PROGRAMME AT A GLANCE

• PA – Parkside Auditorium • P110A – Parkside 110A • PG04 – Parkside G04 • P110B – Parkside 110B

SUNDAY SEPTEMBER 14

1.20 (for 1.30) –4.00pm	**1. Opening Session** Chair: *Leo Radom* • PA			
1.20pm	**Congress Opening**			
2.20pm	*Henry F. Schaefer III* – WATOC Comes of Age			
2.40pm	*Julian Gale* – The Computational Challenge of Crystallisation			
3.20pm	*Pavel Hobza* – Accurate Interaction Energies of Building Blocks of Biomacromolecules: A Quantum Chemical Study			
4.00–4.30pm	AFTERNOON TEA			
4.30–6.30pm	**Poster Session 1 (PP001–PP175)**			
6.30–8.30pm	WELCOME RECEPTION – BALLROOM FOYER, SYDNEY CONVENTION CENTRE			

MONDAY SEPTEMBER 15

8.30–9.50am	**2. Plenary Session** Chair: *Brian Yates* • PA			
8.30am	*Peter M. W. Gill* – Recent Developments in Electron Correlation and Density Functional Theory			
9.10am	*Anna Krylov* – **2007 Dirac Medal Lecture**: Glancing for Concerted, Conical for Stepwise: The Role of the Excited State Topology in Three-Body Dissociation of Triazine Explained by EOM-CC			
9.50–10.20am	MORNING TEA			
10.20am–12.40pm	**3.1 Thermochemistry** • PA	**3.2 Transition Metal Chemistry** • P110A	**3.3 NMR/Mössbauer/Relativity** • PG04	**3.4 Biological Structures & Simulations I** • P110B
12.40–2.00pm	LUNCH BREAK			
2.00–3.40pm	**4.1 Electron Correlation** • PA	**4.2 Unusual Molecules I** • P110A	**4.3 Carbon Nanostructures** • PG04	**4.4 Drug Design** • P110B
3.40–4.10pm	AFTERNOON TEA			
4.10–5.30pm	**5.1 Methods for Large Systems I** • PA	**5.2 Unusual Molecules II** • P110A	**5.3 Surfaces I** • PG04	**5.4 Methods for Biological Simulations I** • P110B
5.30–7.30pm	**Poster Session 2 (PP176–PP350)**			

TUESDAY SEPTEMBER 16

8.30–9.50am	**6. Plenary Session** Chair: *Walter Thiel* • PA			
8.30am	*Sason Shaik* – **2007 Schrödinger Medal Lecture**: Concepts and Applications in Chemical Reactivity			
9.10am	*Kenneth Ruud* – **2008 Dirac Medal Lecture**: A General Response Theory Framework for Calculating Higher-Order Molecular Properties			
9.50–10.20am	MORNING TEA			
10.20am–12.40pm	**7.1 Theory I** • PA	**7.2 Organometallic Chemistry** • P110A	**7.3 Rovibrational Spectroscopy** • PG04	**7.4 Methods for Biological Simulations II** • P110B
12.40–2.00pm	LUNCH BREAK			
2.00–3.40pm	**8.1 Quantum Monte Carlo** • PA	**8.2 Radicals in Biology** • P110A	**8.3 Surfaces II** • PG04	**8.4 Self Assembly** • P110B
3.40–4.10pm	AFTERNOON TEA			
4.10–5.30pm	**9.I Methods for Large Systems II** • PA	**9.2 Organic Reactions I** • P110A	**9.3 Kinetics/Dynamics** • PG04	**9.4 Biological Structures & Simulations II** • P110B
5.30–7.30pm	**Poster Session 3 (PP351–PP525)**			

• PA – Parkside Auditorium • P110A – Parkside 110A • PG04 – Parkside G04 • P110B – Parkside 110B

WEDNESDAY SEPTEMBER 17

8.30–10.30am	**10.1 Software Symposium A** • PA	**10.2 Software Symposium B** • P110A	**10.3 Novel Inorganic Compounds** • PG04	**10.4 Concepts** • P110B
10.30–11.00am	MORNING TEA			
11.00am–12.40pm	**11.1 Software Symposium C** • PA	**11.2 Software Symposium D** • P110A	**11.3 Liquids** • PG04	**11.4 Charge Transport/Quantum Coherence** • P110B
12.40pm	LUNCH BREAK/EXCURSION			

THURSDAY SEPTEMBER 18

8.30–9.50am	**12. Plenary Session** Chair: *Mark Gordon* • PA			
8.30am	*Rodney Bartlett* – **2008 Schrödinger Medal Lecture:** How Close Can We Come to a Correlated Orbital Shell Model of Molecules?			
9.10am	*Lucas Visscher* – **2006 Dirac Medal Lecture:** Relativistic Electronic Structure Theory			
9.50–10.20am	MORNING TEA			
10.20am–12.40pm	**13.1 Theory II** • PA	**13.2 Intermolecular Interactions** • P110A	**13.3 Organic & Inorganic Photochemistry** • PG04	**13.4 Biological Structures & Simulations III** • P110B
12.40–2.00pm	LUNCH BREAK			
2.00–3.40pm	**14.1 Mechanisms/Potential Energy Surfaces** • PA	**14.2 Hydrogen Bonds/Acids and Bases** • P110A	**14.3 Optical Material Properties** • PG04	**14.4 Biological Structures & Simulations IV** • P110B
3.40–4.10pm	AFTERNOON TEA			
4.10–5.30pm	**15.1 Biological Photochemistry** • PA	**15.2 Organic Reactions II** • P110A	**15.3 Protein Folding** • PG04	**15.4 Solvation** • P110B
7.00pm	CONGRESS BANQUET – DOCKSIDE, COCKLE BAY WHARF, DARLING HARBOUR			

FRIDAY SEPTEMBER 19

8.30–9.50am	**16. Plenary Session** Chair: *Henry F. Schaefer III* • PA
8.30am	*Martin Head-Gordon* – Tractable Valence Space Models for Strong Electron Correlations
9.10am	*Shigeru Nagase* The Important Interplay between Theoretical Calculations and Experiment
9.50–10.20am	MORNING TEA
10.20am–12.30pm	**17. Closing Session** Chair: *Peter M. W. Gill* • PA
10.20am	*Tim Clark* **–** Simulating Biological Signal Transduction
11.00am	*Donald G. Truhlar* **– 2006 Schrödinger Medal Lecture:** New Density Functionals with Broad Applicability for Thermochemistry, Thermochemical Kinetics, Noncovalent Interactions, Transition Metals, and Spectroscopy
11.40am–12.30pm	CLOSING CEREMONY

