Ninth Conference of the Asia-Pacific Association of Theoretical and Computational Chemists

PROGRAMME BOOK

PROGRAMME AT A GLANCE

MONDAY 30 SEPTEMBER 2019			
12.30-7.45pm	Registration open - *Foyer, Abercrombie Business School (ABS)*		
	ABS Auditorium (B2010)		
2.00-3.20pm	**Opening Ceremony** Welcome to Country by Uncle Chicka Madden Welcome from Professor Leo Radom, Chair, APATCC 2019 Welcome by The Hon. Gabrielle Upton, MP Welcome from Professor Barbara Messerle, Provost, University of Sydney Welcome from Professor Leo Radom, President APATCC		
3.20-4.00pm	**Plenary Session 1**		
3.20pm	**PL001**	*Kazuo Kitaura*	**Morokuma Lecture** - Honoring the Late Professor Keiji Morokuma
3.40pm	**PL002**	*Addy Pross*	How Could Life Have Emerged?
4.00-4.30pm	Afternoon Tea and Poster Viewing - *ABS Upper Foyer*		
4.30-6.00pm	**Plenary Session 2**		
4.30pm	**PL003**	*Amanda Barnard*	Materials Intelligence
5.00pm	**PL004**	*Yi Qin Gao*	**2016 Pople Medal** - A Phase Separation Perspective for Chromatin Structure Change In Development, Differentiation, Senescence And Certain Diseases
5.30pm	**PL005**	*Kazuo Takatsuka*	**2019 Fukui Medal** - Time-Domain Quantum Chemistry Beyond the Born-Oppenheimer Paradigm
6.15-8.15pm	Poster Session (P001-P076) and Mixer - *ABS Upper Foyer.* Please refer to the additional booklet **"POSTERS - AUTHORS - PARTICIPANTS"** in your satchels for the full poster list, Index of all authors and the list of Participants.		

TUESDAY 1 OCTOBER 2019

8.00am-7.45pm	Registration open - *Foyer, Abercrombie Business School (ABS)*			
	ABS Lecture Theatre 1040	*ABS Case Study Lecture Theatre 1050*	*ABS Case Study Lecture Theatre 1060*	*ABS Case Study Lecture Theatre 1070*
9.00-10.20am	**DFT**	**Chemical Reactivity A**	**Condensed Phase Chemistry A**	**Biomolecules**
10.20-10.50am	Morning Tea			
10.50am-12.30pm	**Electronic Structure**	**Reaction Paths**	**Condensed Phase Methods**	**Heavy Elements**
12.30-2.00pm	Lunch			
2.00-3.20pm	**Modeling Electronic Structures**	**Dispersion**	**Low Dimensional Materials**	**Drug Design**
3.20-3.50pm	Afternoon Tea and Poster Viewing			
3.50-5.30pm	**Computational Technology**	**Chemical Reactivity B**	**Catalysis and Surface Chemistry**	**Modeling Biological Functions**
6.00-8.00pm	Poster Session (P077-P149 and Mixer - *ABS Upper Foyer.* Please refer to the additional booklet **"POSTERS - AUTHORS - PARTICIPANTS"** in your satchels for the full poster list, Index of all authors and the list of Participants.			

WEDNESDAY 2 OCTOBER 2019

8.00am-7.45pm	Registration open - *Foyer, Abercrombie Business School (ABS)*			
	ABS Lecture Theatre 1040	*ABS Case Study Lecture Theatre 1050*	*ABS Case Study Lecture Theatre 1060*	*ABS Case Study Lecture Theatre 1070*
9.00-10.20am	**Large Systems**	**Catalysis A**	**Machine Learning & Supercomputers**	**Metals in Biology**
10.20-10.50am	Morning Tea			
10.50am-12.30pm	**Excited States A**	**Chemical Structure**	**Condensed Phase Chemistry B**	**Structure and Reactivity**
12.40pm	*Bus transfers to Sydney Harbour Lunch Cruise depart from ABS (pre-bookings essential)*			
1.30pm	*Sydney Highlights and Bondi Beach Bus Tour departs from ABS (pre-bookings essential)*			
7.30pm	*West Side Story @ Sydney Opera House (tickets sold out) - Joan Sutherland Theatre*			

