POSTERS

Poster Session and Mixer 1

Time: 18:15 - 20:15
Date: Monday September 30, 2019
Location: Upper ABS Foyer

P001

A Molecular Simulation Study of Carbon Dioxide Adsorption in Two Interpenetrated Metal-Organic Frameworks: LMOF-201 and 202

Ankit Agrawal[1], Mayank Agrawal[2], Donguk Suh[1], Yunsheng Ma[3], Ryotaro Matsuda[3], Wei-Lun Hsu[1], Hirofumi Daiguji[1]
[1]University of Tokyo, Tokyo, Japan. [2]Georgia Institute of Technology, Atlanta, USA. [3]Nagoya University, Nagoya, Japan

P002

Investigating Luminescent Metal Complexes using Computational Methods

Johnny Agugiaro, David Wilson
La Trobe University, Melbourne, Australia

P003

Theoretical Investigation of Ring-Expansion of N-Heterocyclic Carbenes (NHCs) Containing C, P, O, S Heteroatoms

Khalidah Al-Furaiji, David Wilson
La Trobe Institute for Molecular Science, Melbourne, Australia

P004

Roby-Gould Bond Indices as a Tool in Chemistry

Khidhir Alhameedi
School of Molecular Sciences, The University of Western Australia, Perth, Australia

P006

Toroidal States in an Isosceles Spin Triangle Without Spin-Orbit Coupling: Applications in a Molecular Spintronics Device

Jared Ashtree, Shashank Rao, Alessandro Soncini
University of Melbourne, Parkville, Australia

P007

Valence and Core Electron Spectroscopy for the Conformational Study of Bio-active Pyridine Derivatives

Fred Backler[1], Hanan Sa'adeh[2,3], Kevin Prince[3], Feng Wang[1]
[1]Swinburne University of Technology, Melbourne, Australia. [2]The University of Jordan, Amman, Jordan. [3]Elettra Sincrotrone, Trieste, Italy

P008

Effect of Ca-Dopant on Lithium Ion Conductivity in $Li_7P_3S_{11}$ and Li_3PS_4 Solid Electrolytes

Ardeshir Baktash[1], Debra Searles[1,2]
[1]Centre for Theoretical and Computational Molecular Science, Australian Institute for Bioengineering and Nanotechnology, the University of Queensland, Queensland , Brisbane, Australia. [2]School of Chemistry and Molecular Biosciences, the University of Queensland, Queensland , Brisbane, Australia

P009

Towards an Understanding of Field Effects in the G-Quadruplex/Hemin DNAzyme Peroxidation Catalysis.

Clare Birch, Meredith Jordan
The University of Sydney, Sydney, Australia

P010

Theoretical Progress Towards pH-Switchable Electrostatic Catalysis

Mitchell Blyth, Michelle Coote
Research School of Chemistry, Australian National University, Canberra, Australia

P011

Fine Tuning of Ligand Field Splitting in Iron(II) Complexes

Luca Bondi[1,2], Federico Totti[2], Paul Jerabek[3], Anna Garden[1], Sally Brooker[1]
[1]University Of Otago, Dunedin, New Zealand. [2]University Of Florence, Florence, Italy. [3]Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany

P012

Microscopic Mechanism of SEI Film Formation in Highly Concentrated Electrolytes Based on Nonflammable Trimethyl Phosphate Solvent

Amine Bouibes[1], Norio Takenaka[2], Soumen Saha[3], Masataka Nagaoka[1]
[1]Nagoya University, Nagoya, Japan. [2]University of Tokyo, Tokyo, Japan. [3]Kyoto University, Nagoya, Japan

P013

On the Application of the Hubbard-U Correction in Modelling Semiconductors for Solar Water Splitting

Joshua Brown, Alister Page
The University of Newcastle, Newcastle, Australia

P014

Effect of Magnetic Anisotropy on Direct Chiral Discrimination in Paramagnetic NMR Spectroscopy

Simone Calvello[1,2], Alessandro Soncini[1]
[1]The University of Melbourne, Melbourne, Australia. [2]Australia's Nuclear Science and Technology Organisation, Sydney, Australia

P015

The Full Potential Energy Surface for N-H Tautomerisation in Free-Base Porphyrin

Peter Canfield[1,2,3], Jeffrey Reimers[4,3], Maxwell Crossley[1]
[1]The School of Chemistry, University of Sydney, Sydney, Australia. [2]ORAinnova, Sydney, Australia. [3]International Centre for Quantum and Molecular Structures, Shanghai University, Shanghai, China. [4]University of Technology Sydney, Sydney, Australia.

P016

Long-Range Corrected Double Hybrid Density Functionals Optimised for Electronic Excitations

Marcos Casanova-Páez, Lars Goerigk
The University of Melbourne, Melbourne, Australia

P017

Towards an Accurate Description of Solvent Effects

Junbo Chen[1], Yihan Shao[2], Bun Chan[3], Junming Ho[1]
[1]University of New South Wales, Sydney, Australia. [2]University of Oklahoma, Norman, USA.
[3]Nagasaki University, Nagasaki, Japan

P018

Molecular Vibrational Spectroscopy Study by Path Integral Liouville Dynamics

Zifei Chen, Zhijun Zhang, Xinzijian Liu, Kangyu Yan, Haifeng Zheng, Jian Liu
Institute of Theoretical and Computational Chemistry, College of Chemistry and Molecular Engineering, Peking University, Beijing, China

P019

Computational Insights into the Role of BINOL-Derived Catalysts in Asymmetric Nazarov Cyclisations

Yuk Ping Chin, Elizabeth Krenske
[1]School of Chemistry and Molecular Biosciences, The University of Queensland, Australia

P020

An In-Silico Investigation of Menthol Metabolism

Taweetham Limpanuparb, Wanutcha Lorpaiboon, Kridtin Chinsukserm
Mahidol University, Salaya, Thailand

P021

Recent Development of Automatized Density-Functional Tight-Binding Parameterization for Metal-Containing Systems

Chien-Pin Chou[1], Aditya Sakti[2], Hiromi Nakai[1,2,3]
[1]Waseda Research Institute for Science and Engineering (WISE), Waseda University, Tokyo, Japan.
[2]Element Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, Kyoto, Japan.
[3]Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University, Tokyo, Japan

P022

Collisional Energy Transfer Between Hot CH_3CHO/CH_2CHOH and N_2

Maggie Corrigan, Isabella Russell, Meredith Jordan
School of Chemistry, the University of Sydney, Sydney, Australia

P023

Predicting NMR Spectra Using Mixed Pseudoramp-Gaussian Basis Sets

Claudia Cox[1], Juan Camilo Trujillo[2,1], Laura McKemmish[1]
[1]UNSW, Sydney, Australia. [2]Universidad Icesi, Cali, Colombia

P024

fragHAR: Towards Ab Initio Quantum Crystallographic X-Ray Structure Refinement for Polypeptides and Proteins

Justin Bergmann[1], Max Davidson[2], Esko Oksanen[3], Ulf Ryde[1], Dylan Jayatilaka[2]
[1]Lund University, Lund, Sweden. [2]University of Western Australia, Perth, Australia. [3]European Spallation Source, Lund, Sweden

P025

Electronic Structure Understanding of the Mechanically Induced Selectivity in Acid Catalyzed Chitin Hydrolysis

Danjo De Chavez[1], Horikazu Kobayashi[2], Atsushi Fukuoka[2], Jun-ya Hasegawa[2]
[1]Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan. [2]Institute for Catalysis, Hokkaido University, Sapporo, Japan

P026

Studies of Peroxide Intermediate Structure and Mechanism of the Aryl Nitration Reaction in Nonheme N-Oxygenase CmlI – A Theoretical Study

Salai Kalaiselvi Dhanasekaran, Senthilnathan Dhurairajan
Centre for Computational Chemistry, CRD, PRIST Deemed to be University, Thanjavur, India

P027

Computational Design of Highly Activating Ligands for Atom-Transfer Radical Polymerisation

Phuong Doan, Benjamin Noble, Alfred Fung, Michelle Coote
ARC Centre of Excellence for Electromaterials Science, Research School of Chemistry, Australian National University, Canberra, Australia

P028

Effect of Liquid Phase on Heterogeneous Catalytic Reactions

Swarit Dwivedi[1], Samir Mushrif[2], Alan Chaffee[1], Akshat Tanksale[1]
[1]Monash University, Melbourne, Australia. [2]University of Alberta, Edmonton, Canada

P029

Exploring the Structure and Mechanism of Transport of the Human Sodium Proton Exchanger Isoform One (NHE1)

Nehad El Salamouni[1,2,3], Michael Kelso[1,2,3], Haibo Yu[1,2,3]
[1]School of Chemistry and Molecular Bioscience, , University of Wollongong , Wollongong, Australia. [2]Molecular Horizons, University of Wollongong, Wollongong, Australia. [3]Illawarra Health and Medical Research Institute, Wollongong, Australia

P030

Molecular Dynamics Simulations of Specific Ion Effects at Interfaces

Gareth Elliott, Grant Webber, Erica Wanless, Alister Page
University of Newcastle, Callaghan, Australia

P031

Predicting the Basicity of *N*-Heterocyclic Carbenes

Alicia Evans, Jason Harper, Junming Ho
UNSW, Sydney, Australia

P032

Accurate Approach in Simulating the Electronic Absorption Cross Section of Small to Medium Molecules

Sara Farahani, Joseph Lane
University of Waikato, Hamilton, New Zealand

P033

Energy-Based Automatic Fragmentation in the Linear-Scaling Divide-and-Conquer Electron Correlation Calculations

Toshikazu Fujimori[1], Masato Kobayashi[2,3,4], Tetsuya Taketsugu[1,2,3,4]
[1]Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan. [2]Faculty of Science, Hokkaido University, Sapporo, Japan. [3]WPI-ICReDD, Hokkaido University, Sapporo, Japan. [4]ESICB, Kyoto University, Kyoto, Japan

P034

Machine Learning Study for Optimization of Reaction Conditions Including Discrete Variables with Small Number of Experiments

Mikito Fujinami[1], Hiroki Maekawara[1], Junji Seino[2,3], Hiromi Nakai[1,2,4]
[1]Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University, Tokyo, Japan. [2]Waseda Research Institute for Science and Engineering, Waseda University, Tokyo, Japan. [3]PRESTO, Japan Science and Technology Agency, Saitama, Japan. [4]Element Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, Kyoto, Japan

P035

Mechanism and Optimisation of Nitroxide Mediated Photopolymerisation

Melinda Fule[1], Nicholas Hill[1,2], Michelle Coote[1,2]
[1]Australian National University, Canberra, Australia. [2]ARC Centre of Excellence for Electromaterials Science, Wollongong, Australia

P036

Parallel MP2 by Quadrature

Giuseppe Barca, Simon McKenzie, Andrew Gilbert, Nathaniel Bloomfield, Peter Gill
Australian National University, Canberra, Australia

P038

Decomposing Specific-Ion Interactions

Kasimir Gregory, Erica Wanless, Grant Webber, Alister Page
The University of Newcastle, Callaghan, Australia

P039

Molecular Modelling of Non-Ionic Surfactant ($C_{12}E_6$) Aqueous Phase Behaviour

Amali Guruge[1], Dallas Warren[2], Colin Pouton[2], David Chalmers[1]
[1]Medicinal Chemistry, Monash Institute of Pharmaceutical Sciences, Monash University, 381 Royal Parade, Parkville, Victoria 3052, Australia. [2]Drug Delivery, Disposition and Dynamics, Monash Institute of Pharmaceutical Sciences, Monash University, 381 Royal Parade, Parkville, Victoria 3052, Australia

P040

Influence of Sugar and Bases on the Stretching Vibrations of PO_2^- of DNA: A Computational Study with FMO/FDD.