PROGRAMME AT A GLANCE

PL – PLENARY LECTURE | IL – INVITED LECTURE | OC – ORAL COMMUNICATION | PP – POSTER PRESENTATION

SUNDAY SEPTEMBER 14

1.20–4.00pm	**1. Opening Session** Chair: *Leo Radom* PARKSIDE AUDITORIUM	
1.20 for 1.30pm	**Indigenous Welcome** **Welcome from Professor Leo Radom, President of WATOC and Chair of WATOC 2008** **The Australian Youth Choir, conducted by Fiona Gardner** **Official Opening by Professor Margaret Sheil, Chief Executive Officer of the Australian Research Council**	
2.20pm	**PL001**	*Henry F. Schaefer III* – WATOC Comes of Age
2.40pm	**PL002**	*Julian Gale* – The Computational Challenge of Crystallisation
3.20pm	**PL003**	*Pavel Hobza* – Accurate Interaction Energies of Building Blocks of Biomacromolecules: A Quantum Chemical Study
4.00–4.30pm	AFTERNOON TEA	
4.30–6.30pm	**Poster Session 1 (PP001–PP175)**	
6.30–8.30pm	WELCOME RECEPTION – BALLROOM FOYER, SYDNEY CONVENTION CENTRE	

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PL – PLENARY LECTURE | IL – INVITED LECTURE | OC – ORAL COMMUNICATION | PP – POSTER PRESENTATION

MONDAY SEPTEMBER 15

8.30–9.50am	**2. Plenary Session** Chair: *Brian Yates* PARKSIDE AUDITORIUM							
8.30am	**PL004**	*Peter M. W. Gill* – Recent Developments in Electron Correlation and Density Functional Theory						
9.10am	**PL005**	*Anna Krylov* – **2007 Dirac Medal Lecture:** Glancing for Concerted, Conical for Stepwise: The Role of the Excited State Topology in Three-Body Dissociation of Triazine Explained by EOM-CC						
9.50–10.20am	MORNING TEA							
10.20am–12.40pm	**3.1 Thermochemistry** Chair: *Kimihiko Hirao* PARKSIDE AUDITORIUM		**3.2 Transition Metal Chemistry** Chair: *Gernot Frenking* PARKSIDE 110A		**3.3 NMR/Mössbauer/Relativity** Chair: *Peter Pulay* PARKSIDE G04		**3.4 Biological Structures & Simulations I** Chair: *Tim Clark* PARKSIDE 110B	
10.20am	**IL001**	*Stefan Grimme* Status and Perspectives of Double-Hybrid Density Functionals	**IL008**	*Helmut Schwarz* High-Valent Iron-Oxo and Iron-Nitrido Cations: Intraligand Bond Activation, Intermolecular Oxygen- and Nitrogen-Atom Transfer, Nitrile-Alkyne Metathesis, and More …	**IL013**	*Janet Del Bene* A Comparison of Computed SOPPA and EOM-CCSD Spin-Spin Coupling Constants Experimental Data for Molecules H_mXYH_n and Selected F^- Derivatives, for X, Y = ^{13}C, ^{15}N, ^{17}O, and ^{19}F	**IL018**	*Ian Williams* Computational Modelling of Glycosidase Mechanisms
10.40am	**IL002**	*Jan Martin* Robust, Generally Applicable, Double Hybrid Functionals: A "Third Way" for Reliable Thermochemistry and Thermochemical Kinetics	**IL009**	*Peter Schwerdtfeger* The Elusive Chromium Dihalide Structures – A Combined Computational and Gas Phase Electron Diffraction Study	**IL014**	*Wenjian Liu* Relativistic Theory for NMR Parameters	**IL019**	*Avital Shurki* Hydrolysis Caused by Mutation – The Story of Nerve Agents and Other Organophosphate Esters
11.00am	**IL003**	*Larry Curtiss* Assessment of Gaussian-4 Theory and Related Methods	**IL010**	*Max Holthausen* Bioinorganic Models for Dinuclear Copper Proteins: Aliphatic and Aromatic Hydroxylation from a Quantum Chemical Point of View	**IL015**	*Michael Filatov* First Principles Calculation of Hyperfine Parameters for Mössbauer Spectroscopy	**IL020**	*Darrin York* Theoretical Studies of RNA Catalysis
11.20am	**IL004**	*George Petersson* Towards a Quick and Clean CCSD(T)/CBS Limit: The CBS-Wes1P Model	**IL011**	*Shigeyoshi Sakaki* Geometry and Bonding Nature of Transition Metal Complexes: Theoretical Study with Frontier-Orbital-Consistent Effective Potentials (FOC-EP)	**IL016**	*Markus Reiher* Recent Developments in Douglas-Kroll-Hess Theory: Molecular Properties with a Focus on Mössbauer Spectroscopy	**IL021**	*Yirong Mo* Ammonium Deprotonation Mechanism in Escherichia coli Ammonium/Ammonia Transport Protein (AmtB)

PROGRAMME • MONDAY SEPTEMBER 15

PL – PLENARY LECTURE | IL – INVITED LECTURE | OC – ORAL COMMUNICATION | PP – POSTER PRESENTATION

MONDAY SEPTEMBER 15

11.40am	**IL005**	*John Stanton* The HEAT Family of Methods for Theoretical Thermochemistry	**OC001**	*Antonio Largo* Cyanide vs. Isocyanide Competition in Transition Metal Complexes	**OC005**	*Juha Vaara* Theory of Nuclear Magnetic Resonance Chemical Shift in an Arbitrary Electronic Spin State	**OC009**	*Vicent Moliner* Enzyme Promiscuity
			OC002	*Nicola Gaston* The Lattice Structures of the Group 12 Metals: A Local Correlation Treatment	**OC006**	*Oleg Poleshchuk* Application of DFT to Analysis of the Hyperfine Interactions and Bonding in Various Complexes	**OC010**	*Zexing Cao* Broad Substrate Specificity and Reaction Mechanism of Pseudomonas stutzeri L-Rhamnose Isomerase: Insight from QM/MM Molecular Dynamics Simulations
12.00pm	**IL006**	*Wesley Allen* A Hierarchy of Homodesmotic Reactions for Thermochemistry	**IL012**	*Rob Deeth* Molecular Modelling for Systems Containing Transition Metal Centres	**IL017**	*Martin Kaupp* Local Hybrid Functionals and the Highest Oxidation States of the 5d Elements	**OC011**	*Viktorya Aviyente* A Computational Approach to the Deamidation Mechanism of Asparagine in Peptides and Proteins
							OC012	*Jan Saam* Dynamic Oxygen Access Pathways in Proteins
12.20pm	**IL007**	*Angela Wilson* Quantitative Modelling Across the Periodic Table: The Correlation Consistent Composite Approach (ccCA)	**OC003**	*Nurbosyn U. Zhanpeisov* Structure and Chemical Activity of Transition Metal and Metal Oxide Catalysts: A Theoretical DFT Study	**OC007**	*Trond Saue* 2- and 4-Component Relativistic DFT Linear and Quadratic Response Theory	**OC013**	*Janez Mavri* Calculation of H/D Isotope Effects: Application to Lipoxygenase
			OC004	*Hazel Cox* Insights Into Metal Ion Solvation Using TDDFT	**OC008**	*Fabio Pichierri* Golden Nanoclusters: Molecular Design with Density Functional Theory	**OC014**	*Ewa Broclawik* Smart Catalysis on Enzymes with an Iron-Oxo Cores: Theory Behind Electronic Structure
12.40–2.00pm	LUNCH BREAK							
2.00–3.40pm	**4.1 Electron Correlation** Chair: *Bogumil Jeziorski* PARKSIDE AUDITORIUM		**4.2 Unusual Molecules I** Chair: *Shigeru Nagase* PARKSIDE 110A		**4.3 Carbon Nanostructures** Chair: *Julian Gale* PARKSIDE G04		**4.4 Drug Design** Chair: *David Winkler* PARKSIDE 110B	
2.00pm	**IL022**	*Piotr Piecuch* Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell and Large Systems	**IL027**	*Gernot Frenking* The Chemistry of Divalent Carbon(0) Compounds – A Challenge for Experiment	**IL031**	*Keiji Morokuma* Growth Process of Single-Walled Carbon Nanotubes from Metal Cluster: Density Functional Tight-Binding Molecular Dynamics Simulation	**IL036**	*Leif Eriksson* Molecular Photochemistry in Medicine – The Photodegradation of Non-Steroid Anti-Inflammatory Drugs (NSAIDs)