PROGRAMME AT A GLANCE

PROGRAMME AT A GLANCE

THURSDAY 3 OCTOBER 2019				
8.00am-7.45pm	Registration open - *Foyer, Abercrombie Business School (ABS)*			
	ABS Lecture Theatre 1040	*ABS Case Study Lecture Theatre 1050*	*ABS Case Study Lecture Theatre 1060*	*ABS Case Study Lecture Theatre 1070*
9.00-10.20am	**Non-bonded interactions**	**Molecular Design**	**Materials Design**	**Biological Mechanisms**
10.20-10.50am	Morning Tea			
10.50am-12.30pm	**DMRG**	**Excited States B**	**Clusters and Bulk**	**New Tools for Modeling Biology**
12.30-1.40pm	Lunch			
1.40-2.20pm	**Challenging Molecules**	**Electrostatic Effects**	**Catalysis B**	**Complex Biomolecules**
2.20pm	Changeover time			
2.30-3.30pm	**Plenary Session 3**			
	ABS Auditorium (B2010)			
2.30pm	**PL006** *Carmay Lim*	Metal Ions & Brain Signaling		
3.00pm	**PL007** *Jian Liu*	**2019 Pople Medal** - A Unified Thermostat Scheme for Efficient Configurational Sampling for Classical/Quantum Canonical Ensembles via Molecular Dynamics: From the Single-Electronic-State System to the Non-Adiabatic System		
3.30-4.00pm	Afternoon Tea			
4.00-4.30pm	**Plenary Session 4**			
	ABS Auditorium (B2010)			
4.00pm	**PL008** *Martin Head-Gordon*	Progress and Problems in the Design of Density Functionals		
4.30-5.10pm	**Prize Presentations and Closing Ceremony**			
7.00-11.00pm	**Conference Banquet at Le Montage** (bookings essential) - *Le Montage, 38 Frazer Street, Lilyfield NSW 2040 (Waterfront Entrance), Deanah's View room*			

PROGRAMME • Monday 30 September

PL - Plenary Lecture | IL - Invited Lecture | IC - Invited Communication | P - Poster Presentation

MONDAY 30 SEPTEMBER 2019			
12.30-7.45pm	Registration open - *Foyer, Abercrombie Business School (ABS)*		
	ABS Auditorium (B2010)		
2.00-3.20pm	**Opening Ceremony** *Chair: Leo Radom* Welcome to Country by Uncle Chicka Madden Welcome from Professor Leo Radom, Chair, APATCC 2019 Welcome by The Hon Gabrielle Upton, MP Welcome from Professor Barbara Messerle, Provost, University of Sydney Welcome from Professor Leo Radom, President APATCC		
3.20-4.00pm	**Plenary Session 1** *Chair: Leo Radom*		
3.20pm	**PL001**	*Kazuo Kitaura*	**Morokuma Lecture** - Honoring the Late Professor Keiji Morokuma
3.40pm	**PL002**	*Addy Pross*	How Could Life Have Emerged?
4.00-4.30pm	Afternoon Tea and Poster Viewing - *ABS Upper Foyer*		
4.30-6.00pm	**Plenary Session 2** *Chair: Yundong Wu*		
4.30pm	**PL003**	*Amanda Barnard*	Materials Intelligence
5.00pm	**PL004**	*Yi Qin Gao*	**2016 Pople Medal** - A Phase Separation Perspective for Chromatin Structure Change In Development, Differentiation, Senescence And Certain Diseases
5.30pm	**PL005**	*Kazuo Takatsuka*	**2019 Fukui Medal** - Time-Domain Quantum Chemistry Beyond the Born-Oppenheimer Paradigm
6.15-8.15pm	Poster Session (P001-P076) and Mixer - *ABS Upper Foyer*. Please refer to the additional booklet **"POSTERS - AUTHORS - PARTICIPANTS"** in your satchels for the full poster list, Index of all authors and the list of Participants.		

PROGRAMME • Tuesday 1 October

PL - Plenary Lecture | IL - Invited Lecture | IC - Invited Communication | P - Poster Presentation

TUESDAY 1 OCTOBER 2019

8.00am-7.45pm	Registration open - *Foyer, Abercrombie Business School (ABS)*			
	ABS Lecture Theatre 1040	*ABS Case Study Lecture Theatre 1050*	*ABS Case Study Lecture Theatre 1060*	*ABS Case Study Lecture Theatre 1070*
9.00-10.20am	**DFT** *Chair: Lars Goerigk*	**Chemical Reactivity A** *Chair: Bun Chan*	**Condensed Phase Chemistry A** *Chair: Alister Page*	**Biomolecules** *Chair: Junming Ho*
9.00am	**IL001** *Peter Gill* Rebuilding the Foundations of Density Functional Theory	**IL004** *Yun-Dong Wu* Mechanistic Understanding of Catalysis by Combining Computation and Mass Spectrometry	**IL007** *Julian Gale* Exploring the Stable Pre-Nucleation Species for Calcium Phosphate Materials	**IL010** *Jiali Gao* Allosteric Regulation of Biological Function from Multistate Density Functional Theory
9.20am	**IL002** *Henryk Witek* Uniform Electron Gas on a 3-Sphere	**IL005** *Kazunari Yoshizawa* Orbital Concept for Methane Activation	**IL008** *Hirofumi Sato* Understanding the Self-Assembly Process: A Global and Local Approach	**IL011** *Stacey Wetmore* Modeling Human DNA Repair Processes
940am	**IL003** *Eunji Sim* Benefits of Inconsistent Density Functional Calculations	**IL006** *Satoshi Yabushita* Quantum Interference Effects in ICN Photodissociation Reaction	**IL009** *Yun Hee Jang* Ionic Liquids for PEDOT:PSS Conductivity Enhancement: Multiscale Molecular Modeling	**IL012** *Joseph Lane* Bonder: Convenient Analysis of Non-Covalent Interactions
10.00am	**IC001** *Stephen Dale* Complete Basis Set Limit Convergence for Finite Uniform Electron Gases	**IC003** *Manikandan Paranjothy* Competing Molecular and Radical Pathways in the Dissociation of Halons via Direct Chemical Dynamics Simulations	**IC005** *Hemant Kashyap* Thermodynamic Phases and Structural Organization of Ionic Liquids within Nanoscale Solvophobic Confinement	**IC007** *Kimichi Suzuki* Multistructural Microiteration Technique Adopting the Electrostatic Embedding Scheme
10.10am	**IC002** *Hiroyuki Nakashima* Implementation of Slater-Type One-Center Atomic Integrals for Accurate Variational Calculations of Small Atoms by Free Complement Theory	**IC004** *Yi Zhao* Theoretical Simulation of Carrier Quantum Dynamics in Organic Materials	**IC006** *Kentaro Yamamoto* A Chemical Mechanism of Unidirectional Proton Transfers Driven by Coupled Proton and Electron-Wavepacket Transfers	**IC008** *Susmita De* TCR Recognition in Chronic Beryllium Disease – Molecular level Understanding of Be2+ Binding to HLADP2-Peptide Complex

