns of site substitutions in protein evolution**		SL John Brady **Molecular Dynamics and Neutron Diffraction Studies of the Structuring of Water by Carbohydrates and Other Solutes**	SL Shigeru Nagase **Large Spaces and Flexible Structures Provided by Nanomolecular Systems**	SL Notker Rösch Metal and Oxide-Supported Metal Catalysis: Materials and Reactivity Aspects	SL Henry F. Schaefer
09:30-10:00	I Neil Ostlund HyperProtein: A New Software Tool at the Interface Between Molecular Modeling and Bioinformatics		I Valerie Daggett Towards Characterization of Protein Folding/Unfolding at Atomic Resolution	I Kwang S. Kim Nanomaterials, Nanodevices, and Nanosensors: De Novo Design Approach based on Nanorecognition.	I Francesc Illas Unraveling molecular mechanisms in heterogeneous catalysis models through strong theory and experiment interaction	I Holger Bettinger Mechanistic Investigations on the Sidewall-Addition to Carbon Nanotubes
10:00-10:30	Break					
10:30-11:00	I David Pollock Structure, Function, and Context-Dependent Evolution in Vertebrate Mitochondrial Genomes		I Michael Levitt Protein Structure Prediction	I William A. Lester, Jr. Recent Developments in Quantum Monte Carlo for Electronic Structure: Methods and Applications to Bio and Other Systems.	I Peijun Hu A Density Functional Theory Study of CO Oxidation on Au-Based Catalysts	I Paul Geerlings Reactivity Descriptors from Density Functional Theory : Application in Organic and Inorganic Chemistry
11:00-11:30	I Christopher Voigt Synthetic Design of Bacterial Pathogens		I Tom Woolf Molecular Dynamics of Membrane Systems: Membrane Proteins, Salt, Peptide Folding, and Fusion	I Hans Peter Lüthi "Measuring" Electron Delocalization in Linearly p-conjugated Systems.	I Gianfranc Pacchioni METAL ATOMS AND CLUSTERS ON OXIDE THIN FILMS: MODEL SYSTEMS OF SUPPORTED CATALYSTS	I Bill Hase Direct dynamics simulations of atomic-level gas-phase organic reaction mechanisms. post-transition state dynamics
11:30-12:00	IC Siegfried Höfinger A Poisson-Boltzmann Solver running on the specialized computer chip MD-GRAPE-2: a case study on the effect of explicit consideration of counter ions.		I Axel Brunger Structure and mechanism of the ATPase VCP/p97: computational challenges for structure determination at low resolution	I Mark S Gordon Scalable Electronic Structure Theory: Methods and Applications	I Malgorzata Witko Heterogeneity of surface of oxide-based catalysts. Cluster DFT Studies	I David Sherrill Energy Landscapes from Pi-Stacking to Bond-Breaking
12:00-12:30	IC Jörg Grunenberg Direct Assessment of Interresidue Forces in Biomolecules Using Theoretical Compliance Constants		IC Patricia Hunt Solute-Solvent and Solvent-Solvent Interactions of Molecular Liquids	I Kazuo Kitaura Fragment molecular orbital (FMO) method for all electron calculations of very large molecules.	I Georgi N. Vayssilov Density functional model studies of local structure and chemical behavior of metal species in zeolites	I Greg Tschumper Toward ab Initio Theoretical Predictions of Chemical Reactions
12:30-14:00	Lunch					