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MONDAY SEPTEMBER 15

2.20pm	**IL023**	*Debashis Mukherjee* Development of a Novel Spin-Free Combinatoric Open-Shell Coupled Cluster (COS-CC) Theory to Single-Reference CSFs: Application to a Doublet State	**IL028**	*Yitzhak Apeloig* NMR Characterization of Low-Coordination Silicon Compounds. Experiment and Theory	**IL032**	*Elena Bichoutskaia* Multiscale Modelling of Carbon Based Nanomaterials and Applications to Nanoelectronics and Data Storage	**IL037**	*Narahari Sastry* On the Reliability and Relevance of Computational Approaches in Drug Design: Some Case Studies
2.40pm	**IL024**	*Mark Hoffmann* Inclusion of Triple and Quadruple Excitations into MRCISD	**OC015**	*Miriam Karni* Resonance and Aromaticity of N-Heterocyclic Carbenes, Silylenes and Germylenes	**IL033**	*Kwang Kim* Super-Magnetoresistance in Graphene Nanoribbon Spin Valve Devices	**OC017**	*Ngai Ling Ma* Prioritization of Anti-Tubercular Agents: A Model for Minimum Inhibitory Concentration (MIC) Prediction
			OC016	*Henry Rzepa* Intrinsically Chiral Aromaticities. Twist, Writhe and Linking Number as Fundamental Properties of Higher-Order Möbius Annulenes			**OC018**	*Anna K. Croft* Discovering Structural Features of Mycolic Acids from Mycobacterium Tuberculosis
3.00pm	**IL025**	*Jiri Pittner* State-Specific Mukherjee's Multireference Coupled Cluster Method with Non-Iterative Triples: Theory, Efficient Implementation, and Applications	**IL029**	*Jean-Marie Andre* Simple Mathematical Models that Lead to Non Equilibrium, Fractals and Möbius Structures in Organic Chemistry	**IL034**	*Nigel Marks* Self-Assembly of sp^2-Bonded Carbon Nanostructures: The Role of Topological Constraints Arising from Geometry	**IL038**	*Supot Hannongbua* Drug-Target Interactions in Avian Influenza Virus A Subtype H5N1: Molecular Modelling
3.20pm	**IL026**	*Edward Valeev* Universal Perturbative Explicitly Correlated Correction for Accurate Electronic Structure Methods	**IL030**	*Rainer Herges* Are there Stable, Unsubstituted Möbius Annulenes? Calculations and Experiments	**IL035**	*Kim Baldridge* Structure, Dynamics, and Properties of Corannulene Derivatives in Condensed Phases and on Metallic Surfaces	**OC019**	*Martine Prévost* Structure-Based Design of a New Inhibitor for D-Alanine:D-Alanine Ligase
							OC020	*Vladimir Palyulin* Neuroprotectors as Cognition Enhancers: From Theoretical Predictions to Drugs
3.40–4.10pm	AFTERNOON TEA							
4.10–5.30pm	**5.1 Methods for Large Systems I** Chair: *Donald G. Truhlar* PARKSIDE AUDITORIUM		**5.2 Unusual Molecules II** Chair: *Henry Rzepa* PARKSIDE 110A		**5.3 Surfaces I** Chair: *Petr Čársky* PARKSIDE G04		**5.4 Methods for Biological Simulations I** Chair: *Alan Mark* PARKSIDE 110B	
4.10pm	**IL039**	*Michael Collins* Ab Initio Energies by Systematic Fragmentation of Molecules	**IL043**	*Manuel Yáñez* Pentacovalent Carbon Atoms and Other Beauties of Gas-Phase Ion Chemistry	**IL047**	*Irene Yarovsky* Theoretical Nanoscale Design of Contamination Resistant Surfaces	**IL049**	*Wilfred van Gunsteren* Methodological Advances in Computer Simulation of Biomolecular Systems

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MONDAY SEPTEMBER 15

4.30pm	**IL040**	*Shuhua Li* Energy-Based Fragmentation Approaches to Ab Initio Quantum Chemistry Calculations of Very Large Systems	**IL044**	*Athanassios Nicolaides* Thermochemistry of a Homologous Series of Tertiary Pyramidal Alkyl Radicals	**OC021**	*Cheol Ho Choi* Mechanistic Understanding of Surface Reactions	**IL050**	*Yun-Dong Wu* Progress in Developing a United-Atom Protein Force Field in a Coarse-Grained Solvent
					OC022	*Oliver Warschkow* Water on the Silicon (001) Surface: C-Defects and the Initial Steps of Surface Oxidation		
4.50pm	**IL041**	*Hiromi Nakai* Development of Linear-Scaling Electronic Structure Calculations based on the Divide-and-Conquer Method	**IL045**	*Alexander Boldyrev* Developing Paradigms of Chemical Bonding: Adaptive Natural Density Partitioning	**OC023**	*Javier Fernández Sanz* Gold Atoms Deposited on N-Doped TiO_2 (110) Rutile Surfaces	**IL051**	*Kevin Naidoo* Toward the Development of Free Energy Based Mean Field Long Range Interaction Potentials
					OC024	*Jin Yong Lee* Understanding of Fluorescent Chemosensor Functions and CO Vibration Changes upon Tip-Surface Field: Computational Studies		
5.10pm	**IL042**	*Kimihiko Hirao* Towards Linear Scaling Density Functional Theory	**IL046**	*Gabriel Merino* Planar Tetracoordinate Carbon Atoms: Brave New World of C_5^{2-}	**IL048**	*Jean-Claude Rayez* Some Theoretical Contributions in Heterogeneous Chemistry	**OC025**	*Michele Cascella* Topologically-Based Multipolar Reconstruction of Electrostatic Interactions in Multiscale Simulations of Proteins
							OC026	*Tell Tuttle* Semiempirical Methods for the Description of Biochemical Systems
5.30–7.30pm	**Poster Session 2 (PP176–PP350)**							