10.20-10.50am	Morning Tea			
10.50am-12.30pm	**Electronic Structure** *Chair: Yuxiang Bu*	**Reaction Paths** *Chair: Shigeru Nagase*	**Condensed Phase Methods** *Chair: Jing Ma*	**Heavy Elements** *Chair: Russell Boyd*
10.50am	**IL013** *Seiichiro Ten-no* Full Coupled-Cluster Reduction for Strongly Correlated Electrons	**IL017** *Koichi Ohno* Quantum Chemical Exploration of Novel Chemistry on Potential Energy Surfaces	**IL021** *Shigeyoshi Sakaki* Proposal of Periodic-QM/MM Method and Its Application to a Molecular Crystal Consisting of a Transition Metal Complex	**IL025** *Peter Schwerdtfeger* The Year of the Periodic Table - Going Superheavy
11.10am	**IL014** *Debashis Mukherjee* Interlacing and Avoided Crossings of a Manifold of Potential Energy Surfaces Studied by a Spin-Free State Specific Many-Body Approach	**IL018** *Satoshi Maeda* Understanding Reaction Mechanisms Using Reaction Path Networks Generated by the Artificial Force Induced Reaction Method	**IL022** *Bun Chan* Computational Fullerene Thermochemistry	**IL026** *Masahiro Ehara* Coordination Asymmetry: Frenkel-Exciton Decomposition Analysis of Circular Dichroism and Circularly Polarized Luminescence for Multichromophoric Systems
11.30am	**IL015** *Sourav Pal* Effects of Triples in Fock Space Coupled Cluster: Fourth Order Perturbation Corrections to Electron Affinity and Excitation Energy	**IL019** *Tetsuya Taketsugu* Reaction Path Concept: Intrinsic Reaction Coordinate, Anharmonic Downward Distortion Following, and Ab Initio MD	**IL023** *Debra J. Searles* Calculation of Local Diffusion Coefficients for Inhomogeneous Systems	**IL027** *Alessandro Soncini* Ab Initio Models for Lanthanide Complexes in Molecular Magnetism
11.50am	**IL016** *Wenjian Liu* Iterative Configuration Interaction with Selection	**IL020** *Eluvathingal Jemmis* MECP (Minimum Energy Crossing Point) Barrier Controls Reductive Coupling of Isocyanides Mediated by Cr-Cr Quintuple Bond: A DFT Study Involving 50 Intermediates, 23 Transition States and a Range of Spin Multiplicities	**IL024** *Irene Suarez-Martinez* Transferability of Carbon Interatomic Potentials: Lessons from Amorphous Carbon & Graphitization	**IL028** *Liviu Ungur* Ab Initio Crystal Field for Lanthanides