Eunice Gwee[1,2,3], Kamila Kochan[1,3], Glen Deacon[1], Bayden Wood[1,3], Ekaterina Izgorodina[1,2]
[1]Monash University, Melbourne, Australia. [2]Monash Computational Chemistry Group, Melbourne, Australia. [3]Centre of Biospectroscopy, Melbourne, Australia

P041

Theoretical Study of Ni Catalysts for H_2 Oxidation and Production via the Minimum Energy Intersystem Crossing Point

Sarinya Hadsadee[1], Manussada Ratanasak[2], Siriporn Jungsuttiwong[1], Jun-ya Hasegawa[2]
[1]Ubon Ratchathani University, Ubon Ratchathani, Thailand. [2]Hokkaido University, Hokkaido, Japan

P042

Electronic Transport Investigation of Redox-Switching Azulenequinones/Hydroquinones via First-Principles Studies

El-Abed Haidar[1], Sherif Tawfik[2], Catherine Stampfl[1], Kimihiko Hirao[3], Kazunari Yoshizawa[4], Safinaz El-Demerdash[5], Takahito Nakajima[3], Ahmed El-Nahas[3,4,5]
[1]School of Physics, The University of Sydney, Sydney, New South Wales 2006, Australia, Sydney, Australia. [2]School of Science, RMIT University, GPO Box 2476 Melbourne, Victoria 3001 Australia, Melbourne, Australia. [3]RIKEN, Advanced Institute for Computational Science, 7-1-26 Minatojima-minami, Chuo, Kobe 650-0047, Japan, Kobe, Japan. [4]Institute for Materials Chemistry and Engineering, Kyushu University, Nishi-ku, Fukuoka 819-0395, Japan, Fukuoka , Japan. [5]Chemistry Department, Faculty of Science, Menoufia University, Shebin El-Kom 32512, Egypt, Shebin El-Kom, Egypt

P043

Normal Mode Analysis for Vibrational Motions in Liquid Water

Zheng Haifeng, Yi Shasha
Peking University, Beijing, China

P044

Transport Properties of Ionic Liquids from MD Simulations with a Self-Consistent Atomic Charge Determination

Lukman Hakim[1,2,3], Yoshiki Ishii[2], Nobuyuki Matubayasi[2]
[1]Elements Strategy Initiative for Catalysts and Batteries, Kyoto University, Kyoto, Japan. [2]Graduate School of Engineering Science, Osaka University, Osaka, Japan. [3]Department of Chemistry, Brawijaya University, Malang, Indonesia

P045

Ab Initio Examination of Nitrogen Gas Solubility in Fluorinated Ionic Liquid Clusters

Peter Halat, Douglas MacFarlane, Katya Pas
Monash University, Clayton, Australia

P046

Assessing Noncovalent Interactions in Electronic Excited States

Amy Hancock, Lars Goerigk
University of Melbourne, Melbourne, Australia

P047

Finding and Analyzing Interfacial Amorphous Carbon Structures in CNT-Based Functional Materials by Artificial Force Induced Reaction Method

Taisuke Hasegawa[1], Makito Takagi[2], Yosuke Sumiya[3], Satoshi Maeda[3,1]
[1]NIMS, Tsukuba, Japan. [2]Yokohama City University, Yokohama, Japan. [3]Hokkaido University, Sappro, Japan

P048

Understanding the Extent of Ionicity in Diamine Protic Ionic Liquids

Fairuz Hashim[1], Steven Pas[2], Douglas MacFarlane[1], Ekaterina Izgorodina[1]
[1]Monash University, Melbourne, Australia. [2]Defence Science and Technology Organisation, Melbourne, Australia

P049

Tuning of the Dielectric Constant to Correct for Delocalisation Error: Development and Preliminary Testing of a Novel Computational Method

Luke Hemmingsen[1], Oliver Hervir[1], Stephen Dale[1,2]
[1]Australian National University, Canberra, Australia. [2]University of Sydney, Sydney, Australia

P050

Internal Oriented Electric Fields as a Strategy for Selectively Modifying Photochemical Reactivity

Nicholas Hill[1,2], Michelle Coote[1,2]
[1]Australian National University, Canberra, Australia. [2]ARC Centre of Excellence for Electromaterials Science, Wollongong, Australia

P051

Importance of Li Distribution on High Li Conductivity in $Li_x(Ge,P)_3S_{12}$

Yoyo Hinuma[1,2], Takeshi Yajima[3], Satoshi Hori[4], Rui Iwasaki[3], Zenji Hiroi[3], Ryoj Kanno[4]
[1]Chiba University, Chiba, Japan. [2]National Institute for Materials Science, Tsukuba, Japan. [3]University of Tokyo, Kashiwa, Japan. [4]Tokyo Institute of Technology , Yokohama, Japan

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P052

Effect of Protonation on the Reaction Mechanism of Fragmentation and 1,3-Rearrangement *via* Breslow Intermediates

Ming-Hsiu Hsieh[1,2], Jen-Shiang Yu[1,2,3]
[1]Department of Biological Science and Technology, National Chiao Tung University, Hsinchu, Taiwan. [2]Institute of Bioinformatics and Systems Biology, National Chiao Tung University, Hsinchu, Taiwan. [3]Center for Intelligent Drug Systems and Smart Bio-devices (IDS2B), National Chiao Tung University, Hsinchu, Taiwan

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P053

Without Compromising Efficiency and Accuracy: Solving the Nuclear Schrödinger Equation Using Path Integral Monte Carlo Simulation with Modified Shepard Interpolation

Gavin Huang, Meredith Jordan
The University of Sydney, Sydney, Australia

P054

Molecular Spintronics with Single-Molecule Magnets Under Irradiation

Kieran Hymas, Alessandro Soncini
The University of Melbourne, Melbourne, Australia

P055

A Systematic Study on Bond Activation Energies of NO, N_2, and O_2 Catalyzed by Eight Transition Metal Hexamers

Tomoya Ichino[1], Satoshi Maeda[1,2,3]
[1]Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo, Japan. [2]Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University, Sapporo, Japan. [3]Research and Services Division of Materials Data and Integrated System (MaDIS), National Institute for Materials Science (NIMS), Tukuba, Japan

P056

Key Factor of the S_0/S_1 Minimum Energy Conical Intersection

Mayu Inamori[1], Yasuhiro Ikabata[2], Takeshi Yoshikawa[2], Hiromi Nakai[1,2,3]
[1]Department of Chemistry and Biochemistry, Waseda University, Tokyo, Japan. [2]WISE, Waseda University, Tokyo, Japan. [3]ESICB, Kyoto University, Kyoto, Japan

P057

The Production of Formic Acid and Formaldehyde From CO_2 Using Boron-Doped Diamond: A Theoretical Study

Yuwanda Injongkol[1,2], Siriporn Jungsuttiwong[1], Alejandro Montoya[2]
[1]Department of Chemistry, Faculty of Science, Ubon Ratchathani University, Ubon Ratchathani, Thailand. [2]School of Chemical and Biomolecular Engineering, The University of Sydney, Sydney, Australia

P058

The Role of Solvation in Predicting Protein–Ligand Binding Affinities: Validating the Automated Topology Builder

Kasey Ireland, Nicole Wheatley, Martin Stroet, Alan Mark
University of Queensland, Brisbane, Australia

P059

An Exploration of Bifurcation on a Reaction Route Network of a Diels–Alder Reaction Based on the AFIR Method

Takuma Ito[1], Yu Harabuchi[2,3,4], Satoshi Maeda[2,4,5]
[1]Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan. [2]Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo, Japan. [3]JST, PRESTO, Saitama, Japan. [4]WPI-ICReDD, Sapporo, Japan. [5]NIMS, Tsukuba, Japan

P060

Investigating the Mechanism of High Performing Dielectric Materials

Lilit Jacob, Terry Frankcombe
UNSW, Canberra, Australia

P061

Identifying Binding Modes of Neurosteroids at an Intra-Subunit Pocket on $GABA_A$ Receptors

Tian Jiang[1,2], Ali Kusay[1,2], Thomas Balle[1,3]

[1]Sydney School of Pharmacy, Faculty of Medicine and Health, The University of Sydney, Sydney, Australia. [2]Brain and Mind Centre, The University of Sydney, Sydney, Australia. [3]Brain and Mind, The University of Sydney Centre, Sydney, Australia

P062

Implications of Hybrid Organic–Inorganic Functionalized Dodecaborane Dianions in Lithium and Magnesium Ion Batteries

Meenakshi Joshi[1,2], Tapan Ghanty[1,2]

[1]Homi Bhabha National Institute, Mumbai, India. [2]Theoretical Chemistry Section, Chemistry Group, Bhabha Atomic Research Centre, Mumbai, India

P063

Computational Insights into the Origin of Enantioselectivity in a Palladium Catalyzed Dynamic Kinetic Asymmetric Transformation of Racemic Biaryls

Surya K, Raghavan Sunoj

Indian Institute of Technology Bombay, Mumbai, India

P064

Stabilising Molecular Fragments of Group 13, 15 Heteronuclear Diatomics

Aishvaryadeep Kaur, David Wilson

La Trobe University, Melbourne, Australia

P065

Examination of Statistical Methods for Analyzing Fragment Molecular Orbital Calculation Results on Ligand-Protein Interactions.