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TUESDAY SEPTEMBER 16

8.30–9.50am	**6. Plenary Session** Chair: *Walter Thiel* PARKSIDE AUDITORIUM						
8.30am	**PL006**	*Sason Shaik* – **2007 Schrödinger Medal Lecture:** Concepts and Applications in Chemical Reactivity					
9.10am	**PL007**	*Kenneth Ruud* – **2008 Dirac Medal Lecture:** A General Response Theory Framework for Calculating Higher-Order Molecular Properties					
9.50–10.20am	MORNING TEA						
10.20–12.40am	**7.1 Theory I** Chair: *Martin Head-Gordon* PARKSIDE AUDITORIUM		**7.2 Organometallic Chemistry** Chair: *Odile Eisenstein/Michael Hall* PARKSIDE 110A		**7.3 Rovibrational Spectroscopy** Chair: *Suehiro Iwata* PARKSIDE G04		**7.4 Methods for Biological Simulations II** Chair: *Keiji Morokuma* PARKSIDE 110B	
10.20am	**IL052**	*Hiroshi Nakatsuji* Solving the Schrödinger Equation of General Atoms and Molecules: Towards Confidently Predictive Quantum Chemistry	**IL058**	*Feliu Maseras* **2008 Chemical Society Reviews Lecture:** The Complex Mechanism of Cross-Coupling Reactions	**IL063**	*R. Benny Gerber* Anharmonic Quantum Calculations of Large-Molecule Vibrations: Algorithms and Spectroscopic Applications	**IL069**	*Ulf Ryde* Accurate Energies in Proteins by Combining QM Fragment Calculations and MM with Polarisabilities and Multipole Expansions
10.40am	**IL053**	*Wim Klopper* Slater-Type Geminals in Molecular Electronic-Structure Theory	**IL059**	*Matthias Bickelhaupt* Origin of Reaction Barriers and Rational Design in Chemistry	**IL064**	*Petr Čársky* Use of Quantum Chemistry Methods for Calculations of Vibrational Spectra by Electron Impact	**IL070**	*Kazuo Kitaura* Quantum Chemical Calculations of Protein-Ligand Interactions with the Fragment Molecular Orbital Method
11.00am	**IL054**	*Garnet Chan* Ab Initio Density Matrix Renormalization Group and Tensor Network Wavefunctions	**IL060**	*Brian Yates* Breaking Chemistry's Strongest Bonds	**IL065**	*Yoon Sup Lee* Towards Accurate Calculations of Vibrational Frequencies and Structures for Low-Lying States of Halomethane Cations	**IL071**	*Jonathan Essex* Hit Identification and Binding Mode Predictions by Rigorous Free Energy Calculations
11.20am	**IL055**	*Vitaly Rassolov* Polynomial Scaling of the Spin Problem	**IL061**	*Michael Hall* Carbon-Hydrogen Bond Activation	**OC033**	*Robert Berger* Vibronic Structure Methods for Systems with Hundreds of Atoms	**OC035**	*Dušanka Janežič* Binding-Sites Prediction Assisting Protein-Protein Docking
					OC034	*Marek J. Wójcik* Dynamics of Protons in Hydrogen Bonds Studied by Theoretical Methods and Vibrational Spectroscopy	**OC036**	*Jaroslav Koča* TRITON – Software for In Silico Engineering of Carbohydrate Binding Proteins

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TUESDAY SEPTEMBER 16

11.40am	**IL056**	*Seiichiro Ten-no* The Use of the Yukawa Potential in Ab Initio and Semi-Empirical Quantum Chemistry	**OC029**	*Sven Tobisch* Unravelling the Function of the Lewis Acid in the Tungsten Imido-Catalysed Dimerisation of Alpha-Olefins: A DFT Study	**IL066**	*Tim Lee* Calculation of Highly Accurate Rovibrational Spectra for Molecules Containing a Large-Amplitude Motion: Ammonia	**OC037**	*Shin Nakamura* Ab Initio NMR Chemical-Shift Calculations on Proteins Using the FMO Method
			OC030	*Laurent Maron* Organometallic Catalysis: An Example of Interplay Between Theory and Experiment			**OC038**	*Shigenori Tanaka* Molecular Recognition in Influenza Viral Hemagglutinin Systems Analyzed by the Fragment Molecular Orbital Method
12.00pm	**IL057**	*So Hirata* Electronic and Vibrational Many-Body Methods for Molecules and Macromolecules	**OC031**	*Matthias Lein* Theory and Experiment of Linear Agostic Interactions: A New Motif in an Old Concept	**IL067**	*Attila Császár* Variationally Computed Molecular Spectra	**OC039**	*Dmitri Fedorov* Quantum-Mechanical Calculations of Proteins: Why and How
			OC032	*Mark Buntine* Production of Acrylic Acid Through Nickel-Mediated Coupling of Ethylene and Carbon Dioxide – A DFT Study			**OC040**	*Michelle Kuttel* Developing Novel Molecular Visualizations for Complex Molecules
12.20pm	**OC027**	*Takeshi Yanai* Canonical Transformation for An Efficient Multireference Electronic Structure Method	**IL062**	*Odile Eisenstein* Hydrogenation and Dehydrogenation Reactions of Organic Molecules in the Presence of Metallic Fragments from a DFT Perspective	**IL068**	*Henrik Kjaergaard* Molecular Spectroscopy of the Water Dimer	**IL072**	*Jill E. Gready* Computational Solution to the Holy Grail of Plant Science – Successful Re-engineering of Improved Rubisco
	OC028	*Ilya Kaplan* Theoretical Studies of the Electron Affinities of the Alkaline-Earth Dimers, Trimers, and Tetramers						
12.40–2.00pm	LUNCH BREAK							
2.00–3.40pm	**8.1 Quantum Monte Carlo** Chair: *Janet Del Bene* PARKSIDE AUDITORIUM		**8.2 Radicals in Biology** *Sponsored by the ARC Centre of Excellence for Free Radical Chemistry and Biotechnology* Chair: *Russell Boyd* PARKSIDE 110A		**8.3 Surfaces II** Chair: *Tom Ziegler* PARKSIDE G04		**8.4 Self Assembly** Chair: *Robin Garrell* PARKSIDE 110B	
2.00pm	**IL073**	*William A. Lester, Jr.* Selected Developments in Quantum Monte Carlo: Methods and Applications	**IL076**	*David Smith* Computational Investigations of Enzyme Mechanisms: An Application to the Dehydration of 1,2-Diols	**IL080**	*Notker Rösch* Uranyl Adsorption on Solvated Surfaces of Kaolinite	**IL084**	*Michael Klein* Large Scale Molecular Dynamics Simulations for Self Assembling Systems