PROGRAMME • Tuesday 1 October

12.10pm	**IC009** *Xiuwen Zhou* Predicting the Emission Efficiency of Phosphorescent Emitters in OLEDs	**IC011** *Toshiaki Matsubara* Insight into the Chemical Reactions from the Molecular Dynamics Simulation	**IC013** *Chien-Pin Chou* Density-Functional Tight-Binding Metadynamics Study of Oxy-Carbon Diffusion on (100)-g-Al2O3 Surface	**IC015** *Asaph Widmer-Cooper* Colloidal Stability of Apolar Nanoparticles: Insights from Simulations and Theory
12.20pm	**IC010** Hyeonho Choi Computational Strategies to Achieve Highly Efficient and Stable OLEDs: An Industrial Perspective	**IC012** *Gabriel da Silva* Decomposition of PFOS and PFOA: A Density Functional Theory and Transition State Theory Study	**IC014** *David Huang* Entrance Effects in Concentration Gradient-Driven Flow Through an Ultrathin Porous Membrane	**IC016** *Muhammad Alif Mohammad Latif* The Structural and Dynamics Properties of Enzyme Encapsulated in Metal-Organic Framework
12.30-2.00pm	Lunch			
2.00-3.20pm	**Modeling Electronic Structures** *Chair: Amir Karton*	**Dispersion** *Chair: Shridhar Gadre*	**Low Dimensional Materials** *Chair: Aloysius Soon*	**Drug Design** *Chair: Binju Wang*
2.00pm	**IL029** Wei Wu Combining Ab Initio Valence Bond Method with Density Functional Theory	**IL032** *Hyungjun Kim* uMBD: A Materials-Ready Dispersion Correction that Uniformly Treats Metallic, Ionic, Covalent, and van der Waals Bonding	**IL035** *Michael Ford* Theoretical Spectroscopy of Semiconductor Defects with Application to 2D hBN Nanophotonics	**IL038** *Supa Hannongbua* Identification of Absolute Configuration of Diptoindonesin D by Quantum Chemical Calculations and interaction with Penicillin-Binding Protein 2a, Based on Molecular Docking
2.20pm	**IL030** *Xin Xu* Extended Koopmans' Theorem at the Second Order Perturbation Theory: From Wave Function Theory to Density Functional Theory	**IL033** *John Dobson* Dispersion Interactions Between "Zero Dimensional Metals"	**IL036** *Jijun Zhao* Eighteen Functional Monolayer Metal Oxides: Wide-Bandgap 2D Semiconductors with Superior Oxidation Resistance and Ultrahigh Carrier Mobility	**IL039** *Thanyada Rungrotmongkol* Anticancer Drug Screening and Development
2.40pm	**IL031** *Deborah Crittenden* A New Minimal-Determinant Electronic Structure Model that Interpolates Between Molecular Orbital and Valence Bond Theories	**IL034** *Jeffrey Reimers* The van der Waals Force: How it Can Outcompete Covalent and Ionic Bonding, and How it Can Be Switched Off	**IL037** *Nicola Gaston* How Stable is 2D gallium, aka Gallenene? Electronic and Thermodynamic Aspects	**IL040** *Luhua Lai* Ligand Design for Intrinsically Disordered Proteins

3.00pm	**IC017** *Mario Piris* Natural Orbital Functional for Multiplets	**IC019** *Peifeng Su* Origin of Intermolecular Interactions in Open Shell Singlet State	**IC021** *Pieremanuele Canepa* High-Stability and Fast-ion Transport in Mg-based Compounds for Mg batteries from First-Principles Calculations	**IC023** *Andrew Christofferson* The Michaelis Complex for Nitroaromatic Substrates in Bacterial Nitroreductases Determined by Molecular Dynamics Simulations
3.10pm	**IC018** *Manolo Per* Benchmarking Real-Space Quantum Monte Carlo for Quantum Chemistry	**IC020** *Takashi Tsuchimochi* Second-Order Perturbation Theory with Spin-Projected Hartree-Fock	**IC022** *Ravichandar Babarao* Metal-Organic Frameworks for Energy and Environmental Applications: From Molecular Modeling to Mass Production	**IC024** *Hui-Chung Tai* Gene Silencing Mechanisms Revealed by Dynamics of Guide, Target and Duplex Binding to Argonaute
3.20-3.50pm	Afternoon Tea and Poster Viewing			
3.50-5.30pm	**Computational Technology** *Chair: Roger Amos*	**Chemical Reactivity B** *Chair: Chin-Hui Yu*	**Catalysis and Surface Chemistry** *Chair: Shigeyoshi Sakaki*	**Modeling Biological Functions** *Chair: Stacey Wetmore*
3.50pm	**IL041** Hiromi Nakai How Can Artificial Intelligence Help Quantum Chemists?	**IL044** *Minori Abe* Theoretical Study of Uranium Isotope Fractionation by Bacteria	**IL047** *Michelle Spencer* Effect of Defects on the Gas Sensing Reaction of CH2O and H2S with ZnO Nanostructures	**IL050** *Jaeyoung Sung* Chemical Dynamics in Living Cells
4.10pm	**IL042** *Ivan Kassal* Simulating Non-Adiabatic Chemical Dynamics on Quantum Computers	**IL045** *Parameswaran Pattiyil* Rule Breaking Main Group Compounds Stabilized by Donor-Acceptor Interactions	**IL048** *Supawadee Namuangruk* Formaldehyde Oxidation over Metal-Supported Titanium Dioxide	**IL051** *Megan O'Mara* Does the Choice of Molecular Dynamics Forcefield or Starting Crystal Structure Influence Membrane Protein Dynamics?
4.30pm	**IL043** *Gino DiLabio* Atom-Centred Potentials: A Tool for Fast and Accurate Modelling of Molecular Systems	**IL046** *Richard Wong* Fluorine as Halogen Bonding Donor?	**IL049** *David Henry* Coordination of Ligands to Gallium Nanoclusters: Structure, Stability and Reactivity	**IL052** *Hsiao-Ching Yang* Unravelling how Enzyme Channel Drives Stepwise Translocation and Optimal Binding of Prostaglandin H2 for Cyclization