Yusuke Kawashima[1], Nanami Mori[1], Hirotomo Moriwaki[2], Norihito Kawashita[3], Yu-Shi Tian[1], Tatsuya Takagi[1]

[1]Graduate School of Pharmaceutical Sciences, Osaka University, Suita, Japan. [2]RIKEN Center for Biosystems Dynamic Research, Yokohama, Japan. [3]Faculty of Science and Engineering, Kindai University, Higashi Osaka, Japan

P066

HACA Accelerated: The Role of the Submerged Barrier in the Rate of Radical–Acetylene Addition Reactions

Patrick Kelly[1], Oisin Shiels[1], Aislinn Turner[1], Brett Burns[1], Cameron Bright[1], Stephen Blanksby[2], Gabriel da Silva[3], Adam Trevitt[1]
[1]University of Wollongong, Wollongong, Australia. [2]Queensland University of Technology, Brisbane, Australia. [3]University of Melbourne, Melbourne, Australia

P067

Control of Ziegler–Natta Catalyst Activity by the Structural Design of External Donor

Vikas Khatri[1], Gurmeet Singh[2], Hemant Kashyap[1]
[1]Indian Institute of Technology, Delhi, India. [2]R&D Center, IndianOil Corporation Ltd, Faridabad, India

P068

Size-Dependent Level Alignment Between Anatase and Rutile TiO_2 Nanoparticles

Kyoung Chul Ko
Chonnam National University, Gwangju, Korea, Republic of

P069

Practical Excited-State Simulation of Thousands of Atoms

Nana Komoto[1], Takeshi Yoshikawa[2], Junichi Ono[2], Yoshifumi Nishimura[2], Hiromi Nakai[1,2,3]
[1]Department of Chemistry and Biochemistry, Waseda University, Tokyo, Japan. [2]WISE, Waseda University, Tokyo, Japan. [3]ESICB, Kyoto University, Kyoto, Japan

P070

Catalysis by Pure Graphene - From Supporting Actor to Protagonist through π–π Interactions

Asja Kroeger, Amir Karton
The University of Western Australia, Perth, Australia

P071

Role of Atmospheric Molecular Clusters in the Atmosphere

Jakub Kubečka, Theo Kurtén, Hanna Vehkamäki
University of Helsinki, Helsinki, Finland

P072

Towards Selective nAChR Therapeutics: Identifying the Binding Mode of CMPI and NS9283 in α4β2 nAChRs

Ali Kusay[1,2], Thomas Balle[1,2]
[1]Sydney School of Pharmacy, Faculty of Medicine and Health, The University of Sydney, Sydney, Australia. [2]Brain and Mind Centre, The University of Sydney, Sydney, Australia

P073

Calculating the Exact Ground-State Wave Function of Two-Electron Atoms via Analytic Perturbation Theory

Johanna Langner, Henryk Witek
National Chiao Tung University, Hsinchu, Taiwan

P074

Insights into $MoTe_2$ Intrinsic Defects from Ab Initio Calculations

Martina Lessio[1], Alexander Kerelsky[2], Abhay Pasupathy[2], David Reichman[2]
[1]University of Sydney, Sydney, Australia. [2]Columbia University, New York, USA

P075

Scaffold-Based Molecular Design Using Graph Generative Model

Jaechang Lim, Sang-Yeon Hwang, Seungsu Kim, Seokhyun Moon, Woo Youn Kim
KAIST, Daejeon, Korea, Republic of

P076

Investigating the Effects of Membrane Lipid Composition on Neurotransmitter Transport Function

Yiechang Lin, Katie Wilson, Megan O'Mara
Australian National University, Canberra, Australia

Poster Session and Mixer 2

Time: 18:00 - 20:00
Date: Tuesday October 1, 2019
Location: Upper ABS Foyer

P077

Finding Electrons: Transforming Chemical Thought by Analysing Wavefunctions

Yu Liu
The Univeristy of New South Wales, Sydney, Australia

P078

Spin Crossover Induced by Non-Covalent Interaction of a Metal–Organic Complex with N-Doped Graphene

Bruno Torre[1], Martin Švec [1], Rabindranath Lo[2], Debashree Manna[2], Amrit Sarmah[2], Dana Nachtigallová[2], Radek Zbořil[3], Pavel Hobza[2,3], Pavel Jelínek[1], Prokop Hapala[1]
[1]Institute of Physics of the Czech Academy of Sciences, Prague 6, Czech Republic. [2]Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Prague 6, Czech Republic. [3]Regional Centre of Advanced Technologies and Materials, Palacký University, Olomouc, Czech Republic

P079

The One-Electron Self-Interaction Error in 50 Density Functional Approximations

Dale Lonsdale, Lars Goerigk
The University of Melbourne, Melbourne, Australia

P080

The Effect of Ionic Liquids on the H_2 Splitting Capacity of Frustrated Lewis Pairs: Computational Insights

Kaycee Low[1], Lucy Brown[2], Małgorzata Swadźba-Kwaśny[2], Ekaterina Izgorodina[1]
[1]School of Chemistry, Monash University, Clayton, Australia. [2]The QUILL Research Centre, University of Belfast, Belfast, Ireland

P081

Effect of Factors on Ethylene Epoxidation by Oxoiron(IV) Porphyrin π-Cation Radical Complex in High Spin States: A DFT Study

Zhifeng Ma[1], Hiroshi Fujii[2], Masahiko Hada[1]
[1]Tokyo Metropolitan University, Tokyo, Japan. [2]Nara Women's University, Nara, Japan

P082

Determining the Mechanism of a Novel Class of Mitochondrial Uncoupler

Hugo MacDermott-Opeskin, Megan O'Mara
ANU, Canberra, Australia

P083

Theoretical Insights into CO_2 Hydrogenation to Methanol by a Mn–PNP Complex

Shyama Mandal[1], Kuber Rawat[1], Surajit Nandi[1], Biswarup Pathak[1,2]
[1]Discipline of Chemistry, Indian Institute of Technology Indore, Indore, India. [2]Discipline of Metallurgy Engineering and Materials Science, Indian Institute of Technology Indore, Indore, India

P084

Correlation Effects in the Photoelectron Spectrum and Photoionization Dynamics of OsO_4

Soumitra Manna, Sabyashachi Mishra
Indian Institute of Technology Kharagpur, Kharagpur, India

P085

Investigating the Effect of Protonation Site on Photostability

Samuel Marlton[1], Benjamin McKinnon[1], Boris Ucur[1], Stephen Blanksby[2], Adam Trevitt[1]
[1]UOW, Wollongong, Australia. [2]QUT, Queensland, Australia

P086

Polarisation of Water in Hydrated Choline Dihydrogen Phosphate and Related Ionic Liquids

Thomas Mason[1], Zoe Seeger[1], Anh Nguyen[1], Kyoko Fujita[2], Ekaterina Pas[1]
[1]Monash University, Melbourne, Australia. [2]Tokyo University of Pharmacy and Life Sciences, Tokyo, Japan

P087

MP2-Q-F12-SOS: A Novel Efficient Method to Compute the MP2-F12 Correlation Energy

Simon McKenzie, Peter Gill
University of Sydney, Sydney, Australia

P088

Photostability of Protonated Pyridine Derivatives in the Gas Phase

Benjamin McKinnon[1], Samuel Marlton[1], James Bezzina[1], Stephen Blanksby[2], Adam Trevitt[1]
[1]University of Wollongong, Wollongong, Australia. [2]Queensland Institute of Technology, Queensland, Australia

P089

Boron Nitride Nanotube Nucleation During Ni-Catalysed Chemical Vapour Deposition: Non-Equilibrium Molecular Dynamics

Ben McLean, Grant Webber, Alister Page
University of Newcastle, Callaghan, Australia

P090

A Mirror-Image Approach to Spin Contamination in Single-Determinant Wave Functions

Michael McTigue[1], Giuseppe Barca[1], Andrew Gilbert[1], Peter Gill[2]
[1]Australian National University, Canberra, Australia. [2]University of Sydney, Sydney, Australia

P091

Exploring the Applicability of Density Functional Approximations: The Most Comprehensive Benchmark Study of Double Hybrids and Application of Low-Cost DFT to Clam-Like Cyclotricatechylene Capsules

Nisha Mehta, Brendan Abrahams, Lars Goerigk
The University of Melbourne, Melbourne, Australia

P092

Full Atomistic Simulation of Ethylene/1-Octene Copolymerization Reaction Process Catalyzed by (Pyridylamido)Hf(IV) Complex

Nana Misawa[1], Yuichi Suzuki[1], Nobuaki Koga[1,2], Masataka Nagaoka[1,2,3,4]
[1]Nagoya University, Nagoya, Japan. [2]Future Value Creation Research Center, Nagoya University, Nagoya, Japan. [3]ESICB, Kyoto University, Kyoto, Japan. [4]JST-CREST, Tokyo, Japan

P093

Molecular Level Explanation of the Conversion of Regiospecificity (8R to 12S) in Lipoxygenase by a Single Mutation L434F

Vipin Mishra, Sabyashachi Mishra
Indian Institute of Technology, Kharagpur, India

P094

pH-Switchable Electrostatic Catalysis of Organo-SOMO Reactions

Ahmed Elaaf Mohamed, Michelle Coote
Australian National University, Canberra, Australia

P095

Theoretical Insights to Novel Beryllium Reactivity

Andrew Molino, David Wilson
La Trobe University, Melbourne, Australia

P096

Colloidal Stability of Apolar Nanoparticles

Debora Monego[1], Thomas Kister[2], Nicholas Kirkwood[3], Tobias Kraus[2], Paul Mulvaney[3], Asaph Widmer-Cooper[1]
[1]ARC Centre of Excellence in Exciton Science, University of Sydney Nano Institute, School of Chemistry, University of Sydney, Sydney, Australia. [2]INM Leibniz Institute for New Materials, Saarbrücken, Germany. [3]ARC Centre of Excellence in Exciton Science, School of Chemistry, University of Melbourne, Melbourne, Australia

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Alyssa Dwight, Sooin Byeon, Damian Moran
Macquarie University, North Ryde, Australia

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Sebastian Muraru[1], Emil Slusanschi[2], Jorge Burns[1,3], Mariana Ionita[1]
[1]Faculty of Medical Engineering, University Politehnica of Bucharest, Gh Polizu 1-7, 011061, Bucharest, Romania. [2]Computer Science Department and Engineering, Faculty of Automatic Control and Computers, Bucharest, Romania. [3]Laboratory of Cellular Therapies, Department of Medical and Surgical Sciences for Children & Adults, University Hospital of Modena and Reggio Emilia, Modena, Italy

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Hitoshi Nabata[1], Makito Takagi[2], Kenichiro Saita[3], Satoshi Maeda[3,4,5]
[1]Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan. [2]Graduate school of NanoBioSystems Science, Yokohama City University, Yokohama, Japan. [3]Faculty of Science, Hokkaido University, Sapporo, Japan. [4]Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University, Sapporo, Japan. [5]National Institute for Materials Science (NIMS), Tsukuba, Japan

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Anh Nguyen, David Wilson
La Trobe Institute for Molecular Sciences (LIMS), La Trobe University, Melbourne, Australia

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Yoshio Nishimoto
Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto, Japan

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Soichiro Nishio, Yuki Kurashige
Kyoto University, Kyoto, Japan

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Masaki Okoshi[1,2,3], Hitoshi Washizu[2,3], Hiromi Nakai[3,4,5]
[1]Research Organization for Information Science and Technology, Tokyo, Japan. [2]Graduate School of Simulation Studies, University of Hyogo, Hyogo, Japan. [3]Elements Strategy Initiative for Catalysts & Batteries, Kyoto University, Kyoto, Japan. [4]Department of Chemistry and Biochemistry, Waseda University, Tokyo, Japan. [5]Waseda Research Institute for Science and Engineering, Waseda University, Tokyo, Japan