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TUESDAY SEPTEMBER 16

2.20pm	**IL074**	*James Anderson* Correlated Sampling in Correction Calculations with Diffusion Quantum Monte Carlo	**IL077**	*Kazunari Yoshizawa* Computational Mutation Analysis of Coenzyme B_{12}-Dependent Diol Dehydratase	**IL081**	*Cathy Stampfl* Predicting Surface Phase-Diagrams of Sub-Nanoscale Oxidation Catalysts from First-Principles	**IL085**	*Alan Mark* Simulating Self-Organization in Biomolecular Systems
2.40pm	**IL075**	*Meredith Jordan* The Proton Affinities of Methane and Ethane: A Challenge to Theory	**OC045**	*Greg Sandala* Theoretical Investigations of the Rearrangement Mechanism Catalyzed by Methylmalonyl-CoA Mutase	**IL082**	*Axel Gross* Methanol Oxidation and Synthesis on Cu(110): A Detailed Microscopic Picture	**IL086**	*David Winkler* Complexity, Systems Chemistry, and Stem Cell Fate
			OC046	*E. Laura Coitino* Assessing the Effect of Polarizing Environments on Hydrogen Abstraction from Substrate in the Process Catalyzed by Ethanolamine Ammonia-Lyase/B_{12}				
3.00pm	**OC041**	*Ellak von Nagy-Felsobuki* Ab Initio Trends in the Structures and Stabilities of MH_2^{n+} (M = Li – K, Be – Ca; n = 1, 2)	**IL078**	*Arvi Rauk* The Chemistry of Alzheimer's Disease: What's a (Retired) Computational Chemist To Do?	**OC047**	*Hong Seok Kang* First-Principles Study of NOx Adsorption on Armchair and Zigzag Nanotubes	**IL087**	*Siewert-Jan Marrink* Fascinating Vesicles
	OC042	*Masanori Tachikawa* Geometric Isotope Effect on the $N_2H_7^+$ Cation by Ab Initio Path Integral Molecular Dynamics Simulation			**OC048**	*Kangnian Fan* Oxidative Dehydrogenation (ODH) of Light Alkanes (Propane and Ethane) Over the V_2O_5 (001) Surface		
3.20pm	**OC043**	*Tapio Rantala* The Path-Integral Monte Carlo Approach to Molecular Electronic Structure	**IL079**	*H. Bernhard Schlegel* An Exploration of Mechanisms for the Transformation of 8-Oxoguanine to Guanidinohydantoin and Spiroiminodihydantoin	**IL083**	*Francesc Illas* Mechanism of Heterogeneously Catalyzed Ethene and Propene Epoxidation: Role of Halogens as Selectivity Promoters	**OC049**	*Joonkyung Jang* Dynamics of Self-Assembled Monolayer Growth in Soft Nanolithgoraphy
	OC044	*Alejandro Ramírez-Solís* Basis Set-Free Excitation Degree-Free Thermochemistry: An Efficient CASSCF/Fixed Node Multireference Quantum Monte Carlo Threshold Selection Scheme. Application to the $O_4 \rightarrow 2O_2$ Reaction					**OC050**	*Fabio Mavelli* Stochastic Simulations of Proto-Cell Dynamics
3.40–4.10pm	AFTERNOON TEA							

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TUESDAY SEPTEMBER 16

	9.I Methods for Large Systems II Chair: *Wei Wu* PARKSIDE AUDITORIUM		9.2 Organic Reactions I Chair: *Yun-Dong Wu* PARKSIDE 110A		9.3 Kinetics/Dynamics Chair: *Meredith Jordan* PARKSIDE G04		9.4 Biological Structures & Simulations II Chair: *Sason Shaik* PARKSIDE 110B	
4.10pm	**IL088**	*Frank Neese* Computationally Efficient Simplified Single Reference Correlation Methods for Larger Molecules	**IL091**	*Kendall Houk* Distortion/Interaction Energies of Bimolecular Reactions	**IL094**	*Martin Quack* Quantum Chemical Kinetics and Intramolecular Primary Processes Derived from High Resolution Spectroscopy of Simple Polyatomic Molecules and Clusters	**IL098**	*Arieh Warshel* Computer Simulations of Biological Functions
4.30pm	**IL089**	*Joachim Sauer* Accurate Energies of Transition State Structures and Intermediates by Hybrid MP2:DFT and DFT+Disp Calculations	**IL092**	*Peter R. Schreiner* Sugars in Space?	**IL095**	*Dong Hui Zhang* Accurate Theoretical Study of Chemical Reaction Dynamics	**IL099**	*Nino Russo* Density Functional Theory Approaches in Enzymology
4.50pm	**IL090**	*Krishnan Raghavachari* QM/QM Electronic Embedding Models for Materials Chemistry	**IL093**	*Allan East* Some Computational Chemistry Studies of Petroleum Cracking Mechanisms	**IL096**	*Veronique Van Speybroeck* First Principle Chemical Kinetics: From Isolated Molecules to Supramolecular Systems	**OC055**	*Milan Hodošček* Determination of the MurD Mechanism Through Ab Initio QM/MM Analysis of Enzyme Complexes
							OC056	*Denis Bucher* Polarization of Water Molecules in Biological Systems
5.10pm	**OC051**	*Visit Vao-soongnern* Development of a Multiscale Modelling Method to Simulate Polymeric Materials: The Polyethylene Oxide System	**OC053**	*Marzio Rosi* Ab Initio Investigations on Systems Relevant for the Chemistry of the Atmosphere	**IL097**	*António Varandas* Accurate Potential Energy Surfaces and Dynamics: Clues for a Cost-Effective General Strategy	**OC057**	*Wenning Wang* The Conformational Change and Translocation Mechanism of ATP-Binding Cassette (ABC) Transporters
	OC052	*Anatole von Lilienfeld* From Molecular Grand-Canonical Density Functional Theory Towards the Rational First Principles Design of Chemical Compounds	**OC054**	*Imre Papai* On the Reactivity of Frustrated Lewis Pairs			**OC058**	*Geoffrey Wood* Can We Probe the Solution Structure of Amyloid-Beta by using Replica Exchange Molecular Dynamics Simulations?
5.30–7.30pm	**Poster Session 3 (PP351–PP525)**							