PROGRAMME • Tuesday 1 October

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4.50pm	**IC025**	*Terry Frankcombe*	Gaussian Basis Function Methods for Propagating Molecular Wave Functions: BEL MCG	**IC029**	*Benjamin Noble*	Electrochemical Alkoxyamine Cleavage; a 'On-Demand' Source of Radicals and Cations for Synthesis	**IC033**	*Qinghong Yuan*	Enhanced Catalytic Performance of Ni(111) surface doped with Cu for the decomposition of CH4	**IC037**	*Ricky Nellas*	CGMD Approach: Mutation Studies on the Thermostability and Activity Improvement of a Plant Fructosyltransferase from Pachysandra terminalis
5.00pm	**IC026**	*Lin Ji*	Macroscopic Combustion Mechanism Representation Method Based on Complex Network Theory and Feedback Analysis	**IC030**	*Richmond Lee*	Halogenophilic Nucleophilic Substitution Reaction from a Theoretical Perspective	**IC034**	*Yoyo Hinuma*	Density Functional Theory Calculations on Surface Oxygen Vacancy Formation in Metal Oxides	**IC038**	*Evelyne Deplazes*	A New, Flexible Enhanced Sampling Method to Predict Binding Free Energy of Small Molecules – Membrane Systems
5.10pm	**IC027**	*Junichi Ono*	Large-Scale Quantum-Mechanical Molecular Dynamics Simulations for the Long-Distance Proton Transfer in Bacteriorhodopsin	**IC031**	*Fengyi Liu*	Photochemistry of Criegee Intermediate Revealed by Multireference Ab Initio Calculation and Nonadiabatic Molecular Dynamics	**IC035**	*Marlies Hankel*	Carbon Nitride Materials as Anodes in Lithium Ion Batteries	**IC039**	*Ronan Bureau*	The Pharmacophore Network: A Computational Method for Exploring Structure–Activity Relationships from a Large Chemical Data Set
5.20pm	**IC028**	*Masanori Tachikawa*	Path Integral Simulation for Accurate Calculation of Hyperfine Coupling Constants of Muoniated Molecules	**IC032**	*Debashree Manna*	Isolated Iron(II) Phthalocyanine Exhibits Quintet Ground-State: A Nexus between Theory and Experiment	**IC036**	*Manussada Ratanasak*	Theoretical Investigation for the Mechanism of Copolymerization of CO2 and Cyclohexene Oxide Catalyzed by Novel Bifunctional Al(III) Porphyrin Catalyst	**IC040**	*Yves Lansac*	Protamine-Triggered DNA Self-Assembly Unveiled at the Molecular Level by Molecular Dynamics Simulations
6.00-8.00pm	Poster Session (P077-P149 and Mixer - *ABS Upper Foyer.* Please refer to the additional booklet **"POSTERS - AUTHORS - PARTICIPANTS"** in your satchels for the full poster list, Index of all authors and the list of Participants.											

PROGRAMME • Wednesday 2 October

PL - Plenary Lecture | IL - Invited Lecture | IC - Invited Communication | P - Poster Presentation

WEDNESDAY 2 OCTOBER 2019

8.00am-7.45pm	Registration open - *Foyer, Abercrombie Business School (ABS)*			
	ABS Lecture Theatre 1040	*ABS Case Study Lecture Theatre 1050*	*ABS Case Study Lecture Theatre 1060*	*ABS Case Study Lecture Theatre 1070*
9.00-10.20am	**Large Systems** *Chair: Krishnan Raghavachari*	**Catalysis A** *Chair: Richard Wong*	**Machine Learning & Supercomputers** *Chair: Steven Kirk*	**Metals in Biology** *Chair: Brian Smith*
9.00am	**IL053** *Michael Collins* Systematic Molecular Fragmentation by Annihilation	**IL046** *Richard Wong* QMTSDock - Automatic Conformational Search of Transition States for Catalytic Reactions Using Genetic Algorithm	**IL059** *Yousung Jung* Materials Discovery using Computational and Data-Driven Approaches	**IL062** *Elizabeth Krenske* Insights into the Mechanisms of Cytochrome P450-Catalyzed Hydroxylations from Studies on an Ultrafast Probe Substrate
9.20am	**IL054** *Shuhua Li* "Cluster-in-Molecule" Local Correlation Approach for Large Molecules and Periodic Systems	**IL057** *Hajime Hirao* Computational Studies of Chemical Reactions in Various Catalytic Environments	**IL060** *Miho Hatanaka* Database and Machine-Learning Enabled New Insights into the Lanthanide Luminescence Materials	**IL063** *Jen-Shiang Yu* Singly-bonded Dimanganese Coordination Complexes and Manganese-binding Proteins
9.40am	**IL055** *Ekaterina Pas* Studying Large-Scale Systems with Wavefunction-based Methods: Improving Accuracy	**IL058** *Raghavan B. Sunoj* Transition State Models for Asymmetric Catalysis and Rational Predictions	**IL061** *Rika Kobayashi* Computational Chemistry at the NCI Supercomputer Facility	**IL064** *Shigehiko Hayashi* Atomistically Deciphering Functional Processes of Photo-Receptor and Redox Proteins with Molecular Simulations
10.00am	**IC041** *Giuseppe Barca* Q-MP2-OS: an Inherently Parallel MP2 by Quadrature	**IC043** *Kaito Takahashi* Theoretical View on Gas Phase Water Catalysis at Room Temperature	**IC045** *Masato Kobayashi I* Surface Model Calculation Database for Predicting Catalytic Activity: An Application to Methane Steam Reforming	**IC047** *Russell Boyd* A Brief Account of My Encounters with Exchange in Computational Chemistry