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Cihan Ozen[1], Yoshiaki Shoji[2], Takanori Fukushima[2], Satoshi Maeda[1]
[1]Hokkaido University, Sapporo, Japan. [2]Tokyo Institute of Technology, Yokohama, Japan

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Gareth Elliott, Kas Gregory, Alister Page, Simone Waite
The University of Newcastle, Callaghan, Australia

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Ishara Peiris, Evan Robertson, David Wilson
La Trobe Institute for Molecular Science, La Trobe University, Melbourne 3086, Australia

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Joshua Pryor, Stephen Bosi, Erica Smith
University of New England, Armidale, Australia

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Madhuranga Rathnayake[1], Stefano Bernardi[1], Asaph Widmer-Cooper[1,2]
[1]ARC Centre of Excellence in Exciton Science, School of Chemistry, The University of Sydney, Sydney, Australia. [2]The University of Sydney Nano Institute, Sydney Nanoscience Hub, The University of Sydney, Sydney, Australia

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Michael Robinson, Andrew Wright, Andrea Robinson, Katya Pas
Monash University, Melbourne, Australia

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Fergus Rogers, Michelle Coote
RSC, ANU, Canberra, Australia

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Tanglaw Roman[1,2], James Reid[2], Debra Searles[2,3]
[1]School of Mathematics and Physics, The University of Queensland, Brisbane, Australia. [2]Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, Brisbane, Australia. [3]School of Chemistry and Molecular Biosciences, The University of Queensland, Brisbane, Australia

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Ras Baizureen Roseli, Ilene Allison, Atul Shukla, Ebinazar Namdas, Shih-Chun Lo, Elizabeth Krenske
The University of Queensland, Brisbane, Australia

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Keiran Rowell[1], Scott Kable[1], Meredith Jordan[2]
[1]The University of New South Wales, Sydney, Australia. [2]The University of Sydney, Sydney, Australia

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Charlie Ruffman[1], Calum Gordon[1], Egill Skúlason[2], Anna Garden[1]
[1]University of Otago, Dunedin, New Zealand. [2]University of Iceland, Reykjavík, Iceland

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Matthew Sale[1,2], Chris Ling[1], Maxim Avdeev[2,1]
[1]School of Chemistry, University of Sydney, Sydney, Australia. [2]Australian Center for Neutron Scattering (ACNS), Australian Nuclear Science and Technology Organisation (ANSTO), Sydney, Australia

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W. M. C. Sameera[1], Feliu Maseras[2]
[1]Hokkaido University, Sapporo, Japan. [2]Institute of Chemical Research of Catalonia (ICIQ), Tarragona, Spain

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Isolde Sandler, Daniel Notaras, Junming Ho
School of Chemistry, University of New South Wales, Sydney, Australia

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Zoe Seeger, Ekaterina Izgorodina
Monash University, Melbourne, Australia

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Junji Seino[1,2], Ryo Kageyama[1], Mikito Fujinami[1], Yasuhiro Ikabata[1], Hiromi Nakai[1,3]
[1]Waseda University, Tokyo, Japan. [2]JST-PRESTO, Saitama, Japan. [3]ESICB, Kyoto University, Kyoto, Japan

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Takafumi Shiraogawa[1], Masahiro Ehara[1,2,3]
[1]SOKENDAI, The Graduate University for Advanced Studies, Okazaki, Japan. [2]Institute for Molecular Science, Research Center for Computational Science, Okazaki, Japan. [3]ESICB (Element Strategy Initiative for Catalysts and Batteries), Okazaki, Japan

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Catherine Simpson[1], Heather Aitken[1], Naomi Haworth[1], Nadim Darwish[2], Simone Ciampi[2], Michelle Coote[1]

[1]ARC Centre of Excellence for Electromaterials Science, Research School of Chemistry, Australian National University, Canberra, Australia. [2]Nanochemistry Research Institute, Department of Chemistry, Curtin University, Perth, Australia

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Abhishek Singh, Ekaterina Izgorodina

Monash University, Melbourne, Australia

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Sukriti Singh, Monika Pareek, Avtar Changotra, Sayan Banerjee, Bangaru Bhaskararao, Palaniappan Balamurugan, Raghavan Sunoj

Indian Institutuion of Technology Bombay, Mumbai, India

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Yuichi Suzuki[1,2], Hiroaki Yagoshi[1], Nobuaki Koga[1,3], Masataka Nagaoka[1,2,3,4]

[1]Nagoya University, Nagoya, Japan. [2]NEDO, Tokyo, Japan. [3]Future Value Creation Research Center, Nagoya University, Nagoya, Japan. [4]ESICB, Kyoto University, Kyoto, Japan

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Anna-Maree Syme, Maria Cunningham, Laura McKemmish

UNSW, Sydney, Australia

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Makito Takagi[1], Satoshi Maeda[2,3,4], Masanori Tachikawa[1]
[1]Graduate school of NanoBioSystems Science, Yokohama City University, Yokohama, Japan. [2]Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo, Japan. [3]Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University, Sapporo, Japan. [4]National Institute for Materials Science (NIMS), Tsukuba, Japan

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Masato Takenaka[1], Yoshikazu Hashimoto[2], Takeshi Iwasa[1,3,4], Tetsuya Taketsugu[1,3,4], Gediminas Seniutinas[5,6], Armandas Balcytis[5,6], Saulius Juodkazis[5,6,2], Yoshiaki Nishijima[2]
[1]Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan. [2]Department of Electrical and Computer Engineering, Yokohama National University, Yokohama, Japan. [3]Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo, Japan. [4]Elements Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, Kyoto, Japan. [5]Melbourne Centre for Nanofabrication (MCN), Australian National Fabrication Facility, Clayton, Australia. [6]Centre for Micro-Photonics, Faculty of Engineering and Industrial Sciences, Swinburne University of Technology, Hawthorn, Australia

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Siu Min Tan, Davin Tan, Richmond Lee
Singapore University of Technology and Design, Singapore, Singapore

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Sherif Tawfik, Dale Osborne, Michelle Spencer
School of Science, RMIT University, Melbourne, Australia

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Patrick Taylor, Sherif Tawfik, Michelle Spencer
RMIT University, Melbourne, Australia

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Yoshiaki Tsunekawa[1], Sadaiwa Yorimoto[2], Akira Tsubouchi[2], Haruki Mizoguchi[3], Hideaki Oikawa[1], Tomoya Ichino[1], Satoshi Maeda[1,4], Hiroki Oguri[2]
[1]Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo, Japan. [2]Department of Applied Chemistry, Graduate School of Engineering, Tokyo University of Agriculture and Technology, Koganei, Japan. [3]Graduate School of Natural Science and Technology, Okayama University, Okayama, Japan. [4]Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University, Sapporo, Japan

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Hiroki Uratani[1], Chien-Pin Chou[2], Hiromi Nakai[1,2,3]
[1]Department of Chemistry and Biochemistry, Waseda University, Tokyo, Japan. [2]WISE, Waseda University, Tokyo, Japan. [3]ESICB, Kyoto University, Kyoto, Japan

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Rahul Verma[1], Shilendra Sharma[2,3], Shilpi Saxena[2,3], Raj Pala[2,3], sri sivakumar[2,3], Nisanth Nair[1]
[1]Department of Chemistry, Indian Institute of Technology Kanpur, kanpur, India. [2]Department of Chemical Engineering, Indian Institute of Technology Kanpur, kanpur, India. [3]Material Science and Programme, Indian Institute of Technology Kanpur, kanpur, India

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Luigi Villani[1], Patrick Robertson[2,1], Evan Robertson[1], David Wilson[1]
[1]La Trobe University, Melbourne, Australia. [2]University of Bristol, Bristol, United Kingdom

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Simone Waite, Alister Page
University of Newcastle, Newcastle, Australia

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Chun-I Wang[1], Chao-Ping Hsu[1], Gil Claudio[2], Ignasius Joanito[1], Chang-Feng Lan[1], Mac Kevin Braza[2]
[1]Institute of Chemistry, Academia Sinica, Taipei, Taiwan. [2]Institute of Chemistry, University of the Philippines Diliman, Quezon City, Philippines

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Lily Wang, Megan O'Mara
Australian National University, Canberra, Australia

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Dominique Wappett, Lars Goerigk
The University of Melbourne, Melbourne, Australia

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Nicole Wheatley, Kasey Ireland, Martin Stroet, Alan Mark
University of Queensland, Brisbane, Australia

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Jared Wood[1,2,3], Yawei Liu[1,2], Miguel Modestino[4], Asaph Widmer-Cooper[1,2,3]
[1]University of Sydney, Sydney, Australia. [2]ARC Centre of Excellence in Exciton Science, Sydney, Australia. [3]University of Sydney Nano Institute, Sydney, Australia. [4]NYU Tandon School of Engineering, New York, USA

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Luke Wylie[1], Kenichi Oyaizu[2], Amir Karton[3], Masahiro Yoshizawa-Fujita[4], Ekaterina Izgorodina[1]
[1]Monash University, Melbourne, Australia. [2]Waseda University, Tokyo, Japan. [3]University of Western Australia, Perth, Australia. [4]Sophia University, Tokyo, Japan

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Longkun Xu, Michelle Coote
ARC Centre of Excellence for Electromaterials Science, Research School of Chemistry, Australian National University, Canberra, Australian Capital Territory, 2601,, Australia

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Naoto Furuhashi, Satoshi Yabushita
Department of Chemistry, Keio University, Yokohama, Japan

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Likun Yang[1], Jeffrey Reimers[1,2], Rika Kobayashi[3,1], Noel Hush[4,5]
[1]International Centre for Quantum and Molecular Structures and Department of Physics, Shanghai University, Shanghai, China. [2]School of Mathematical and Physical Sciences, University of Technology Sydney, Sydney, Australia. [3]Supercomputer facility, The Australian National University, Canberra, Australia. [4]School of Molecular Biosciences, The University of Sydney, Sydney, Australia. [5]School of Chemistry, The University of Sydney, Sydney, Australia

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Takeshi Yoshikawa[1], Toshiki Doi[1], Hiromi Nakai[1,2]
[1]Waseda University, Tokyo, Japan. [2]ESICB, Kyoto, Japan

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Li-Juan Yu, Mitchell Blyth, Michelle Coote
Australian National University, Canberra, Australia

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Linxing Zhang[1], Kun An[2], Xinhao Zhang[1], Qing-Wei Zhang[3], Zhi-Xiang Yu[4], Wei He[2], Yun-Dong Wu[1,5]
[1]Lab of Computational Chemistry & Drug Design, State Key Laboratory of Chemical Oncogenomics, Peking University Shenzhen Graduate School, Shenzhen, China. [2]School of Pharmaceutical Sciences, Tsinghua University, Beijing, China. [3]Department of Chemistry, University of Science and Technology of China, Hefei, China. [4]Beijing National Laboratory for Molecular Sciences, Key Laboratory of Bioorganic Chemistry and Molecular Engineering of Ministry of Education, College of Chemistry, Peking University, Beijing, China. [5]College of Chemistry and Molecular Engineering, Peking University, Beijing, China