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WEDNESDAY SEPTEMBER 17

8.30–10.30am	10.1 Software Symposium A Chair: *Manuel Yáñez* PARKSIDE AUDITORIUM		10.2 Software Symposium B Chair: *Elfi Kraka* PARKSIDE 110A		10.3 Novel Inorganic Compounds Chair: *Josef Michl* PARKSIDE G04		10.4 Concepts Chair: *Dulal Chandra Ghosh* PARKSIDE 110B	
8.30am	**IL100**	*Evert Jan Baerends* The Amsterdam Density Functional Program Suite ADF: What is Old, What is New	**IL106**	*Alan Mark* Modelling the Dynamic Behaviour of Large Scale Biomolecular Systems: The GROMOS and GROMACS Simulation Packages	**IL112**	*Pekka Pyykkö* Predicting New Inorganic Compounds	**IL116**	*Shridhar Gadre* Conceptualizing Chemistry through Electrostatics
8.50am	**IL101**	*Martin Head-Gordon* Quantum Chemical Advances in the Q-Chem Program Package	**IL107**	*Kenneth Merz* The Past, Present and Future of the AMBER Biomolecular Modelling Package	**IL113**	*Laura Gagliardi* Multiconfigurational Quantum Chemistry for Transition Metals and Actinides	**IL117**	*Paul Geerlings* Conceptual DFT: The Woodward Hoffmann Rules Revisited
9.10am	**IL102**	*Peter Pulay* Quantum Chemistry in Parallel with PQS	**IL108**	*Andreas Klamt* COSMO-RS: Much More Than Just COSMO	**OC059**	*Jen-Shiang Yu* Theoretical Investigations on the Structural Distortion in Quintuply-Bonded Dichromium Complexes	**OC063**	*Brian Duke* The Nature of the Chemical Bond Through the Differing Views of Ruedenberg and Bader: Can the Controversy be Resolved?
					OC060	*Ivan Černušák* Dimers of InN and GaN. An MP2 and CCSD(T) Study	**OC064**	*András Stirling* The Spin Repulsion Phenomenon
9.30am	**IL103**	*Christof Hättig* Coupled-Cluster Response Theory for Large Molecules with TURBOMOLE: On the Performance of Spin-Component Scaled CC2 Approaches	**IL109**	*Jeremy Greenwood* A Brief Introduction to Schrödinger's 2008 Modelling Suite	**OC061**	*Tamás Veszprémi* Formation of Phosphaethyne Dimers and Trimers. A Mechanistic Study	**IL118**	*Luis Arnaut* Understanding Chemical Reactivity: A Bridge Between Qualitative Concepts and Numerical Values
					OC062	*Tony Ford* The Complexes of Boron Trifluoride with Phosphine and its Methyl Derivatives. An Ab Initio Study		
9.50am	**IL104**	*Michael W. Schmidt* Parallel Quantum Chemistry with the GAMESS Code	**IL110**	*Neil Ostlund* Design Ideas in HyperChem and HyperProtein	**IL114**	*Eluvathingal Jemmis* Condensation of Polyhedral Boranes: Electron Counting Rules and Compatibility of Orbitals in Overlap	**IL119**	*Marco Nascimento* The Chemical Bond as a Quantum Interference Phenomenon

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WEDNESDAY SEPTEMBER 17

10.10am	**IL105**	*Wibe de Jong* NWChem: Pushing the Scientific Envelope on Large Computing Platforms	**IL111**	*Bernard Brooks* Using CHARMM for Multiscale Modelling and Examining Complex Reactions	**IL115**	*Jesus Ugalde* Sandwich Complexes of Functionalized Aromatic Aluminium Rings	**OC065**	*Akitomo Tachibana* The QED Stress Tensor Description of Chemical Bonds – Formulation of a Non-Classical Bond Order Concept			
							OC066	*Richard Harcourt* 6 Electron 4-Centre and 4-Electron 3-Centre Bonding: Valence Bond Structures for N_2O_4 and S_3O_2 Isomers, and $S_2I_4^{2+}$			
10.30–11.00am	MORNING TEA										
11.00am–12.40pm	**11.1 Software Symposium C** Chair: *Rika Kobayashi* PARKSIDE AUDITORIUM		**11.2 Software Symposium D** Chair: *Notker Rösch* PARKSIDE 110A		**11.3 Liquids** Chair: *Robert MacLagan* PARKSIDE G04		**11.4 Charge Transport/Quantum Coherence** Chair: *Kangnian Fan* PARKSIDE 110B				
11.00am	**IL120**	*Daniel Crawford* The PSI3 Program Package: An Open-Source Quantum Chemistry Suite	**IL125**	*Alessandro Curioni* CPMD: New Frontiers for Ab Initio Molecular Dynamics in the Petaflop Era	**IL130**	*Theresa Windus* Dynamical Nucleation Theory Using Ab Initio Potentials	**IL134**	*Michel Dupuis* Charge Transport in Metal Oxides: A Multi-Scale Investigation			
11.20am	**IL121**	*Trygve Helgaker* The Dalton Quantum-Chemistry Program: Current Capabilities and Ongoing Development	**IL126**	*Jürgen Hafner* Ab Initio Simulations of Materials Using VASP: Density Functional Theory and Beyond	**IL131**	*P. Mark Rodger* Finding Infrequent Events with MD: Methods for Studying Crystal Nucleation	**OC069**	*Ria Broer* The State of Transition Metals in Transition Metal Oxides			
							OC070	*Marie-Liesse Doublet* New Concepts of Redox Centers in Electrode Materials for Li-Ion Batteries			
11.40am	**IL122**	*Hans Lischka* COLUMBUS: An Efficient Quantum Chemical Tool for Multireference Configuration Interaction	**IL127**	*Julian Gale* The SIESTA Approach to Linear-Scaling Density Functional Theory	**IL132**	*Teresa Head-Gordon* Experimental and Simulation Studies of Bulk Water and Hydration Water at Interfaces	**IL135**	*Carlo Adamo* Molecular Spintronics from a Theoretical Point of View			
12.00pm	**IL123**	*Roland Lindh* The MOLCAS Package: A Platform for Application and Development of Ab Initio Methods	**IL128**	*James Stewart* Current Status of the Semiempirical Program MOPAC2007	**IL133**	*Patricia Hunt* When Does a Reduction in Hydrogen Bonding Lead to an Increase in Viscosity?	**OC071**	*Ross McKenzie* Electronic Excited States in Optically Active Biomolecules: Quantum Systems with a Tuneable Environment Interaction			
							OC072	*Gemma Solomon* When Things are not as They Seem: Quantum Interference Turns Molecular Electron Transfer "Rules" Upside Down.			

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WEDNESDAY SEPTEMBER 17

12.20pm	**IL124**	*Jürgen Gauss* ACES2: Computational Chemistry with State-of-the-Art Coupled-Cluster Techniques	**IL129**	*George Fitzgerald* Towards Multiscale Modelling of Materials: Quantum Mechanics-Based Methods for Extremely Large Systems using Materials Studio	**OC067**	*Ekaterina Izgorodina* Design of Novel Ionic Liquids: An Ab Initio Approach	**OC073**	*Ben Powell* Strong Correlations in Organic Molecular Superconductors: What Role for First Principles Calculations?
					OC068	*Antonio Tilocca* Classical and Car-Parrinello Molecular Dynamics Studies of Bioactive Glasses	**OC074**	*Manuel Fernández-Gómez* Theoretical Study of Phenyl-thiadiazol Derivatives as Candidates for Electron-Conducting Polymers
12.40pm–	LUNCH BREAK / EXCURSION							