14:00-14:50	Plenary Lecture: Rodney Bartlett "From ab Initio DFT to Coupled-CLuster Theory and NMR Coupling Constants"					
15:00-15:20	C Holger Merlitz High Throughput in-silico screening against flexible protein receptors.		C Arthur Mc Gready Novel Computational Methodology for analysing protein ligand/binding sites by use of Vicinity Analysis	C Benedetta Mennucci Excitation energy transfers in condensed phases	C Justin T. Fermann xxx	C Daniel Peeters Some substituent effects in Diels-Alder reactions
15:20:15:40	C T. Khayamian Wavelet Neural Network Modeling in Quantitative Structure Property Relationship		C xxx xxx	C Rubén Contreras Scalar Couplings as Probe to Study s-Hyperconjugative Interactions in 1-F,4-X-Cubanes and 1-X-3-CH3-bicyclo[1.1.1]-pentanes: A DFT and Experimental Study.	C Kaido Sillar Computational modelling of the reaction centres in extended systems: The study of the acid sites in zeolite ZSM-5 using the ONIOM method	C Noah ASARE-DONKOR SEMI - EMPIRICAL PM3(tm) MOLECULAR ORBITAL (MO) STUDY OF ETHYLENE INSERTION INTO THE M CH3 BOND OF HOMOGENEOUS ANSA BIS (INDENYL) GROUP IV METALLOCENE CATALYSTS
15:40-16:00	C Francesco Luigi Gervasio Flexible Docking in Solution Using Metadynamics		C Jörg Grunenberg Direct Assessment of Interresidue Forces in Biomolecules Using Theoretical Compliance Constants	C Jurgen Stohner Parity Violation in Chiral Molecules: Immediate Consequences in Molecular Spectroscopy.	C Edward Jeffery Keto-enol isomerisation on the surfaces of transition metals: A periodic DFT study	C Anatoly Stepanov Simulation of proton transfer dynamics in the hydrogen bond of benzoic acid dimmers at low temperatures
16:00-16:20	Break					
16:20-16:40	C Mehran Jalaie Molecular Chopper: An Automated Scaffold Linker Replacement Program.		C Dusanka Janezic Analytical - Numerical Approach to Molecular Dynamics Integration	C Ulrike Salzner Excited and Charged States of Conjugated p-Systems	C Thomas Strassner Inverse Isotope Effects of a late Transition Metal Olefin Polymerization Catalyst- a DFT Study	C Marialore Sulpizi Electron Transfer Induced Dissociation of Chloro-Cyano-Benzene Radical Anion: Driving Chemical Reactions via Charge Restraint
16:40-17:00	C Marcus C. Durrant Darwin meets Schrödinger: Quantum-Directed Virtual Evolution.		C Hendrick Heinz Atomic Charges for Classical Simulations of Polar Systems	C Kristine Pierloot Role of the molybdopterin ligand in the catalytic activity of oxomolybdenum enzymes: a theoretical investigation on (Tp)MoO(S-S) model compounds.	C Rudy Coquet Methane activation over MoO3(010), an ab initio study	C Shin NAKAMURA Theoretical Study of Organic Functional Molecules; on the Role of Conical Intersection
17:00-17:20	C Gemma L. Holliday Analysing Nature's Catalytic Diversity		C Olivier Lamarche An Anisotropic Force Field based on Quantum Chemical Topology	C Robert Berger Two-component approach to parity violating energy differences between mirror-image molecules	C Micael Baudin The role of transient distortions in modeling reactivity of metal oxide surfaces.	C T. Veszprémi Dimerization and trimerization of Phosphaacetylene. A mechanistic study