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Wenting (Judy) Zhu
The University of Sydney, Sydney, Australia

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Movva Babu, Alister Page
The University of Newcastle, Callaghan, Australia

AUTHORS

PL – Plenary
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IC - Invited Communication
P – Poster

Author Name	Program Codes*
Abdul Rahman, Mohd Basyaruddin	IC016
Abe, Minori	IL044
Abell, Andrew	IC062
Abrahams, Brendan	P091
Aghajamali, Alireza	IL024
Agrawal, Ankit	P001
Agrawal, Mayank	P001
Agugiaro, Johnny	P002
Aitken, Heather	P121
Al-Furaiji, Khalidah	P003
Alexov, Emil	IC071
Alhameedi, Khidhir	P004
Allison, Ilene	P112
Allison, Jane	IL107
An, Kun	P147
Aoki, Yuriko	IL106
Ashtree, Jared	P006
Assabumrungrat, Suttichai	IL083
Avdeev, Maxim	P115
Babarao, Ravichandar	IC022
Babu, Movva	P149

Author Name	Program Codes*
Backler, Fred	P007
Backler, Frederick	IC068
Baktash, Ardeshir	P008
Balamurugan, Palaniappan	P123
Balcytis, Armandas	P127
Balle, Thomas	P061, P072
Banerjee, Sayan	P123
Barca, Giuseppe	IC041, P036, P090
Barfoot, Shelley	IL115
Barnard, Amanda	PL003
Basumallick, Suhita	IL015
Bergmann, Justin	P024
Bernardi, Stefano	P108
Bernhardt, Debra	IC033
Bezzina, James	P088
Bhaskararao, Bangaru	P123
Bhattacharjee, Ishita	IL071
Birch, Clare	P009
Biswas, Parbati	IL116
Blanksby, Stephen	P066, P085, P088
Bloomfield, Nathaniel	IC041, P036

Author Name	Program Codes*
Blyth, Mitchell	P010, P146
Bondì, Luca	P011
Bosi, Stephen	P107
Bouibes, Amine	P012
Bourke, Tom	IL074
Bowman, Michael	IL110
Boyd, Russell	IC047
Braza, Mac Kevin	P136
Bright, Cameron	P066
Brooker, Sally	P011
Brown, Joshua	P013
Brown, Lucy	P080
Bu, Yuxiang	IL098
Bureau, Ronan	IC039
Burns, Brett	P066
Burns, Jorge	P098
Byeon, Sooin	P097
C, Bun	P017
Calvello, Simone	IL027, P014
Canepa, Pieremanuele	IC021
Canfield, Peter	P015

Author Name	Program Codes*
Cao, Zexing	IL108
Casanova-Páez, Marcos	IL066, P016
Cazorla, Claudio	IC069
Chaffee, Alan	P028
Chai, Jeng-Da	IL067
Chakraborty, Debashree	IL103
Chakravarti, Dibyajyoti	IL014
Chakravorty, Arghya	IC071
Chalmers, David	IC072, P039
Chan, Bun	IL022, IL065
Changotra, Avtar	P123
Chen, Fang	IC062
Chen, Junbo	P017
Chen, Zifei	P018
Cheng, Guijuan	IL004
Cheng, Yuan-Chung	IC049
Chibotaru, Liviu	IL028
Chin, Yuk Ping	P019
Chinsukserm, Kridtin	IC058, P020
Choi, Changwon	IL009
Choi, Cheol Ho	IL097

Author Name	Program Codes*
Choi, Hyeonho	IC010
Chou, Chien-Pin	IC013, P021, P132
Christofferson, Andrew	IC023
Chu, Pei-Chuan	IL063
Ciampi, Simone	IC029, P121
Ciavardini, Alessandra	IC068
Claudio, Gil	P136
Cleland, Deidre	IC018
Collins, Michael	IL053
Condic-Jurkic, Karmen	IL051
Coote, Michelle	IC029, IL111, P010, P027, P035, P050, P094, P110, P121, P142, P146
Coreno, Marcello	IC068
Corminboeuf, Clémence	IC059
Corrigan, Maggie	IL100, P022
Cox, Claudia	P023
Crittenden, Deborah	IL031
Crossley, Maxwell	P015
Crumbie, Robyn	IC052
Cuissart, Bertrand	IC039
Cunningham, Maria	P125

Author Name	Program Codes*
da Silva, Gabriel	IC012, P066
Da, Lintai	IC063
Daiguji, Hirofumi	P001
Dale, Stephen	IC001, IL002, P049
Darwish, Nadim	P121
Davidson, Max	P024
Dawson, William	IC050
De Chavez, Danjo	P025
de Izarra, Ambroise	IL009
de Tomas, Carla	IL024
De, Susmita	IC008
Deacon, Glen	P040
Demichelis, Raffaella	IL007
Deng, Jingyuan	IC036
Deplazes, Evelyne	IC038
Dhanasekaran, Salai Kalaiselvi	P026
Dhattarwal, Harender	IC005
Dhurairajan, Senthilnathan	P026
DiLabio, Gino	IL043
Doan, Phuong	P027
Dobson, John	IL033

Author Name	Program Codes*
Doi, Toshiki	P145
Dua, Arti	IL091
Dwight, Alyssa	P097
Dwivedi, Swarit	P028
Ebisawa, Shuichi	IL019
Ehara, Masahiro	IL026, P120
El Salamouni, Nehad	P029
El-Demerdash, Safinaz	P042
El-Nahas, Ahmed	P042
Elliott, Gareth	IL074, P030, P105
Ema, Tadashi	IC036
Evans, Alicia	P031
Fang, Wei-Hai	IL078
Farahani, Sara	P032
Filatov, Michael	IL097, IL099
Ford, Michael	IL035
Frankcombe, Terry	IC025, IL070, P060
Fronzi, Marco	IL035
Fujii, Hiroshi	P081
Fujimori, Toshikazu	P033
Fujinami, Mikito	P034, P119

Author Name	Program Codes*
Fujita, Kyoko	P086
Fujita, Takatoshi	IC054
Fukuoka, Atsushi	P025
Fukushima, Takanori	P104
Fule, Melinda	P035
Fung, Alfred	P027
Furuhashi, Naoto	P143
Furukawa, Shinya	IC034
Gadre, Shridhar	IL102
Gale, Julian	IL007
Gao, Jiali	IL010
Gao, Yi Qin	PL004
Garcia, Natalya	IL007
Garden, Anna	P011, P114
Gaston, Nicola	IL037
Ghanty, Tapan	P062
Ghorai, Sagar	IL020
Ghosh, Debashree	IL071, IL093
Gilbert, Andrew	IC041, P036, P090
Gill, Peter	IC001, IC041, IL001, IL002, P036, P087, P090

Author Name	Program Codes*
Glover, William	IC042
Godara, Sumitra	IC003
Goerigk, Lars	IL066, P016, P046, P079, P091, P138
Gordon, Calum	P114
Gould, Tim	IL068
Gregory, Kas	P105
Gregory, Kasimir	IL074, P038
Griffith, Renate	IC052
Griffiths, Thomas	IL092
Gryn'ova, Ganna	IC059
Guruge, Amali	P039
Gwee, Eunice	P040
Hada, Masahiko	IL044, P081
Hadsadee, Sarinya	P041
Haidar, El-Abed	P042
Haifeng, Zheng	P043
Hakim, Lukman	IC070, P044
Halat, Peter	P045
Hammill, Chelsey	IC029
Han, Wei	IL075
Hancock, Amy	P046

Author Name	Program Codes*
Hankel, Marlies	IC035
Hannongbua, Supa	IL038
Hapala, Prokop	P078
Harabuchi, Yu	IC067, P059
Harper, Jason	P031
Hartono, Herodion	IC072
Hasegawa, Jun-ya	IC036, P025, P041
Hasegawa, Taisuke	P047
Hashim, Fairuz	P048
Hashimoto, Yoshikazu	P127
Hatanaka, Miho	IL060
Haworth, Naomi	P121
Hayashi, Shigehiko	IL064
Hazra, Koustav	IL014
He, Wei	P147
He, Xiao	IC042
Head-Gordon, Martin	PL008
Hemmingsen, Luke	P049
Henchman, Richard	IC071
Henry, David	IL049
Hervir, Oliver	P049

Author Name	Program Codes*
Higham, Jon	IC071
Hill, Nicholas	P035, P050
Hinuma, Yoyo	IC034, P051
Hirao, Hajime	IL057
Hirao, Kimihiko	IL065, P042
Hiroi, Zenji	P051
Ho, Junming	IL082, P017, P031, P117
Hobza, Pavel	IC032, P078
Hoffmann, Mark	IL016
Hori, Satoshi	P051
Hsieh, Ming-Hsiu	IL063, P052
Hsu, Chao-Ping	IL067, P136
Hsu, Wei-Lun	P001
Huang, David	IC014
Huang, Gavin	P053
Huang, Gou-Tao	IL063
Huang, Xuhui	IL090
Huh, Joonsuk	IL079
Hunter, Michelle	IC033
Hunter, Michelle A.	IL023
Hush, Noel	P144

Author Name	Program Codes*
Hutama, Aulia	IC051
Hwang, Sang-Yeon	P075
Hymas, Kieran	P054
Ichino, Tomoya	P055, P131
Ikabata, Yasuhiro	IC065, P056, P119
Inamori, Mayu	P056
Injongkol, Yuwanda	P057
Ionita, Mariana	P098
Ireland, Kasey	P058, P139
Ishii, Yoshiki	P044
Ismail, Mohd Farid	IC016
Ito, Takuma	P059
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Izgorodina, Ekaterina	P040, P048, P080, P118, P122, P141
Ja'o, Aliyu	IC057
Jacob, Lilit	P060
Jang, Yun Hee	IC040, IL009
Jayatilaka, Dylan	P024
Jelínek, Pavel	P078
Jemmis, Eluvathingal	IL020

Author Name	Program Codes*
Jenkins, Samantha	IL080
Jerabek, Paul	IL025, P011
Ji, Lin	IC026
Jiang, Tian	P061
Jin, Shan	IC062
Jin, Xinsheng	IC042
Joanito, Ignasius	P136
Jordan, Meredith	IL100, P009, P022, P053, P113
Joshi, Meenakshi	P062
Jung, Yousung	IL059
Jungsuttiwong, Siriporn	P041, P057
Juodkazis, Saulius	P127
K, Surya	P063
Kable, Scott	IL100, P113
Kageyama, Ryo	P119
Kamachi, Takashi	IC034
Kamiya, Muneaki	IC050
Kanno, Ryoj	P051
Karton, Amir	IL081, P070, P141
Kashimura, Tatsuhiko	IL006
Kashyap, Hemant	IC005, P067

