

RACI PHYSICAL CHEMISTRY 2016 MEETING



2-5 FEBRUARY 2016
UNIVERSITY OF CANTERBURY NEW ZEALAND

www.physchem2016.com

Tuesday 2 February 2016

Jack Mann Auditorium, University of Canterbury

8:00 am	Registration Desk Opens	Jack Mann Foyer
8:45 am	Official Conference Opening Remarks	Jack Mann Auditorium
	PLENARY SESSION	Jack Mann Auditorium
9:00 am	<p>Professor Natalie Stingelin, Imperial College London, United Kingdom</p> <p><i>The Principles of Manipulating the Phase Transformations, Solid-State Order and Properties of Organic Functional Matter</i></p>	
	CONTRIBUTED PAPERS	Jack Mann Auditorium
10:00 am	<p>Professor Jeffrey Reimers, University of Technology Sydney, Australia</p> <p><i>Gold Surfaces and Nanoparticles are Protected by Au(0)-thiol Species but Destroyed When Au(I)-thiolates Form</i></p>	
10:15 am	<p>Professor Mark Buntine, Curtin University, Australia</p> <p><i>Ligand-Mediated Influence of the Surface Plasmon Resonance in Copper Nanoparticles Generated by Laser Ablation</i></p>	
10:30 am	<p>Dr Peggy Williams, Queensland University of Technology, Australia</p> <p><i>An Examination of Charge Proximity on the Gas Phase Reactivity of Distonic Arylperoxyl Radical Ions</i></p>	
10:45 am	<p>Professor Timothy Schmidt, University of New South Wales, Australia</p> <p><i>Dicarbon – 214 Years On</i></p>	
11:00 am	Morning Refreshments	Jack Mann Drama Room
	KEYNOTE SESSION	Jack Mann Auditorium
11:30 am	<p>Professor Gregory Metha, University of Adelaide, Australia</p> <p><i>Combining theory and experiment to understand the photocatalytic potential of atomically precise metal clusters on titania</i></p>	
	CONTRIBUTED PAPERS	Jack Mann Auditorium
12:00 pm	<p>Dr Justin Hodgkiss, Victoria University of Wellington, New Zealand</p> <p><i>Photocatalyst Thermalization and Cooling in Organometal Halide Perovskites</i></p>	
12:15 pm	<p>Dr Deborah Crittenden, University of Canterbury, New Zealand</p> <p><i>A New Method for Scaling Harmonic Frequencies to Match Experiment</i></p>	

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12:30 pm	Dr Viktoras Dryza, University of Melbourne, Australia <i>Spiropyran-Cyclodextrin Coated Metal Oxide Nanoparticles for Photochromic Light-Harvesting Applications</i>	
12:45 pm	Professor Huai Yong Zhu, Queensland University of Technology, Australia <i>Visible Light Photocatalysts of Gold and Palladium Alloy Nanoparticles for Synthesis of Fine Organic Chemicals under Mild Conditions</i>	
1:00 pm	Lunch	Jack Mann Drama Room
	KEYNOTE SESSION	Jack Mann Auditorium
2:00 pm	Professor Evan Bieske, University of Melbourne, Australia <i>Shape Shifting Molecules: Photoisomerization Action Spectroscopy of Molecular Ions</i>	
	CONTRIBUTED PAPERS	Jack Mann Auditorium
2:30 pm	Associate Professor Adam Trevitt, University of Wollongong, Australia <i>Laser Action Spectroscopy of Fundamental Aromatic Chromophores</i>	
2:45 pm	Dr Kai Chen, Victoria University of Wellington, New Zealand <i>A New Broadband Ultrafast Photoluminescence Spectroscopy Method and its Application to Light Harvesting Arrays</i>	
3:00 pm	Dr David Marshall, Queensland University of Technology, Australia <i>Shining New Light on Nitroxide-Mediated Photopolymerisation by Photodissociation Action Spectroscopy</i>	
3:15 pm	Dr Ivan Kassal, University of Queensland, Australia <i>Why Charges Separate in Organic Solar Cells</i>	
3:30 pm	Afternoon Refreshments	Jack Mann Drama Room
	CONTRIBUTED PAPERS	Jack Mann Auditorium
4:00 pm	Professor Feng Wang, Swinburne University of Technology, Australia <i>Differentiation of Intramolecular Interactions between Eclipsed and Staggered Ferrocene and Ferrocenium</i>	
4:15 pm	Dr Lars Goerigk, University of Melbourne, Australia <i>Finding a Way Through the Computational-Methods Jungle: Insights, Tips and Developments</i>	
4:30 pm	Dr David Wilson, La Trobe University, Australia <i>Theoretical Study of Low-Oxidation State Donor-Acceptor Complexes</i>	
4:45 pm	Dr Duncan Wild, University of Western Australia, Australia <i>Halogen...Molecule Chemistry: High Level Ab Initio Calculations and Anion Photoelectron Spectroscopy</i>	