Provisional

Tuesday

Time	Informatics	Enzyme Catalysis	Molecular Structure	Electronic Structure	Industrial Catalysis	Reaction Mechanisms
08:00-08:50	Plenary Lecture: Hugh Kubinyi "Changing Paradigms in Drug Discovery"					
	Computational Chemistry - A Vital Tool in Modern Drug Design	**Quantum Mechanical Prediction of Enzyme Mechanisms**	**Theoretical Studies of Conformational Transitions in Biological Systems**	**Electronic Structure of Molecules, Clusters and Solids**		**Reaction Mechanisms in the Condensed Phase III: Biological Systems**
09:00-09:30	SL Mike M Hann **What we can and can not do in Computational Chemistry in support of Drug Discovery.**	SL Kendall Houk **Principles of Enzyme Proficiency and Design: Computational Studies of Enzyme Catalysis**	SL Alex MacKerell **Base flipping and sequence specificity by the (cytosine-C5)-methyltransferase from HhaI**	SL Eluvathingal D. Jemmis **Analogies Between Boron and Carbon: Electronic Structure and Electron Counting Rules.**		SL Jiali Gao
09:30-10:00	I Jonathan S. Mason 3D Pharmacophoric and Biological Fingerprints – Combining information from ligands and protein targets to enhance drug discovery applications.	I William Jorgensen QM/MM Studies of Organic and Enzymatic Reactions	I Michael Feig Implicit Modelling of Heterogeneous Cellular Environments: Applications to Integral Membrane Proteins	I G. Narahiri Sastry Computational studies on siblings en-route to fullerenes: Study of curved polycyclic aromatic hydrocarbons		I Kenneth Merz The Role of Quantum Mechanics in Structure-Based Drug Design
10:00-10:30	Break					
10:30-11:00	I Tim Clark Modeling, QSAR and QSPR based on the electron density.	I Graham Richards Pattern recognition and grid computing in drug discovery	I Ian Gould Molecular Dynamics simulations of LysRS –An Asymmetric State	I Jerzy Leszczynski Interactions of the DNA Fragments with Solvents and Metal Ions		I Piotr Paneth Modeling of Enzyme-catalyzed Reactions Based on Kinetic Isotope Effects
11:00-11:30	I Rod Hubbard Theory in practice: experiences in predictive structure-based drug discovery	I Arieh Warshel How do enzymes really work ;Using Computer Simulations to Examine and Eliminate catalytic Proposals	I Jianpeng Ma New Methods for Simulating, Refining, and Modeling Supermolecular Complexes at Multi-resolution and Multi-length Scales	I Paul v R Schleyer		I Jean-Claude Rayez New perspective in transition state theory
11:30-12:00	I Esin Aki Sener 3D-QSAR studies of topoisomerase II inhibitors using catalyst	I Yun-Dong Wu A Theoretical Study on the Mechanism of the Reductive Half-reaction of Xanthine Oxidase	I Monte Pettitt The role of solute-solvent attraction on the dewetting of large hydrophobic solutes	I Henry S. Rzepa Foliacenes: Ab initio modelling of metallocomplexes exhibiting a unique form of 16-electron, metal-induced aromaticity		I Charles H. Reynolds Mechanistic Approaches to Drug Discovery
12:00-12:30	I Martin Stahl Fragment Spaces in 2D and 3D de novo design	I Max C. Holthausen Mechanistic Insights into the Hydroxylation Activity of Bioinorganic Models for Dinuclear Cu-Proteins	I Robert B. Best Identifying dynamically relevant reaction coordinates in biomolecular transitions	I Alexander I. Boldyrev Multiple Aromaticity - A New Tool in Deciphering Chemical Bonding in Main Group Clusters		I Qiang Cui Theoretical analysis of mechanochemical coupling in myosin
12:30-14:00	Lunch					
14:00-14:50	Plenary Lecture: Martin Quack "Electroweak Quantum Chemistry and Dynamics of Parity Violation in Chiral Molecules"					
15:00-15:20	C Horst Bögel Web-based Computational Network using Java-Tools and Java-WebStart technology.	C Nino Russo Potential Energy Surfaces for Reactions Catalysed by Metal Containing Enzymes from Density Functional Computations	C Wolfgang Wenzel Reproducible in-silico Protein Folding at the all atom level	C Shyi–Long Lee Computational study for the hydrogen bonding 1:1complexes of tetrahydrofuran with water, hydrogen fluoride or ammonia		C Geza Fogarasi Water-mediated Tautomerism in Cytosine: an ab Initio Dynamics Study
15:20:15:40	C Jamie Platts Polar Surface Area: Problems and Opportunities.	C Stefano Piana Molecular mechanism of caspase activity regulation.	C Maria Colombo A study of the structural stability of the apo- and holo-form of the C-terminal domain of the mouse prion protein	C David Danovich Triple Bonds of Carbon and Silicon – A Comparative Study Using Modern Valence Bond Theory.		C K.J. Jalkanen Modeling study the mechanism of DNA repair by the photolyase protein
15:40-16:00	C Christoph Steinbeck Open Content Databases and Open Source Libraries for Chemoinformatics.	C Thomas H. Rod High-level QM/MM free energies for enzymatic reactions.	C Tamás Beke Secondary structure elements of b-peptides using quantum chemical calculations	C Klaus Hermann Ab initio DFT Cluster Studies for Oxygen 1s NEXAFS Spectra at V2O5 and V2O3 Surfaces.		C Xiang-Yuan Li New Theory for Nonequilibrium solvation and Numerical Solution of Poisson Equation
16:00-16:20	C John B.O. Mitchell QSAR Study of Structure-Odour Relationships Using EVA Descriptors.	C Ivano Tavernelli Excited state ab initio MD study of photochemical processes in model compounds	C Roberto D. Lins Influence of the treatment of Long-range Electrostatics Interactions in Peptide Folding	C Chin-Hui Yu Tuning the Hydrogen Bonds through Cooperative Effects.		C Benjamin Gladwin Final Times, First Passage Times and Long Time Scale Least Action
16:00-16:20	Break					
	Posters					