Author Name	Program Codes*
Kassal, Ivan	IL042
Kaur, Aishvaryadeep	P064
Kawashima, Yusuke	P065
Kawashita, Norihito	P065
Kawatsu, Tsutomu	IC028
Kayal, Riya	IL014
Kelly, Patrick	P066
Kelso, Michael	P029
Kerelsky, Alexander	P074
Khan, Yasir	IC012
Khatri, Vikas	P067
Khire, Subodh	IL102
Kilby, Philip	IL070
Kim, Hyungjun	IL032
Kim, Jun Soo	IC055
Kim, Seungsu	P075
Kim, Woo Youn	IL084, P075
Kirk, Steven	IL080
Kirkwood, Nicholas	P096
Kister, Thomas	P096
Kitaura, Kazuo	PL001

Author Name	Program Codes*
Ko, Kyoung Chul	P068
Kobayashi, Horikazu	P025
Kobayashi, Masato	IC045, P033
Kobayashi, Rika	IL035, IL061, P144
Kochan, Kamila	P040
Kodaya, Yoshitomo	IC056
Koga, Nobuaki	P092, P124
Komoto, Nana	P069
Kraus, Tobias	P096
Krenske, Elizabeth	IL062, P019, P112
Kroeger, Asja	IL081, P070
Kubečka, Jakub	P071
Kuo, Jer-Lai	IL077
Kurashige, Yuki	IL096, P102
Kurokawa, Yusaku	IC002
Kurtén, Theo	P071
Kusay, Ali	P061, P072
Lai, Luhua	IL040
Lan, Chang-Feng	P136
Lane, Joseph	IL012, P032
Langner, Johanna	P073

Author Name	Program Codes*
Lankau, Timm	IL069
Lansac, Yves	IC040, IL009
Lee, Jin Yong	IL114
Lee, Richmond	IC030, P128
Lee, Seunghoon	IL097
Lepailleur, Alban	IC039
Lessio, Martina	P074
Li, Jun	IL089
Li, Shuhua	IL054
Li, Yue	IC026
Lim, Carmay	IC024, PL006
Lim, Jaechang	P075
Limpanuparb, Taweetham	IC058, P020
Lin, Yiechang	P076
Ling, Chris	P115
Liu, Fengyi	IC031
Liu, Jian	P018, PL007
Liu, Wenjian	IL016
Liu, Xinzijian	P018
Liu, Ya-Jun	IL076
Liu, Yawei	P140

Author Name	Program Codes*
Liu, Yu	P077
Lo, Rabindranath	IC032, P078
Lo, Shih-Chun	P112
Lonsdale, Dale	P079
Lorpaiboon, Wanutcha	IC058, P020
Low, Kaycee	P080
Luo, Jing	IC062
Ma, Haibo	IL095
Ma, Jing	IL073
Ma, Yunsheng	P001
Ma, Zhifeng	P081
MacDermott-Opeskin, Hugo	P082
MacFarlane, Douglas	P045, P048
Maeda, Chihiro	IC036
Maeda, Satoshi	IC007, IC067, IL018, P047, P055, P059, P099, P104, P126, P131
Maekawara, Hiroki	P034
Maeno, Zen	IC034
Mahalapbutr, Panupong	IL039
Mallik, Bhabani	IL103
Mancera, Ricardo	IC038

Author Name	Program Codes*
Mandal, Shyama	P083
Manjanath, Aaditya	IL067
Manna, Debashree	IC032, P078
Manna, Soumitra	P084
Manzhos, Sergei	IL080
Mark, Alan	IL051, IL115, P058, P139
Marks, Nigel	IL024
Marlton, Samuel	P085, P088
Martinotti, Carlo	IC038
Maseras, Feliu	P116
Mason, Thomas	P086
Masters, Sarah	IC057
Matel, Hosea	IC037
Matsubara, Toshiaki	IC011
Matsuda, Ryotaro	P001
Matsumoto, Masakazu	IC070
Matsuoka, Takahide	IL085
Matubayasi, Nobuyuki	P044
McKemmish, Laura	IL104, P023, P125
McKenzie, Simon	IC041, P036, P087
McKinnon, Benjamin	P085, P088

Author Name	Program Codes*
McLean, Ben	P089
McTigue, Michael	P090
Meftahi, Nastaran	IC046
Mehta, Nisha	P091
Metivier, Jean-Philippe	IC039
Midoro, Yuuki	IC056
Misawa, Nana	P092
Mishra, Sabyashachi	P084, P093
Mishra, Vipin	P093
Mizoguchi, Haruki	P131
Modestino, Miguel	P140
Mohamed, Ahmed Elaaf	P094
Mohammad Latif, Muhammad Alif	IC016
Molino, Andrew	P095
Monego, Debora	IC015, P096
Montoya, Alejandro	P057
Moon, Seokhyun	P075
Moran, Damian	P097
Mori, Nanami	P065
Moriwaki, Hirotomo	P065
Mukherjee, Debashis	IL014

Author Name	Program Codes*
Mulvaney, Paul	P096
Muraru, Sebastian	P098
Mushrif, Samir	P028
Nabata, Hitoshi	P099
Nachtigallová, Dana	IC032, P078
Nagaoka, Masataka	P012, P092, P124
Nagaoka, Masataka	IL087
Nair, Nisanth	P133
Nakai, Hiromi	IC013, IC027, IC065, IL041, P021, P034, P056, P069, P103, P119, P132, P145
Nakajima, Takahito	IC050, IL085, P042
Nakashima, Hiroyuki	IC002
Nakata, Hiroya	IL097
Nakatsuji, Hiroshi	IC002
Nam, Yeonsig	IL114
Namdas, Ebinazar	P112
Namuangruk, Supawadee	IL048
Nandi, Surajit	P083
Nellas, Ricky	IC037
Nguyen, Anh	IL055, P086, P100

Author Name	Program Codes*
Nishijima, Yoshiaki	P127
Nishimoto, Yoshio	P101
Nishimura, Yoshifumi	IC027, P069
Nishio, Soichiro	P102
Noble, Benjamin	IC029, P027
Norcott, Philip	IC029
Notaras, Daniel	P117
Nozaki, Kyoko	IC036
Nudejima, Takuro	IC065
O'Mara, Megan	IC064, IL051, P076, P082, P137
Oakley, Aaron	IL092
Oba, Yuki	IC028
Oguri, Hiroki	P131
Ohno, Koichi	IL017
Oikawa, Hideaki	P131
Okada, Chika	IC027
Okano, Sakura	IC028
Oki, Takuto	IC056
Okoshi, Masaki	P103
Oksanen, Esko	P024
Ono, Junichi	IC027, P069

Author Name	Program Codes*
Ono, Yuriko	IL019
Onoda, Haruka	IC045
Orimoto, Yuuichi	IL106
Ortiz, Christopher Llynard	IC037
Osborne, Dale	P129
Oyaizu, Kenichi	P141
Ozen, Cihan	P104
Page, Alister	IL074, P013, P030, P038, P089, P105, P135, P149
Pal, Sourav	IL015
Pala, Raj	P133
Parameswari, Akshintala	IC061
Paranjothy, Manikandan	IC003
Parasuk, Vudhichai	IL083
Parasuk, Waraporn	IL083
Pareek, Monika	P123
Pas, Ekaterina	IL055, P086
Pas, Katya	P045, P109
Pas, Steven	P048
Pasupathy, Abhay	P074
Pathak, Biswarup	P083

Author Name	Program Codes*
Pattiyil, Parameswaran	IL045
Paul, Ankan	IL071
Pei, Lin-Qi	IC062
Peiris, Ishara	P106
Per, Manolo	IC018
Piccardo, Matteo	IL027
Picciril, Susanna	IC068
Piris, Mario	IC017
Pittalis, Stefano	IL068
Poger, David	IL115
Pomogaeva, Anna	IL106
Pouton, Colin	P039
Powell, Benjamin	IC009
Prince, Kevin	IC068, P007
Priyakumar, U. Deva	IL086
Pross, Addy	PL002
Pryor, Joshua	P107
Puripat, Maneeporn	IL083
Qian, Shu-Li	IC062
Raghavachari, Krishnan	IL105
Raiteri, Paolo	IL007

Author Name	Program Codes*
Rankine, Conor	IC057
Rao, Shashank	IL027, P006
Ratanasak, Manussada	IC036, P041
Rathnayake, Madhuranga	P108
Rawat, Kuber	P083
Reichman, David	P074
Reid, James	P111
Reimers, Jeffrey	IL034, IL035, P015, P144
Remsing, Richard	IC005
Richter, Robert	IC068
Robertson, Evan	P106, P134
Robertson, Patrick	P134
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Rogers, Fergus	P110
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Roseli, Ras Baizureen	P112
Rosson, Lorraine	IL049
Rovira, Carme	IC048
Rowell, Keiran	IL100, P113
Ruffman, Charlie	P114

Author Name	Program Codes*
Rungrotmongkol, Thanyada	IL039
Russell, Isabella	IL100, P022
Ryde, Ulf	P024
S, Jan	IL025
Sa'adeh, Hanan	P007
Saadeh, Hanna	IC068
Sabu, Gopika	IC008
Saha, Soumen	P012
Saita, Kenichiro	P099
Saitow, Masaaki	IC066
Sajid, Ali	IL035
Sakaki, Shigeyoshi	IL021
Sakti, Aditya	IC013, P021
Sale, Matthew	P115
Sameera, W. M. C.	IC044, P116
Sandler, Isolde	P117
Sangpheak, Kanyani	IL039
Saparpakorn, Patchareenart	IL038
Sarmah, Amrit	P078
Sato, Ataru	IL044
Sato, Hirofumi	IL008

Author Name	Program Codes*
Saxena, Shilpi	P133
Schaefer, Henry	IL110
Schmidt, Timothy	IL070, IL070
Schwerdtfeger, Peter	IL025
Scuseria, Gustavo	IL109
Searles, Debra	P008, P111
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Seniutinas, Gediminas	P127
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Sharma, Shilendra	P133
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Shaw, Miranda	IL100
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Shih, Petra	IC049
Shimizu, Ken-ichi	IC034
Shiraogawa, Takafumi	IL026, P120
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Author Name	Program Codes*
Shukla, Atul	P112
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Stampfl, Catherine	P042
Stefanovic, Ryan	IL074
Stevens, Molly	IC053
Stinson, Chris	IL031
Stroet, Martin	P058, P139

Author Name	Program Codes*
Su, Peifeng	IC019
Suarez-Martinez, Irene	IL024
Subramanian, Nandhitha	IL051
Sudto, Kanokorn	IL038
Suh, Donguk	P001
Sumiya, Yosuke	P047
Sung, Jaeyoung	IL050
Sunoj, Raghavan	P063, P123
Sunoj, Raghavan B.	IL058
Suzuki, Kimichi	IC007
Suzuki, Yuichi	P092, P124
Swadźba-Kwaśny, Małgorzata	P080
Švec, Martin	P078
Syme, Anna-Maree	P125
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Tai, Hui-Chung	IC024
Takagi, Makito	P047, P099, P126
Takagi, Tatsuya	P065
Takahashi, Kaito	IC043
Takakusagi, Satoru	IC034
Takatsuka, Kazuo	IC006, PL005