PROGRAMME • Wednesday 2 October

10.10am	**IC042** *William Glover* Fragmentation Approach to Electronic Excitations	**IC044** *W. M. C. Sameera* Exploring Mechanistic Puzzles in Pd-Catalyzed Aziridine Ring-Opening Reactions	**IC046** *Nastaran Meftahi* Development of QSPR machine learning algorithms to predict photovoltaic properties	**IC048** *Binju Wang* The Molecular Mechanisms of Oxygen Activation and Hydrogen Peroxide Formation in Lytic Polysaccharide Monooxygenases
10.20-10.50am	Morning Tea			
10.50am-12.30pm	**Excited States A** *Chair: Ivan Kassal*	**Chemical Structure** *Chair: Sarah Masters*	**Condensed Phase Chemistry B** *Chair: Yousung Jung*	**Structure and Reactivity** *Chair: Megan O'Mara*
10.50am	**IL065** *Kimihiko Hirao* Excitation Energies can be Expressed in Terms of Orbital Energies Obtained from KS-DFT with LC Functionals	**IL069** *Chin-Hui Yu* The Computational Evidence for Homonuclear Dative Bonds	**IL073** *Jing Ma* Efficient Methods for Simulation of Stimuli-Responsive Materials in Condensed Phases	**IL077** *Jer-Lai Kuo* Ab-Initio Anharmonic Algorithms and their Applications to Understand Vibrational Coupling
11.10am	**IL066** *Lars Goerigk* Exploring Time-Dependent Double Hybrids with Range-Separation	**IL070** *Timothy Schmidt* Calculating Lewis-Structures and Curly Arrows from Ab-Initio Wavefunctions	**IL074** *Alister Page* Specific-Ion Effects in Aqueous, Non-Aqueous and Nanostructured Solvents: Multiscale Quantum Chemistry Approaches	**IL078** *Wei-Hai Fang* Quantum Trajectory Mean-Field Approach and its Implementation for Exploring the Dynamics of the Photoinduced Ring-Opening of 2-Thiophenone
11.30am	**IL067** *Chao-Ping Hsu* Excitation Energies from Time-Dependent Thermally-Assisted-Occupation Density Functional Theory	**IL071** *Ankan Paul* The Enigmatic Quadruple Bonding in C2: What do the Excited States Tell?	**IL075** *Wei Han* Multiscale Simulations of Peptide Assembly into Nanostructures	**IL079** *Joonsuk Huh* Quantum Simulation Methods for Molecular Vibronic Spectra
11.50am	**IL068** *Tim Gould* Ensemble Density Functional Theory: Stories from the Quest for a Low-Cost Quantum Chemical Approach for Excitations	**IL072** *David Wilson* Theoretical Analysis of Donor-Acceptor Bonding	**IL076** *Ya-Jun Liu* Computational Bioluminescence - Assignment of Bacterial Bioluminophore	**IL080** *Samantha Jenkins* Beyond Scalar Measures: Directional Chemical Perspective with Next Generation QTAIM

12.10pm	**IC049**	*Yuan-Chung Cheng* Understanding the Ultrafast Qx to Qy Transition in Chlorophylls	**IC051**	*Aulia Hutama* A Density Functional and Wave Function Theory-based Study on the Mechanism of Oxygen Atom Attack on Polycyclic Aromatic Hydrocarbon	**IC053**	*Nevena Todorova* Molecular Modelling Studies as a Complementary Approach to Experiments to Elucidate the Interfacial Bio-Nano Interactions of Biomaterials	**IC055**	*Jun Soo Kim* DNA-Based Brownian Motor for Directional Nanoparticle Delivery – Computational Design
12.20pm	**IC050**	*Muneaki Kamiya* Development of Large-Scale Time-Dependent Density Functional Theory Code Based on Massively-Parallel Sparse-Matrix Library	**IC052**	*Renate Griffith* Exploration of the Differences between Amine and Thiolate Addition to Acetylenedicarboxylates	**IC054**	*Takatoshi Fujita* Development of the Large-Scale GW+Bethe-Salpeter Equation Method Based on Fragment Molecular Orbital Method for Applications to Organic Materials	**IC056**	*Hideo Yamakado* Search for Conformers Using the Number of Molecular Independent Variables Reduction Method by Specifying Discrete Atoms
12.40pm	*Bus transfers to Sydney Harbour Lunch Cruise depart from ABS (pre-bookings essential)*							
1.30pm	*Sydney Highlights and Bondi Beach Bus Tour departs from ABS (pre-bookings essential)*							
7.30pm	*West Side Story @ Sydney Opera House (tickets sold out) - Joan Sutherland Theatre*							