Provisional

Wednesday

Time	Informatics	Enzyme Catalysis	Molecular Structure	Electronic Structure	Industrial Catalysis	Reaction Mechanisms
08:00-08:50	Plenary Lecture: Paul Madden "From First-principles to Material Behaviour: Towards Predictive Modelling of Ionic Systems"					
08:50-09:40	Dirac Medallist (2004) Plenary Lecture: Jan Martin "Computational Thermochemistry: The Right Result for the Right Reason?"					
09:40-10:10	Break					
	Selected Contributed Lectures IV	**Selected Contributed Lectures V**	**Conformational Studies of Small Molecules and Molecular Complexes**	**Selected Contributed Lectures I**	**Selected Contributed Lectures II**	**Selected Contributed Lectures III**
10:10-10:30	C Tanja van Mourik A density functional theory study of guanine quartets.	C Annu Söderholm 3D Structure-Activity Relationships of Non-Steroidal Androgen Receptor Ligands.	SL Tony Ford **Conformational Preferences of the Structures of the Molecular Complexes of Boron Trifluoride with Some Hydrogen Halides, Halogens and Interhalogens**	C Eva Zurek Density Functional Calculations of the 13C NMR Chemical Shifts in (9,0) Single-Walled Carbon Nanotubes.	C Michelle Kuttel Stretching Dynamics of Pyranose Polysaccharides	C Ulf Ryde Accurate geometries and energies for metalloproteins estimated by QM/MM methods
10:30-10:50	C N. Absi Divide and conquer strategy for molecular electronic integrals over Exponential Type Orbitals	C Albérico B.F. da Silva A study on the influence of molecular properties in the psychoactivity of cannabinoid compounds.	I Perry Kaye Experimental and Theoretical Studies of Unexpected Terpenoid Rearrangements	C Berta Fernández Accurate rovibrational spectra of van der Waals complexes.	C Gianfranco La Manna Theoretical study of the insertion of sodium ion into organic tubular structures	C Jan Saam Identification of an Oxygen Channel in Lipoxygenase by Molecular Dynamics.
10:50-11:10	C Alexei V. Arbuznikova "Double local hybrid" exchange-correlation potentials: construction and evaluation in DFT calculations of magnetic-resonance parameters.	C Ming Wah Wong Diels-Alder Reactions Using Chiral Oxazaborolidinone Catalysts: The Roles of p-stacking, Hydrogen Bonding and Donor-Acceptor Interactions.	I Phuti Ngoepe Atomistic simulations of surfaces and interfaces of manganese dioxides	C Hazel Cox What is required to stabilise Al3+? A gas phase perspective.	C Iveta Bártová Molecular Dynamics Simulations on Cyclin Dependent Kinase 2. Solvent Behavior Analysis and Activation and Inhibition by Phosphorylation -Tools to Design New Inhibitors and Contribute to Understanding Mechanism	C Manuel Yanez Gas-Phase Reactions Between Urea and Ca2+: The Importance of Coulomb Explosions
11:10-11:30	C Dmitri G. Fedorov A general fragment-based method for quantum-chemical calculations of large molecules	C Yukihiko Nagae Hydrated Structure of Ammonia-Water Molecule Pair via the Free Energy Gradient Method.	I Gert Kruger Predicted protection of alcohols, amines and hydantoins	C O. Kh. Poleshchuk Application of DFT to analysis of non-transition and transition element complexes electronic structure	C Caterina Ghio Solvent Effects on two Pterocarpans with Biological Activity: a Continuum-discrete Approach	C Bruno Giardina From the Arctic to the fetal life: physiological importance and computational studies of an "additional" chloride binding site in hemoglobin.
11:30-11:50	C Hideo Sekino Polarizability Evaluation by Density Functional Theory (DFT) with Long Range Corrected (LRC)	C Neslihan Canbek Computational Modeling of Interactions of Glutamic Acid with Metal Ions.	I Helder Marques The Conformations of Some Biologically Important Molecules using Molecular Mechanics and Molecular Dynamics Methods	C Tom Leyssens Imaging the metal-phosphorus bond by density differences.	C Claudio Carra Nanosecond Molecular Dynamics Simulations and Structural Analysis of dsDNA-dye Complex in Solution	C Robin Garnell Accurate Protein Secondary Structure Determination from CD and UV Spectra by g-Factor Analysis
11:50-12:10	C Stephen Glover Number A computational investigation of the structure of phenyloxenium ions.	C O. Anatole von Lilienfeld Optimization of Effective Atom Centered Potentia	I Jan Dillen	C Josef Michl Computation of Zero-Field Splitting Parameters: Triplets of Six-Valence-Electron Analogs of Dimethylcarbene and Methylnitrene	C Daniela Niederreiter Pharmacophore Modeling For Selective, Non-Steroidal CYP17 and CYP19 Inhibitors.	C T. Veszprémi Dimerization and trimerization of Phosphaacetylene
12:10-14:00	Lunch					
14:00-?	Excursion					