Author Name	Program Codes*
Takenaka, Masato	P127
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Taketsugu, Tetsuya	IC045, IL019, P033, P127
Takigawa, Ichigaku	IC034
Tan, Davin	P128
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Tanksale, Akshat	P028
Tawfik, Sherif	IL035, P042, P129, P130
Taylor, Patrick	P130
TayRongde, Ian	IL080
Teeraniramitr, Peerayar	IC058
Ten-no, Seiichiro	IL013
Tewary, Subrata	IL065
Thapa, Bishnu	IL105
Thomas, Trayder	IC072
Tian, Tian	IL080
Tian, Yu-Shi	P065
Todorova, Nevena	IC053
Tokoyama, Hiroaki	IC056
Tokuda, Hideki	IC036

Author Name	Program Codes*
Torre, Bruno	P078
Totti, Federico	P011
Toyao, Takashi	IC034
Trevitt, Adam	P066, P085, P088
Trujillo, Juan Camilo	P023
Tsubouchi, Akira	P131
Tsuchimochi, Takashi	IC020
Tsunekawa, Yoshiaki	P131
Tsutsumi, Takuro	IL019
Tuan Kob@Yaakub, Tuan Nurul Azura	IC016
Turner, Aislinn	P066
Ucur, Boris	P085
Ungur, Liviu	IL028
Uratani, Hiroki	P132
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Verma, Rahul	P133
Villani, Luigi	P134
Vo, Nhat Vinh	IC039
Waite, Simone	P105, P135
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Walsh, Tiffany	IL088

Author Name	Program Codes*
Walton, Paul	IC048
Wang, Binju	IC048
Wang, Chun-I	P136
Wang, Feng	IC068, P007
Wang, Jie	IC026
Wang, Lily	IL051, P137
Wang, Wenliang	IC031
Wanless, Erica	IL074, P030, P038
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Wappett, Dominique	P138
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Washizu, Hitoshi	P103
Webber, Grant	IL074, P030, P038, P089
Welsh, Ivan	IL107
Wetmore, Stacey	IL011
Wheatley, Nicole	P058, P139
Widmer-Cooper, Asaph	IC015, P096, P108, P140
Wilson, David	IL072, P002, P003, P064, P095, P100, P106, P134
Wilson, Katie	IC064, P076
Witek, Henryk	IC001, IL002, P073

Author Name	Program Codes*
Wong, Richard	IL046
Wood, Bayden	P040
Wood, Jared	P140
Wright, Andrew	P109
Wu, Wei	IL029
Wu, Xiao-Hui	IC062
Wu, Yun-Dong	IL004, P147
Wylie, Luke	P141
Xu, Longkun	P142
Xu, Tianlv	IL080
Xu, Xin	IL030
Yabushita, Satoshi	IL006, P143
Yagoshi, Hiroaki	P124
Yajima, Takeshi	P051
Yamakado, Hideo	IC056
Yamamoto, Kentaro	IC006
Yan, Feng	IC062
Yan, Kangyu	P018
Yanai, Takeshi	IC066
Yang, Hsiao-Ching	IL052
Yang, Likun	P144

Author Name	Program Codes*
Yao, Nan	IC033
Yarasi, Soujanya	IC061
Yarovsky, Irene	IC053
Yeh, Shu-Hao	IL067
YongBoon, Tan	IL080
Yorimoto, Sadaiwa	P131
Yoshikawa, Takeshi	IC065, P056, P069, P145
Yoshizawa, Kazunari	IL005, P042
Yoshizawa-Fujita, Masahiro	P141
Yu, Chin-Hui	IL069
Yu, Haibo	IL092, P029
Yu, Jen-Shiang	IL063, P052
Yu, Jingxian	IC062
Yu, Li-Juan	P146
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Author Name	Program Codes*
Yuan, Qinghong	IC033, IC033
Zacharias, Martin	IC008
Zbořil, Radek	IC032, P078
Zhang, Linxing	P147
Zhang, Ning	IL016
Zhang, Qing-Wei	P147
Zhang, Xinhao	IL004, P147
Zhang, Zhijun	P018
Zhao, Jijun	IL036
Zhao, Yan	IL101
Zhao, Yi	IC004
Zheng, Haifeng	P018
Zhou, Xiaoshun	IC062
Zhou, Xiuwen	IC009
Zhu, Wenting (Judy)	P148

PARTICIPANTS

List of consenting participants as at 24 September 2019

Dr	Sherif Abdulkader Tawfik	Abbas	RMIT University	Australia	sherif.abbas@rmit.edu.au
Dr	Minori	Abe	Tokyo Metropolitan University	Japan	abeminoriabe@gmail.com
Mr	Ankit	Agrawal	University of Tokyo	Japan	aankit.agrawal1995@gmail.com
Mr	Johnny	Agugiaro	La Trobe University	Australia	j.agugiaro@latrobe.edu.au
Mrs	Khalidah H.M.	Al-Furaiji	La Trobe Institute for Molecular Science	Australia	khalidah1969@gmail.com
Mr	Khidhir	Alhameedi	The University of Western Australia	Australia	khidhir.abdalhussein@gmail.com
A/Prof	Jane	Allison	University of Auckland	New Zealand	j.allison@auckland.ac.nz
Mrs	Hansi	Alwis	Charles Darwin University	Australia	weerakkodigehansisachintha.alwis@cdu.edu.au
Dr	Roger	Amos	NCI	Australia	roger.amos@anu.edu.au
Prof	Yuriko	Aoki	Kyushu University	Japan	aoki.yuriko.397@m.kyushu-u.ac.jp
Mr	Jared	Ashtree	University of Melbourne	Australia	jaredc@student.unimelb.edu.au
Dr	Ravichandar	Babarao	RMIT University	Australia	ravichandar.babarao@rmit.edu.au
Mr	Fred	Backler	Swinburne University of Technology	Australia	fbackler@swin.edu.au
Mr	Ardeshir	Baktash	The University of Queensland	Australia	a.baktash@uq.edu.au
Dr	Giuseppe	Barca	Australian National University	Australia	Giuseppe.Barca@anu.edu.au
Dr	Amanda	Barnard	CSIRO	Australia	amanda.barnard@data61.csiro.au
Prof	Debra	Bernhardt (Searles)	The University of Queensland	Australia	d.bernhardt@uq.edu.au
Ms	Clare	Birch	The University of Sydney	Australia	cbir5622@uni.sydney.edu.au
Prof	Parbati	Biswas	University of Delhi	India	pbiswas@chemistry.du.ac.in
Mr	Mitchell	Blyth	Australian National University	Australia	mitchell.blyth@anu.edu.au
Mr	Luca	Bondi	University of Otago	New Zealand	bonlb235@student.otago.ac.nz
Dr	Amine	Bouibes	Nagoya University	Japan	bouibes@ncube.human.nagoya-u.ac.jp
Prof	Russell	Boyd	Dalhousie University	Canada	Russell.Boyd@Dal.Ca
Mr	Josh J	Brown	The University of Newcastle	Australia	jbrown19@uon.edu.au
Prof Dr	Yuxiang	Bu	Shandong University	China	byx@sdu.edu.cn
Prof	Ronan	Bureau	CERMN, University of Caen	France	ronan.bureau@unicaen.fr
Dr	Simone	Calvello	The University of Melbourne / ANSTO	Australia	simone.calvello@unimelb.edu.au
Prof	Pieremanuele	Canepa	National University of Singapore	Singapore	pcanepa@nus.edu.sg
Mr	Peter	Canfield	The University of Sydney	Australia	peter.canfield@sydney.edu.au
Prof	Zexing	Cao	Xiamen University	China	zxcao@xmu.edu.cn
Mr	Marcos	Casanova -Páez	The University of Melbourne	Australia	mcasanova@student.unimelb.edu.au
Dr	Claudio	Cazorla	The University of New South Wales	Australia	c.cazorla@unsw.edu.au
Dr	Debashree	Chakraborty	National Institute of Technology Karnataka	India	debashree@nitk.edu.in

Dr	David	Chalmers	Monash Institute of Pharmaceutical Sciences	Australia	david.chalmers@monash.edu
Dr	Bun	Chan	Nagasaki University	Japan	bun.chan@nagasaki-u.ac.jp
Mr	Junbo	Chen	The University of New South Wales	Australia	j.chen@unsw.edu.au
Mr	Zifei	Chen	Peking University	China	chenzifei@pku.edu.cn
Prof	Yuan-Chung	Cheng	National Taiwan University	Taiwan	yuanchung@ntu.edu.tw
Miss	Ping	Chin	The University of Queensland	Australia	y.chin@uqconnect.edu.au
Mr	Kridtin	Chinsukserm	Mahidol University	Thailand	kridtin.chi@student.mahidol.edu
Mr	Tony	Chipman	University of Tasmania	Australia	antony.chipman@utas.edu.au
Prof	Cheol Ho	Choi	Kyungpook National University	South Korea	cchoi@knu.ac.kr
Dr	Hyeonho	Choi	Samsung Advanced Institute of Technology	South Korea	hono.choi@samsung.com
Dr	Chien-Pin	Chou	Waseda University	Japan	sol.chou@gmail.com
Dr	Gemma	Christian	Avondale College of Higher Education	Australia	gemma.christian@avondale.edu.au
Dr	Andrew	Christofferson	RMIT University	Australia	andrew.christofferson@rmit.edu.au
Prof	Michael	Collins	Australian National University	Australia	collins@rsc.anu.edu.au
Prof	Michelle	Coote	Australian National University	Australia	michelle.coote@anu.edu.au
Ms	Maggie	Corrigan	The University of Sydney	Australia	mcor3140@uni.sydney.edu.au
Miss	Claudia	Cox	The University of New South Wales	Australia	claudia.cox@unsw.edu.au
Dr	Deborah	Crittenden	University of Canterbury	New Zealand	deborah.crittenden@canterbury.ac.nz
Mr	Lintai	Da	Shanghai Jiao Tong University	China	darlt@sjtu.edu.cn
Dr	Gabriel	da Silva	University of Melbourne	Australia	gdasilva@unimelb.edu.au
Dr	Stephen	Dale	Australian National University	Australia	stephen.dale1990@gmail.com
Mr	Max	Davidson	The University of Western Australia	Australia	max.davidson@research.uwa.edu.au
Dr	Susmita	De	Cochin University of Science and Technology	India	susmita@cusat.ac.in
Mr	Danjo Purio	De Chavez	Institute for Catalysis, Hokkaido University	Japan	dechavezdanjo@gmail.com
Dr	Evelyne	Deplazes	University of Technology Sydney	Australia	Evelyne.Deplazes@uts.edu.au
Miss	Salai Kalaiselvi	Dhanasekara	Prist University	India	kalai.d.sals@gmail.com
Prof	Gino	DiLabio	University of British Columbia	Canada	gino.dilabio@ubc.ca
Mr	Vincent	Doan	Australian National University	Australia	u6057677@anu.edu.au
Emeritus Prof	John	Dobson	Griffith University	Australia	j.dobson@griffith.edu.au
Dr	Arti	Dua	IIT Madras	India	arti@iitm.ac.in
Mr	Swarit	Dwivedi	Monash University	Australia	swarit.dwivedi@monash.edu
Prof	Masahiro	Ehara	Institute for Molecular Science	Japan	ehara@ims.ac.jp
Mr	Gareth	Elliott	The University of Newcastle	Australia	gareth.elliott@uon.edu.au