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5:00 pm	Dr Rika Kobayashi, NCI, Australian National University, Australia <i>Towards Ab Initio NMR Calculations for Large Systems</i>	
5:15 pm	Professor Brian Yates, University of Tasmania, Australia <i>N₂O Reactivity with Vanadium and N-heterocyclic Carbenes: A Computational Approach</i>	
5:30 pm	Dr Jo Lane, University of Waikato, New Zealand <i>Unusual Low-Energy Electronic Transitions in Ferrocenium Complexes</i>	
5:45 pm	Session Close	
6:15 pm – 9:00 pm	Welcome Reception and Poster Session	Ilam Homestead, 86 Ilam Road

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Wednesday 3 February 2016

Jack Mann Auditorium, University of Canterbury

8:00 am	Registration Desk Open	Jack Mann Foyer
	PLENARY SESSION	Jack Mann Auditorium
9:00 am	Professor Dwayne Miller, Max Planck Institute for Structure and Dynamics of Matter, Germany <i>Mapping Atomic Motions with Ultrabright Electrons: The Chemists' Gedanken Experiment Enters the Lab Frame</i>	
	CONTRIBUTED PAPERS	Jack Mann Auditorium
10:00 am	Dr Girish Lakhwani, University of Sydney, Australia <i>Unification of Molecular Exciton and Cholesteric Liquid Crystal Theories</i>	
10:15 am	Professor Elmars Krausz, Australian National University, Australia <i>The Nature and Function of Low Energy States in Photosynthesis</i>	
10:30 am	Professor Ricardo Mancera, Curtin University, Australia <i>What Happens to Proteins at Electrified Liquid Interfaces: The Adsorption and Unfolding of Lysozyme</i>	
10:45 am	Dr Jeremy Hall, Australian National University, Australia <i>Circularly Polarised Luminescence Spectroscopy of Photosystem II</i>	
11:00 am	Morning Refreshments	Jack Mann Drama Room
	KEYNOTE SESSION	Jack Mann Auditorium
11:30 am	Dr Alison Funston, Monash University, Australia <i>Symmetry Breaking and Silver in Gold Nanorod Growth</i>	
	CONTRIBUTED PAPERS	Jack Mann Auditorium
12:00 pm	Dr Toby Bell, Monash University, Australia <i>Correlative Synchrotron Infrared Spectroscopy and Super-Resolution Fluorescence Microscopy for the Detection of Fixation Artefacts in Cells</i>	
12:15 pm	Dr Courtney Ennis, La Trobe University, Australia <i>The Simulation of Titan's Cyanide Haze – Australian Synchrotron Infrared Studies</i>	
12:30 pm	Professor Donald McNaughton, Monash University, Australia <i>Rotational Spectroscopy of Benzoquinolines and the Prediction of Inertial Defects of Extended Aromatic Systems</i>	