Provisional

Thursday

Time	Informatics	Enzyme Catalysis	Molecular Structure	Electronic Structure	Industrial Catalysis	Reaction Mechanisms
08:00-08:50	Schrödinger Medallist (2004) & Plenary lecture: Tom Ziegler "A Computational Approach to Industrial Catalysis"					
		Radicals in Biology		**Recent Advances in Coupled Cluster Based Approach to Excited and Multi-reference Correlation Problem**	**From Molecules to Materials**	**Reaction Mechanisms in the Condensed Phase II: Liquid, Solution and Solid**
09:00-09:30		SL Leo Radom **Number Suicide Inactivation in B12-Mediated Reactions**		SL D. Mukherjee **Contracted and Uncontracted State-specific Multi-reference Coupled Cluster Theories using General Model Spaces**	SL Michael Hall **Carbon-hydrogen Bond Activation by Iridium(III): Oxidative-addition vs. Sigma-bond Metathesis and Catalytic vs. Non-catalytic Alkane Dehydrogenation**	SL Martin Field **Simulating Chemical Reactions in the Condensed Phase using Hybrid Potentials: Developments and Applications**
09:30-10:00		I Russell Boyd Chemical Models for Biological Catalysis		I Anna I. Krylov How unpaired are single electrons in triradicals: Tales of bonding in open-shell compounds by the spin-flip method.	I William Goddard	I Yirong Mo Probing the Electron Transfer Process in Gaseous and Condensed Phases
10:00-10:30	Break					
10:30-11:00		I Sason Shaik One Reagent Many Pathways: Reactivity Patterns of Cytochrome P450 Enzymes and Analogous Catalysts.		I Marcel Nooijen Internally Contracted Multireference Coupled Cluster Theory.	I Keiji Morokuma Recent Progress in Computational Studies of Transition Metal-Catalyzed Element-Element Activation and Addition to Unsaturated Organic Substrates	I Masaru Tateno Investigations of catalytic reaction mechanisms of biological macromolecules by using hybrid methods based on ab initio and classical molecular dynamics simulations
11:00-11:30		I Arvi Rauk The Free Radical Chemistry of Alzheimer's Disease		I Mark R. Hoffmann Generalized Van Vleck Multireference Perturbation Theory for Molecular Electronic Structure.	I Mathew Neurock	I Brian Yates Advances in Computation of pKa Values in Aqueous and Non-aqueous Solvents
11:30-12:00		IO Per Siegbahn Quantum Chemical Studies of Redox-Active Enzymes		I Jürgen Gauss Higher Excitations in the Coupled-Cluster Treatment of Excitation Energies and Excited-State Properties.	I Gyeong Hwang Atomic-level Control of Growth and Catalytic Properties of 1B Metal Nanoparticles on Rutile TiO2(110)	I Darrin York Simuations of phosphoryl transfer reactions using multi-scale quantum models
12:00-12:30		I Vincenzo Barone		I Martin Kaupp Pushing the Envelope in Magnetic Resonance Parameter Calculations	I Axel Gross Number Density functional theory study of the partial oxidation of methanol on copper surfaces	I Laurent Maron Catalysis by lanthanocenes: A combined theoretical and experimental study
12:30-14:00	Lunch					
14:00-14:50	Plenary Lecture: Andrej Sali "Modelling 3D Structures of Proteins and Macromolecular Assemblies"					
15:00-15:20		IO Hendrik Zipse C-H Bond Acidity in Radicals of Biological Interest		C Wesley D. Allen An Improved General Method for Computing Anharmonic Zero-Point Vibrational Energies	C Imre Papai Mechanistic studies on C-C coupling reactions between carbon dioxide and ethylene	C Massimo Mella Effects of Quantum Vibrations and Anharmonicity on the Structure, Stability, and Conversion Mechanisms of Protonated Water Clusters (H2O)nH+
15:20-15:40		I Leif Eriksson Theoretical Studies of Photodynamic Drugs and Phototoxic Reaction.		C Jiri Pittner New Developments in the Multireference Brillouin-Wigner Coupled Cluster Method: Exact Connected Triples, Incomplete Model Space, and Applications	C Jonas Oxgaard Oxidative Hydrogen Migration: a Novel Mechanism for C-H Activation	C Stefano Piana Understanding the barriers to crystal growth: Dynamical simulation of the dissolution and growth of urea from aqueous solution
15:40-16:00		IO David Smith The Substrate Mechanism of Pyruvate Formate-Lyase: The Influence of the Environment on Enzyme-Catalyzed Reactions Involving Free Radicals.		C Rochus Schmid An efficient parallel Car-Parrinello MD Code using "Real-Space" discretized Wavefunctions.	C Michelle L. Coote The Origin of Retardation and Inhibition Effects in the RAFT Polymerization Process	C Dirk Zahn Investigation of Rare Events in Complex Systems from Molecular Dynamics Simulations: Path Sampling of Reactions in Solution and Phase Transitions
16:00-16:20		C Patrick J O'Malley Density Functional Studies of Tyrosyl/Phenoxyl Free Radicals.		C Miroslav Urban Optimized Virtual Orbitals Space (OVOS) as a tool for effective Coupled Cluster calculations of molecular properties.	C Sean Moolman Compatibility of polyvinyl alcohol and poly(methyl vinyl ether-co-maleic acid) blends estimated by Molecular Dynamics.	C Luis Arnaut Absolute Rate Calculations for Atom and Proton Transfer Reaction
16:00-16:20	Break					
	Posters					