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THURSDAY SEPTEMBER 18

8.30–9.50am	**12. Plenary Session** Chair: *Mark Gordon* PARKSIDE AUDITORIUM							
8.30am	**PL008**	*Rodney Bartlett* – **2008 Schrödinger Medal Lecture:** Coupled-Cluster Theory in Quantum Chemistry: The Emergence of a New Paradigm						
9.10am	**PL009**	*Lucas Visscher* – **2006 Dirac Medal Lecture:** Relativistic Electronic Structure Theory						
9.50–10.20am	MORNING TEA							
10.20am–12.20pm	**13.1 Theory II** Chair: *Rodney Bartlett* PARKSIDE AUDITORIUM		**13.2 Intermolecular Interactions** Chair: *Pavel Hobza* PARKSIDE 110A		**13.3 Organic and Inorganic Photochemistry** Chair: *Todd Martínez* PARKSIDE G04		**13.4 Biological Structures & Simulations III** Chair: *Julia Rice* PARKSIDE 110B	
10.20am	**IL136**	*Weitao Yang* Insights and Progress in Density Functional Theory	**IL142**	*Mark Gordon* A General Approach to Intermolecular Interactions: Theory and Applications	**IL148**	*Thorsten Klüner* Surface Photochemistry from First Principles	**IL153**	*Russell Boyd* The Electron Density as an Interpretive Tool in Chemistry
10.40am	**IL137**	*Klaus Ruedenberg* Accurate Ab Initio Anatomy of a Diatomic Potential Energy Curve at Short, Medium and Long Ranges: The Fluorine Molecule	**IL143**	*Dieter Cremer* Efficient and Reliable DFT Treatment of van der Waals Complexes	**IL149**	*Roger Amos* Excitation Energies using a Re-parameterised CAM-B3LYP Functional	**IL154**	*Marcus Elstner* What Governs the Charge Transfer in DNA? The Role of DNA Conformation and Environment
11.00am	**IL138**	*Frank Jensen* Polarization Consistent Basis Sets: An Overview	**IL144**	*Georg Jansen* Density Functional Theory Combined with Symmetry-Adapted Perturbation Theory: Characterization of Intermolecular Interactions and Potential Energy Surfaces	**IL150**	*Leticia González* Photochemistry, Dynamics, and Control in Organic Systems	**OC082** **OC083**	*To be advised* *To be advised*
11.20am	**IL139**	*Poul Jørgensen* A Hierarchical Optimization Strategy for the Kohn-Sham Energy Using a Ground State Directed Optimization Algorithm	**OC077** **OC078**	*Christian Mück-Lichtenfeld* Dispersion-Corrected DFT for van der Waals Interactions of Large Molecules *Gregory Tschumper* Benchmark Interaction Energies and Non-Additivities for Weakly Bound Non-Covalent Clusters: Extending Databases Beyond Dimers	**IL151**	*Wei-Hai Fang* Photodissociation of Aromatic Carbonyl Compounds: A Theoretical Study	**IL156**	*Miroslav Urban* Towards More Extended CCSD(T) Calculations of Model H-Bonded and Stacked Dimers and Electron Affinities. Can We Improve the Electron Affinity of Uracil?

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11.40am	**IL040**	*Alistair Rendell* How Accurate Are Your Integrals? Quantifying Numerical Inaccuracies in Quantum Chemical Calculations	**IL145**	*David Sherrill* Methods for Non-Bonded Interactions	**OC079**	*George Bacskay* Quantum Chemical Computations of Spectroscopic Constants, Oscillator Strengths and Radiative lifetimes for CO and C_2	**OC085**	*Renate Griffith* How Do We Compare? An Assessment of GPCR Modelling.
					OC080	*Kyoung Koo Baeck* Ab Initio Molecular Dynamics Study for Ultrafast Photo-dynamics of Small Polyatomic Molecules	**OC086**	*Michael Shokhen* Rationalization of the Driving Force Controlling the pK_a of Catalytic Residues and Enzyme Acid/Base Catalysis
12.00pm	**IL141**	*Michael Dolg* The Incremental Scheme: A Local Correlation Method for Molecules and Solids	**IL146**	*Jerzy Leszczynski* Beyond 0 K: In Silico Chemistry of Intermolecular Complexes	**IL152**	*Jeffrey Reimers* New Quantum Chemical Techniques for Nanotechnology, Biotechnology, and Photochemistry	**IL157**	*Piotr Paneth* QM and QM/QM Approaches to Mechanisms of Enzymatic Reactions
12.20pm	**OC075**	*Alexei Arbuznikov* Local Hybrid Functionals: New DFT Routes Towards Accurate Thermochemistry, Kinetics, and Response properties	**IL147**	*Bogumil Jeziorski* Coupled-Cluster Approach to Dynamic Density Susceptibility and its Application to van der Waals Interactions	**OC081**	*Paolo Raiteri* Unravelling the Shuttling Mechanism in a Photoswitchable Multi-Component Bistable Rotaxane	**IL158**	*Ursula Röthlisberger* Mixed QM/MM Simulations of Electron Transfer Proteins
	OC076	*Maria Elena Fuentes* CNDOL as a Fast and Reliable Method for the Calculation of Electronic Properties of Very Large Polyatomic Systems			**OC082**	*Koichi Yamashita* Electron-Phonon Coupling and Surface Electronic States of Cs/Cu(111)		
12.40–2.00pm	LUNCH BREAK							
2.00–3.40pm	**14.1 Mechanisms/Potential Energy Surfaces** Chair: *H. Bernhard Schlegel* PARKSIDE AUDITORIUM		**14.2 Hydrogen Bonds/Acids and Bases** Chair: *Tony Ford* PARKSIDE 110A		**14.3 Optical Material Properties** *Sponsored by the US AFOSR/AOARD* Chair: *Marco Nascimento* PARKSIDE G04		**14.4 Biological Structures & Simulations IV** Chair: *David Smith* PARKSIDE 110B	
2.00pm	**IL159**	*Elfi Kraka* The Mechanism of Barrier-less Reactions – Application of the Unified Reaction Valley Approach	**IL163**	*Josef Michl* Enormous Substituent Effects on Brønsted Acidity of the CH vertex in $HC(BH)_{11}(-)$	**IL167**	*Tom Ziegler* Probing the Excited States of Metallo Porphyrins and Phthalocyanines by Magnetic Circular Dichroism. A TD-DFT Study	**IL170**	*Martin Field* Hybrid Quantum Chemical and Molecular Mechanical Potential Simulations of Enzyme Systems
2.20pm	**IL160**	*Alejandro Toro-Labbé* The Reaction Force and Reaction Electronic Flux in Chemistry. Characterization of Reaction Mechanisms	**IL164**	*Chin-Hui Yu* Homo- and Heteronuclear Low Barrier Hydrogen Bonds	**IL168**	*George Schatz* Optical Properties of Metal Nanostructures: Electronic Structure Studies of Plasmon Excitation Effects	**IL171**	*Hualiang Jiang* Mechanical Fundamentals of Channel Gating of Some Important Ion Receptors: Computational Simulations versus Experiments