PROGRAMME • Thursday 3 October

PL - Plenary Lecture | IL - Invited Lecture | IC - Invited Communication | P - Poster Presentation

THURSDAY 3 OCTOBER 2019

8.00am-7.45pm	Registration open - *Foyer, Abercrombie Business School (ABS)*			
	ABS Lecture Theatre 1040	*ABS Case Study Lecture Theatre 1050*	*ABS Case Study Lecture Theatre 1060*	*ABS Case Study Lecture Theatre 1070*
9.00-10.20am	**Non-bonded interactions** *Chair: Ekaterina Pas*	**Molecular Design** *Chair: R.B. Sunoj*	**Materials Design** *Chair: Michelle Spencer*	**Biological Mechanisms** *Chair: Alan Mark*
9.00am	**IL081** *Amir Karton* Graphene Catalysis via Dispersion Interactions and Shape Complementarity	**IL084** *Woo Youn Kim* Deep Generative Models for Smart Molecular Design	**IL087** *Masataka Nagaoka* A Computational Molecular Technology for Complex Chemical Reaction Systems: Red Moon Methodology	**IL090** *Xuhui Huang* Constructing Markov State Models to Elucidate the Functional Conformational Changes of Complex Biomolecules
9.20am	**IL082** *Junming Ho* Solvation Modelling – Are Explicit Solvent Models more Accurate than Continuum Models?	**IL085** *Takahito Nakajima* Materials Design of Hole-Transporting Materials for Perovskite Solar Cells	**IL088** *Tiffany Walsh* Simulations of Materials for Catalysis and Energy Based on Biomolecule-Nano Interfaces	**IL091** *Arti Dua* Transients Generate Memory and Break Hyperbolicity in Single-Enzyme Kinetics
9.40am	**IL083** *Vudhichai Parasuk* Mechanism of Carbon Dioxide Adsorption by Primary and Secondary Amines	**IL086** *U. Deva Priyakumar* Molecular Design using Traditional Computations and Machine Learning	**IL089** *Jun Li* Computational Design of Boron Clusters and Materials	**IL092** *Haibo Yu* Coelenterazine and Oxygen Binding in Obelin: A Computational Study into the Formation of Active Photoproteins
10.00am	**IC057** *Sarah Masters* Structural and Thermochemical Investigation of New Compounds for Hydrogen Storage	**IC059** *Ganna Gryn'ova* Topology-Driven Molecular Electronics Lacking ϖ-Conjugation	**IC061** *Soujanya Yarasi* In Silico Design of Sorbents for Selective Capture of CO2 from Industrial Flue Gases	**IC063** *Lintai Da* Base-Flipping Dynamics from an Intrahelical to an Extrahelical State Exerted by Thymine DNA Glycosylase During DNA Repair Process

10.10am	**IC058** *Taweetham Limpanuparb* When are cis Isomers More Stable Than trans Isomers? A Combinatorial in Silico Investigation on Cyclopropane and A1=A2 where A1, A2 are C, N, P	**IC060** *Mark Waller* Learning the Art of Chemical Synthesis with Deep Neural Networks and Discipline Scale Data	**IC062** *Jingxian Yu* In Situ 2:1 "Sandwich-Type" Complex Formation and Interwire Crosstalk in Single-Molecule Junctions	**IC064** *Katie Wilson* Unveiling the Catch-Bond Mechanism Used by FimH to Tackle Antibiotic Resistance in Uropathogenic *E.coli*
10.20-10.50am	Morning Tea			
10.50am-12.30pm	**DMRG** *Chair: Henry Schaefer III*	**Excited States B** *Chair: Yi Zhao*	**Clusters and Bulk** *Chair: Vinuthaa Murthy*	**New Tools for Modeling Biology** *Chair: Jiali Gao*
10.50am	**IL093** *Debashree Ghosh* **PCCP Emerging Investigator Lecture** - Density Matrix Renormalization Group Studies on Polyaromatic Hydrocarbons – Effect of Spin Frustration and Topology	**IL097** *Cheol Ho Choi* MRSF-TDDFT: An Improved TDDFT for Excited State Properties	**IL101** *Yan Zhao* Development and Applications of the WMS Model Chemistry Method	**IL105** *Krishnan Raghavachari* Exploring Protein–Ligand Interactions using Multilayer Molecules-in-Molecules (MIM) Fragmentation-Based Approach
11.10am	**IL094** *Zhigang Shuai* Hybrid TD-DMRG/TD-Hartree Algorithm for Spectroscopy at Finite Temperature	**IL098** *Yuxiang Bu* Theoretical Characterization of Excess Electrons in Various Loosely-Bound Electron Systems: Structures, Localization Dynamics and the Medium Effects	**IL102** *Shridhar Gadre* A Pragmatic Many-Body Approach for Economic Correlation Energy Estimation of Molecular Clusters	**IL106** *Yuriko Aoki* A Linear Scaling Approach for Efficient Geometry Optimization in Perturbed DNAs
11.30am	**IL095** *Haibo Ma* Dynamic Electron Correlation and Real-Time Simulation for Density Matrix Renormalization Group Quantum Chemistry	**IL099** *Michael Filatov* Computational Design of Photochemistry of Light Driven Molecular Rotary Motors	**IL103** *Debashree Chakraborty* Water and its Anomalous Property: Interplay between Low Density and High Density Water	**IL107** *Jane Allison* CherryPicker: Automated Parameterisation of Large Biomolecules for Molecular Simulation