Provisional

Friday

Time	Informatics	Enzyme Catalysis	Molecular Structure	Electronic Structure	Industrial Catalysis	Reaction Mechanisms
08:00-08:50	Plenary Lecture: Wilfred van Gunsteren "Biomolecular Simulation: (im)possibilities and Perspectives"					
08:50-09:40	Schrödinger Medallist (2003) Plenary Lecture: Peter Pulay "New Computational Methods for Larger Molecules"					
			Molecular Structure and Reactivity in the condensed phase	**Heavy Metal Chemistry**	**Reaction Mechanism of Catalytic Processes**	**Reaction Mechanisms in the Condensed Phase I: Algorithms and Methods**
09:50-10:20			SL Teresa Head-Gordon	SL Kimihiko Hirao **Relativistic Electronic Structure Theory**	SL Gernot Frenking Quantum Chemical Investigations of Transition-Metal Mediated Oxidation Reactions	SL Bernie Brooks
10:20-10:50			I Jeremy Schofield Efficient ab-initio simulation of reactions in condensed phases	I Lucas Visscher Relativistic effects on molecular properties	SL Joachim Sauer	I Martyn Guest Large Scale Electronic Structure Calculations in the Study of the Condensed Phase
10:50-11:20	Break					
11:20-11:50			I John Straub Probing the principles of amyloid protein aggregation	I Pekka.Pyykko New Species of Heavy and Superheavy Elements	I Feliu Maseras Origin of enantioselectivity in the vanadium-catalyzed oxidation of sulfides	I Piotr Piecuch Noniterative Coupled-Cluster Methods for Bond Breaking, Diradicals, and Excited Electronic States
11:50-12:20			I Douglas Tobias Molecular dynamics simulation studies of structure and dynamics on the surface of aqueous electrolyte solutions	I Wenjian Liu Relativistic Time-Dependent Density Functional Theory and Applications	I Shigeyoshi Sakaki Theoretical Study of Catalytic Reactions by Cp2Zr Species. Significant Differences from Late Transition-Metal Complexes	I Paul Sherwood QM/MM Modelling Techniques for Condensed Phase Reactions
12:20-12:50			I Juan Bertrán Towards a Computational Chemistry Rational Design of Antibody Catalysts.	I Yoon Sup Lee Electronic structure calculations of molecules including spin-orbit interactions.	I Sven Tobisch The Stereospecific Polymerization of 1,3-Butadiene Mediated by Early and Late Transition-Metal Catalysts. Towards a Deeper Understanding of the Catalytic Structure-Reactivity Relationships from Theoretical-Mechanistic Studies	IC Alessandro Laio An efficient method to simulate chemical reactions by molecular dynamics
12:50-13:20			I xxx	IC Dominique Guillaumont A quantum chemistry study of lanthanide(III) and actinide(III) complexes with nitrogen ligands.	I Ansgar Schaefer	IC Fabio Mavelli Stochastic Simulation of chemically Reacting Systems
13:20-14:00	Closing					