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12:45 pm	Dr Evan Robertson, La Trobe University, Australia <i>Local and Global Hydrogen Bonding Interactions from Vibrational Spectroscopy of Clusters and Aerosols</i>	
1:00 pm	Lunch	Jack Mann Drama Room
1:15 pm	RACI Physical Chemistry Division Annual General Meeting	Jack Mann Auditorium
	CONTRIBUTED PAPERS	Jack Mann Auditorium
2:15 pm	Associate Professor Gregory Russell, University of Canterbury, New Zealand <i>Termination in Radical Polymerization: The End of the Beginning or the Beginning of the End?</i>	
2:30 pm	Professor Igor Potemkin, Moscow State University, Russia <i>Effect of Solvent Vapours and Polymer-Substrate Interactions on the Structure of Block Copolymer Films</i>	
2:45 pm	Professor Olga Philippova, Moscow State University, Russia <i>Self-Assembled Networks Composed of Polymer and Supramolecular Chains</i>	
3:00 pm	Session Close	
	The remainder of the afternoon is free for independent exploration of Christchurch! What to see and do? Visit the website for more information www.christchurchnz.com	
7:00 pm onwards	The organizing committee will be at the Volstead Trading Company Craft Beer Sanctuary, 55 Riccarton Road, from 7pm, please do join us for some social downtime in town!	http://www.volstead.co.nz

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Thursday 4 February 2016

Jack Mann Auditorium, University of Canterbury

8:00 am	Registration Desk Open	Jack Mann Foyer
	PLENARY SESSION	Jack Mann Auditorium
9:00 am	Professor Scott Kable, University of New South Wales, Australia – Division Medal Winner 2016 <i>Probing dissociation dynamics in H₂CO: Correlated H₂ and CO state distributions measured by ion imaging</i>	
10:00 am	Mr Neville Coughlan, University of Melbourne, Australia – Student Award Winner <i>Identification and Photo-Physical Behaviour of the Primary Degradation Product of Retinal Schiff Base</i>	
	CONTRIBUTED PAPERS	Jack Mann Auditorium
10:15 am	Dr David Henry, Murdoch University, Australia <i>Soil Water Repellence: A Molecular Dynamics Study of Amphiphilic Compounds on Mineral Surfaces</i>	
10:30 am	Dr Krista Steenbergen, Massey University, New Zealand <i>Towards Melting Mercury, Cadmium and Zinc with a Quantum Model</i>	
10:45 am	Dr James Bull, University of Melbourne, Australia <i>Excited State Dynamics of π-Stacked Radical Anions</i>	
11:00 am	Morning Refreshments	Jack Mann Drama Room
	KEYNOTE SESSION	Jack Mann Auditorium
11:30 am	Dr Jane Allison, Massey University, New Zealand <i>Molecular dynamics simulation of protein adsorption at oil/water interfaces</i>	
	CONTRIBUTED PAPERS	Jack Mann Auditorium
12:00 pm	Associate Professor Meredith Jordan, University of Sydney, Australia <i>Accurate First Principles Quantum Simulations of H₂ Adsorbed in MOF-5</i>	
12:15 pm	Dr Terry Frankcombe, Australian National University, Australia <i>Potential Energy Surfaces for Gas–Surface Interactions</i>	
12:30 pm	Dr Elke Pahl, Massey University, New Zealand <i>Melting of Argon under High Pressure: Monte Carlo Simulations on Highly Accurate Potential Curves</i>	
12:45 pm	Lunch	Jack Mann Drama Room