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11.50am	**IL096** *Yuki Kurashige* Excited-State Quantum Dynamics with Time-Dependent Matrix-Product States	**IL100** *Meredith Jordan* The Atmospheric Photochemistry of Acetaldehyde	**IL104** *Laura McKemmish* A Challenge for Quantum Chemistry: Spectroscopic Accuracy for TiO Rovibronic Spectroscopy	**IL108** *Zexing Cao* Global Simulations of Enzymatic Degradation of Organophosphates and Phosphorylation of Sugars
12.10pm	**IC065** *Yasuhiro Ikabata* Machine-Learned Electron Correlation Model for Accurate Reproduction of Correlation Energy at the Basis-Set Limit	**IC067** *Yu Harabuchi* Systematic Exploration of Conical Intersection Geometries Between the Ground and First Excited Electronic States Based on Time Dependent Density Functional Theory: Application to Photoreactions	**IC069** *Claudio Cazorla* Giant Caloric Effects in Fast-Ion Conductors: A Promising Route Towards Ambient Solid-State Cooling	**IC071** *Richard Henchman* Multiscale Method to Calculate the Entropy of Protein Assemblies
12.20pm	**IC066** *Masaaki Saitow* A Reduced-Scaling Multireference Perturbation Theory using DMRG Reference Function	**IC068** *Feng Wang* Decoding Electron Structure of Nicotine, Nicotinamide and Nicotinic Acid from XPS and NMR: Theory and Experiment	**IC070** *Lukman Hakim* On the Negative Thermal Expansion of the EDI Zeolitic Ice	**IC072** *David Chalmers* Markov State Models for Understanding Ligand Binding to G Protein-Coupled Receptors
12.30-1.40pm	Lunch			
1.40-2.20pm	**Challenging Molecules** *Chair: Peter Schwerdtfeger*	**Electrostatic Effects** *Chair: David Wilson*	**Catalysis B** *Chair: Julian Gale*	**Complex Biomolecules** *Chair: Supa Hannongbua*
1.40pm	**IL109** *Gustavo Scuseria* Are Fullerenes Strongly Correlated Molecules?	**IL111** *Michelle Coote* Electrostatic Catalysis of Chemical Reactions	**IL113** *Sean Smith* Understanding the High Activity of Mildly Reduced Graphene Oxide Electrocatalysts in Oxygen Reduction to Hydrogen Peroxide	**IL115** *Alan Mark* Understanding Biological Micro-Machines: From Cytokine Receptors to Viral Fusion

2.00pm	**IL110** *Henry Schaefer III* Some Small Calcium Hydrides		**IL114** *Jin Yong Lee* Influence of Oxygen Vacancy Location on Charge Carrier Dynamics in Reduced TiO_2 Nanoparticles	**IL116** *Parbati Biswas* Hydration Pattern of Intrinsically Disordered Proteins
2.20pm	Changeover time			
2.30-3.30pm	**Plenary Session 3** *Chair: Kimihiko Hirao*			
2.30pm	**PL006** *Carmay Lim*	Metal Ions & Brain Signaling		
3.00pm	**PL007** *Jian Liu*	**2019 Pople Medal** - A Unified Thermostat Scheme for Efficient Configurational Sampling for Classical/Quantum Canonical Ensembles via Molecular Dynamics: From the Single-Electronic-State System to the Non-Adiabatic System		
3.30-4.00pm	Afternoon Tea			
4.00-4.30pm	**Plenary Session 4** *Chair: Peter Gill*			
4.00pm	**PL008** *Martin Head-Gordon*	Progress and Problems in the Design of Density Functionals		
4.30-5.10pm	**Prize Presentations and Closing Ceremony** *Chair: Leo Radom*			
7.00-11.00pm	**Conference Banquet at Le Montage** (bookings essential) - *Le Montage, 38 Frazer Street, Lilyfield NSW 2040 (Waterfront Entrance), Deanah's View room*			

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