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THURSDAY SEPTEMBER 18

2.40pm	**IL161**	*Koichi Ohno* Global Reaction Route Mapping on the Potential Energy Surface via Anharmonic Downward Distortion Following	**IL165**	*Michiel Sprik* Density Functional Calculation of Acidity Constants using Proton Insertion Methods	**OC091**	*Yasushi Honda* Theoretical Studies on the Circular Dichroism Spectra of L-Amino Acids	**OC095**	*Sameer Varma* Mechanisms of Ion Recognition by Biological Molecules
					OC092	*Mike Ford* The Optical Properties of Alkali – Noble – Group 3 Alloys	**OC096**	*Jiri Mareda* Modelling of Synthetic Pore Sensors
3.00pm	**OC087**	*Bernd Ensing* Probing the Minimum Free Energy Pathway of Concerted Chemical Reactions	**IL166**	*Maciej Gutowski* Electron-Driven Acid-Base Chemistry: Proton Transfer from Hydrogen Chloride to Ammonia. Visualization of Molecular Orbitals	**OC093**	*Marko Schreiber* Benchmarks for Electronically Excited States: CASPT2, CC2, CCSD, CC3, TDDFT and DFT-MRCI	**OC097**	*Itamar Kass* From Structure to Function in a Membrane: A Theoretical Approach to Study the Activity of Membrane Proteins
	OC088	*Masataka Nagaoka* Absolute Reaction Rates in Solution via the Free Energy Gradient Method with Molecular Dynamics Simulations			**OC094**	*Ruth Pachter* Nonlinear Optical Absorbing Materials: Time-Dependent Density Functional Theory Calculations of Photophysical Properties	**OC098**	*Ricardo Mancera* Molecular Modelling of the Interactions of Glycosaminoglycans with the PECAM-1 Receptor
3.20pm	**IL164**	*Raghavan Sunoj* Probing the Importance of Explicit Solvents/Additives in Organic Reactions Through Transition State Modelling	**OC089**	*Amalendu Chandra* Hydrogen Bond Dynamics, Proton Transfer and Vibrational Spectral Diffusion in Aqueous Solutions from First Principles	**IL169**	*Dylan Jayatilaka* Refractive Indices for Molecular Crystals Obtained from X-Ray Constrained Wavefunctions	**OC099**	*Jörg Grunenberg* Understanding Carbohydrate Recognition: Towards the Rational Design of Biomimetic Receptors
			OC090	*Jean-Christophe Soetens* Hydrogen Bonding in Supercritical Ammonia as seen by Molecular Dynamics Simulations and Vibrational Spectroscopy			**OC100**	*Henry Woodcock* How Sweet It Is: The Importance of Solvation when Modelling Carbohydrates
3.40–4.10pm	AFTERNOON TEA							
4.10–5.30pm	**15.1 Biological Photochemistry** Chair: *Miroslav Urban* PARKSIDE AUDITORIUM		**15.2 Organic Reactions II** Chair: *Kendall Houk* PARKSIDE 110A		**15.3 Protein Folding** Chair: *Andrew Rohl* PARKSIDE G04		**15.4 Solvation** Chair: *Andreas Klamt* PARKSIDE 110B	
4.10pm	**IL172**	*Walter Thiel* Surface Hopping Studies on Excited State Dynamics of Nucleobases	**IL175**	*Hendrik Zipse* Modelling Reactivity and Selectivity in Organocatalysis	**IL177**	*Jan H. Jensen* Prediction and Rationalization of Protein Stability and Activity	**IL180**	*Benedetta Mennucci* Radiative and Non Radiative Decays of Electronically Excited States in Complex Environments: A Quantum Mechanical Approach

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4.30 pm	**IL173**	*Todd Martínez* Photochemistry and Mechanochemistry from First Principles Dynamics	**IL176**	*Richard M. W. Wong* Understanding Stereoselectivity in Asymmetric Organocatalysis	**IL178**	*Gerhard Hummer* Replica-Exchange Simulations of Protein-Protein Complex Formation	**IL181**	*Brian Smith* Conformational Study of Benzoylureas in Organic Solvents
4.50pm	**IL174**	*Luis Serrano-Andrés* Photostability and Photoreactivity in DNA/RNA Components: Quantum Chemistry of Nucleic Acid Base Monomers and Dimers	**OC103**	*Fernando P. Cossío* Recent Computational Studies on the Staudinger Reaction Between Ketenes and Imines	**OC107**	*Stefano Piana-Agostinetti* Calculation of Folding Kinetics and Thermodynamics with Atomistic Simulations	**IL182**	*Vudhichai Parasuk* From Copper-Water Complex Coordination to Conformations of Keto-Enolate Compounds
			OC104	*David Henry* A DFT Study of H_2 Interactions with Light Metal Clusters	**OC108**	*Francesco Gervasio* Protein Conformational Plasticity: The Closure Mechanism of CDK5		
5.10–5.30pm	**OC101**	*Ines Corral Perez* Generating Singlet Oxygen from Endoperoxides and Phthalocyanines	**OC105**	*Bun Chan* A Zeolite that Catalyzes the Hydrogenation of Carbon Dioxide	**IL179**	*William Swope* Simulations of Protein Folding on the BlueGene Supercomputer at IBM	**OC109**	*Daniel Schofield* Polymorphism in Clathrate Hydrates
	OC102	*Hong Zhang* Quantum Mechanical Investigations of Proton Transfer Dynamics in Green Fluorescent Protein (GFP)	**OC106**	*Mariona Sodupe* Interaction of Amino Acids with Silica Materials			**OC110**	*Mark Iron* A DFT Investigation of the Implausible Probable: A Water-Stable Organic Dianion
7.00pm–	CONGRESS BANQUET – DOCKSIDE, COCKLE BAY WHARF, DARLING HARBOUR							

PROGRAMME • FRIDAY SEPTEMBER 19

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FRIDAY SEPTEMBER 19

8.30–9.50am	**16. Plenary Session** Chair: *Henry F. Schaefer III* PARKSIDE AUDITORIUM	
8.30am	**PL010**	*Martin Head-Gordon* – Tractable Valence Space Models for Strong Electron Correlations
9.10am	**PL011**	*Shigeru Nagase* – The Important Interplay between Theoretical Calculations and Experiment
9.50–10.20am	MORNING TEA	
10.20am–12.30pm	**17. Closing Session** Chair: *Peter M. W. Gill* PARKSIDE AUDITORIUM	
10.20am	**PL012**	*Tim Clark* – Simulating Biological Signal Transduction
11.00am	**PL013**	*Donald G. Truhlar* – **2006 Schrödinger Medal Lecture:** New Density Functionals with Broad Applicability for Thermochemistry, Thermochemical Kinetics, Noncovalent Interactions, Transition Metals, and Spectroscopy
11.40am–12.30pm	CLOSING CEREMONY & POSTER PRIZE PRESENTATIONS	

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