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	PLENARY SESSION	Jack Mann Auditorium
2:00 pm	<p>Professor Rebecca Jockush, University of Toronto, Canada <i>Properties of Gaseous Biomolecular Ions and Complexes Probed using Action Spectroscopy, Fluorescence and Fluorescence Resonance Energy Transfer (FRET)</i></p>	
	CONTRIBUTED PAPERS – STUDENT SESSION I	Jack Mann Auditorium
3:00 pm	<p>Mrs Sophia Ackling, University of Adelaide, Australia <i>Charge Transfer, Photophysics and Intermolecular Interactions of the P3HT/F4TCNQ Polymer/Dopant System</i></p>	
3:15 pm	<p>Mr Izaak Mitchell, University of Newcastle, Australia <i>Mechanisms of Carbon Nanostructure Formation: Ripening versus Surface Diffusion</i></p>	
3:30 pm	<p>Ms Pravindya Haputhanthri, Monash University, Australia <i>A Spectroscopic Investigation into the Binding of Novel Platinum(IV) and Platinum(II) Anticancer Drugs with DNA</i></p>	
3:45 pm	<p>Mr David Perez-Guaita, Monash University, Australia <i>High Resolution FTIR Imaging Provides Automated Discrimination and Detection of Single Malaria Parasite Infected Erythrocytes on Glass</i></p>	
4:00 pm	Afternoon Refreshments	Jack Mann Drama Room
	CONTRIBUTED PAPERS – STUDENT SESSION II	Jack Mann Auditorium
4:30 pm	<p>Mr Nathaniel Gunby, University of Canterbury, New Zealand <i>Development and Demonstration of the New Conformer Ensemble Generation Method UCONGA</i></p>	
4:45 pm	<p>Mr Sui So, University of Melbourne, Australia <i>Oxidation Chemistry of a Distonic Radical Anion: How the Carboxylate Group Directs Peroxyl Radical Reactions</i></p>	
5:00 pm	<p>Ms Julia Melisande Fischer, University of Queensland, Australia <i>Computational Studies of the Interaction of Carbon Dioxide with Graphene Supported Titanium Dioxide</i></p>	
5:15 pm	<p>Mr Matthew Prendergast, University of Wollongong, Australia <i>Ortho-Substituted Phenyl Radical Reactions Leading to PAH Precursors</i></p>	
5:30 pm	<p>Mr Patrick Robertson, La Trobe University, Australia <i>Solvent-Solute Hydrogen Bonding and Infrared Molecular Spectroscopy in Flexible Organic Molecules</i></p>	
5:45 pm	Session Close	
7:00 pm – 10:00 pm	Conference Dinner @ Christchurch Gondola	(Bus Departs Jack Mann Foyer 6:15 pm)

Friday 5 February 2016

Jack Mann Auditorium, University of Canterbury

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8:00 am	Registration Desk Open	Jack Mann Foyer
	PLENARY SESSION	Jack Mann Auditorium
9:00 am	Professor Peter Schwerdtfeger, Massey University, New Zealand <i>From Graphene to Graphyne, Fullerenes, Fulleroids, Gaudienes and their Golden Duals</i>	
	CONTRIBUTED PAPERS	Jack Mann Auditorium
10:00 am	Mr Alireza Kharazmi, University of New South Wales, Australia <i>Phototautomerization of Propanal and Acetone to 1- and 2-Propenol</i>	
10:15 am	Dr Roger Amos, NCI, Australian National University, Australia <i>A TD-DFT Study of the Ring-Opening of Spiropyran</i>	
10:30 am	Associate Professor John Harrison, Massey University, New Zealand <i>Towards State to State Dynamics of the H + Oriented H₂ Reaction</i>	
10:45 am	Morning Refreshments	Jack Mann Drama Room
11:15 am	Dr Gabriel da Silva, University of Melbourne, Australia <i>Formation and Decomposition of a "Doubly Activated" Peroxyl Radical: Master Equation Modelling of the Methacrolein + OH + O₂ Reaction</i>	
11:30 am	Dr Thomas Fallon, Massey University, New Zealand <i>A Deuterium-Labelled Silane as a Simple Mechanism Probe</i>	
	KEYNOTE SESSION	Jack Mann Auditorium
12:00 pm	Associate Professor Tak Kee, University of Adelaide, Australia <i>Pump-Probe & Pump-Repump-Probe Spectroscopy of Conjugated Polymer Chains & Nanostructures – Energy Transfer & Charge Transport</i>	
12:30 pm	Conference Closing Remarks	
1:00 pm	Conference Closed	

The 2016 RACI PhysChem conference reserves the right to amend or alter any advertised details relating to dates, program and speakers if necessary, without notice, as a result of circumstances beyond their control. All attempts have been made to keep any changes to an absolute minimum.