Dr	Nehad	Elsalamouny	University of Wollongong	Australia	nse665@uowmail.edu.au
Ms	Alicia	Evans	The University of New South Wales	Australia	aevansau@gmail.com
Prof	Wei-Hai	Fang	Beijing Normal University	China	Fangwh@bnu.edu.cn
Mrs	Sara	Farahani	University of Waikato	New Zealand	sf112@students.waikato.ac.nz
Dr	Michael	Filatov	Kyungpook National University	South Korea	mike.filatov@gmail.com
Prof	Mike	Ford	University of Technology Sydney	Australia	Mike.Ford@uts.edu.au
Dr	Terry	Frankcombe	The University of New South Wales	Australia	t.frankcombe@adfa.edu.au
Mr	Toshikazu	Fujimori	Hokkaido University	Japan	fuji-0378@eis.hokudai.ac.jp
Mr	Mikito	Fujinami	Waseda University	Japan	m-fujinami@fuji.waseda.jp
Dr	Takatoshi	Fujita	Institute for Molecular Science	Japan	tfujita@ims.ac.jp
Miss	Melinda	Fule	Australian National University	Australia	melinda.fule@anu.edu.au
Prof	Shridhar	Gadre	SPPU Pune	India	gadre@unipune.ac.in
Prof	Julian	Gale	Curtin University	Australia	J.Gale@curtin.edu.au
Prof	Jiali	Gao	Shenzhen Bay Laboratory and University of Minnesota	China	jgao@umn.edu
Mr	Yiqin	Gao	Peking University	China	gaoyq@pku.edu.cn
A/Prof	Nicola	Gaston	University of Auckland	New Zealand	n.gaston@auckland.ac.nz
Prof	Debashree	Ghosh	IACS Kolkata	India	pcdg@iacs.res.in
Dr	Andrew	Gilbert	Australian National University	Australia	andrew.iqmol@gmail.com
Prof	Peter	Gill	The University of Sydney	Australia	peter.gill@anu.edu.au
A/Prof	William	Glover	NYU Shanghai	China	william.glover@nyu.edu
Dr	Lars	Goerigk	The University of Melbourne	Australia	lars.goerigk@unimelb.edu.au
Dr	Tim	Gould	Griffith University	Australia	t.gould@griffith.edu.au
Mr	Kas	Gregory	The University of Newcastle	Australia	kasimir.gregory@uon.edu.au
A/Prof	Renate	Griffith	The University of New South Wales	Australia	r.griffith@unsw.edu.au
Dr	Ganna (Anya)	Gryn'ova	Heidelberg Institute for Theoretical Studies	Germany	ganna.grynova@h-its.org
Ms	Amali	Guruge	Monash Institute of Pharmaceutical Sciences	Australia	amali.galappaththiguruge@monash.edu
Miss	Eunice	Gwee	Monash University	Australia	shu.gwee@monash.edu
Prof	Masahiko	Hada	Tokyo Metropolitan University	Japan	hada@tmu.ac.jp
Miss	Sarinya	Hadsadee	Ubon Ratchathani University	Thailand	subaka29@gmail.com
Mr	El-Abed	Haidar	The University of Sydney	Australia	ehai2584@uni.sydney.edu.au
Mr	Zheng	Haifeng	Peking University	China	zhenghf@pku.edu.cn
Dr	Lukman	Hakim	Brawijaya University	Indonesia	lukman.chemist@ub.ac.id
Mr	Peter	Halat	Monash University	Australia	Peter.Halat@monash.edu
Prof	Wei	Han	Peking University Shenzhen Graduate School	China	hanw@pkusz.edu.cn
Ms	Amy	Hancock	University of Melbourne	Australia	achancock@student.unimelb.edu.au

Dr	Marlies	Hankel	The University of Queensland	Australia	m.hankel@uq.edu.au
Prof	Supa	Hannongbua	Kasetsart University	Thailand	fscisph@ku.ac.th
Prof	Yu	Harabuchi	Hokkaido University	Japan	y_harabuchi@sci.hokudai.ac.jp
Dr	Taisuke	Hasegawa	NIMS	Japan	HASEGAWA.Taisuke@nims.go.jp
Ms	Fairuz	Hashim	Monash University	Australia	fairuz.hashim@monash.edu
A/Prof	Miho	Hatanaka	Nara Institute of Science and Technology	Japan	hatanaka@ms.naist.jp
Prof	Shigehiko	Hayashi	Kyoto University	Japan	hayashig@kuchem.kyoto-u.ac.jp
Prof	Martin	Head-Gordon	University of California Berkeley	USA	mhg@cchem.berkeley.edu
Mr	Luke	Hemmingsen	Australian National University	Australia	u6946812@anu.edu.au
Dr	Richard	Henchman	University of Manchester	United Kingdom	henchman@manchester.ac.uk
A/Prof	David	Henry	Murdoch University	Australia	D.Henry@murdoch.edu.au
Mr	Oliver	Hervir	Australian National University	Australia	u6942736@anu.edu.au
Mr	Nicholas	Hill	Australian National University	Australia	nicholas.hill@anu.edu.au
Dr	Yoyo	Hinuma	Chiba University	Japan	ma7s@yahoo.co.jp
A/Prof	Hajime	Hirao	City University	Hong Kong	hhirao@cityu.edu.hk
Dr	Kimihiko	Hirao	RIKEN & Fukui Institute, Kyoto University	Japan	hirao@riken.jp
Dr	Junming	Ho	The University of New South Wales	Australia	junming.ho@unsw.edu.au
Mr	Ming-Hsiu	Hsieh	National Chiao Tung University	Taiwan	mhhsieh.bt06g@nctu.edu.tw
Prof	Cherri	Hsu	Academia Sinica	Taiwan	cherri@sinica.edu.tw
A/Prof	David	Huang	The University of Adelaide	Australia	david.huang@adelaide.edu.au
Mr	Gavin	Huang	The University of Sydney	Australia	shua9815@uni.sydney.edu.au
Prof	Xuhui	Huang	Hong Kong University of Science & Technology	Hong Kong	xuhuihuang@ust.hk
A/Prof	Joonsuk	Huh	Sungkyunkwan University	South Korea	joonsukhuh@gmail.com
Dr	Aulia Sukma	Hutama	Universitas Gadjah Mada	Indonesia	aulia.sukma.hutama@ugm.ac.id
Mr	Kieran	Hymas	University of Melbourne	Australia	khymas@student.unimelb.edu.au
Dr	Tomoya	Ichino	Hokkaido University	Japan	tichino@eis.hokudai.ac.jp
Dr	Yasuhiro	Ikabata	Waseda University	Japan	ikabata@aoni.waseda.jp
Miss	Mayu	Inamori	Waseda University	Japan	inamori@ruri.waseda.jp
Miss	Yuwanda	Injongkol	Ubon Ratchathani University	Thailand	yuwanda.injongkol@sydney.edu.au
Miss	Kasey	Ireland	The University of Queensland	Australia	kasey.ireland@uq.edu.au
Mr	Takuma	Ito	Hokkaido University	Japan	maru8tito@gmail.com
Miss	Lilit	Jacob	The University of New South Wales (Canberra)	Australia	lilit.jacob@student.adfa.edu.au
Prof	Yun Hee	Jang	DGIST	South Korea	yhjang@dgist.ac.kr
Prof	Dylan	Jayatilaka	The University of Western Australia	Australia	dylan.jayatilaka@uwa.edu.au
Prof	Eluvathingal D.	Jemmis	Indian Institute of Science	India	jemmis@iisc.ac.in

Prof	Samantha	Jenkins	Hunan Normal University	China	samanthajsuman@gmail.com
Mr	Dirk	Jensen	The University of Sydney	Australia	djen0096@uni.sydney.edu.au
Prof	Lin	Ji	Capital Normal University	China	jilin@mail.cnu.edu.cn
Miss	Tian	Jiang	The University of Sydney	Australia	tjia5436@uni.sydney.edu.au
A/Prof	Meredith	Jordan	The University of Sydney	Australia	meredith.jordan@sydney.edu.au
Miss	Meenakshi	Joshi	Homi Bhabha National Institute	India	imeenakshijoshi16@gmail.com
Prof	Yousung	Jung	KAIST	South Korea	ysjn@kaist.ac.kr
Miss	Surya	K	Indian Institute of Technology Bombay	India	srk1684@gmail.com
A/Prof	Muneaki	Kamiya	Gifu University	Japan	m_kamiya@gifu-u.ac.jp
A/Prof	Amir	Karton	The University of Western Australia	Australia	amir.karton@uwa.edu.au
Dr	Hemant K	Kashyap	Indian Institute of Technology Delhi	India	hkashyap@chemistry.iitd.ac.in
Dr	Ivan	Kassal	The University of Sydney	Australia	ivan.kassal@sydney.edu.au
Miss	Aish	Kaur	La Trobe university	Australia	Aishvaryakaur8@gmail.com
Mr	Yusuke	Kawashima	Osaka University	Japan	kawashima-y@phs.osaka-u.ac.jp
Mr	Paddy	Kelly	University of Wollongong	Australia	pdk917@uowmail.edu.au
Mr	Vikas	Khatri	Indian Institute of Technology Delhi	India	cyz168232@iitd.ac.in
Prof	Hyungjun	Kim	KAIST	South Korea	linus16@kaist.ac.kr
Prof	Jun Soo	Kim	Ewha Womans University	South Korea	jkim@ewha.ac.kr
Prof	Woo Youn	Kim	KAIST	South Korea	wooyoun@kaist.ac.kr
Prof	Steven Robert	Kirk	Hunan Normal University	China	stevenrkirk@gmail.com
Dr	Kazuo	Kitaura	RIKEN	Japan	kazuo.kitaura@riken.jp
Prof	Kyoung Chul	Ko	Chonnam National University	South Korea	kcko1982@jnu.ac.kr
Dr	Masato	Kobayashi	Hokkaido University	Japan	k-masato@sci.hokudai.ac.jp
Dr	Rika	Kobayashi	NCI	Australia	Rika.Kobayashi@anu.edu.au
Miss	Nana	Komoto	Waseda University	Japan	nana070412@fuji.waseda.jp
A/Prof	Elizabeth	Krenske	The University of Queensland	Australia	e.krenske@uq.edu.au
Ms	Asja	Kroeger	The University of Western Australia	Australia	asja.kroeger@research.uwa.edu.au
Mr	Jakub	Kubečka	University of Helsinki	Finland	jakub.kubecka@helsinki.fi
Prof	Jer-Lai	Kuo	IAMS, Academia Sinica	Taiwan	jlkuo@pub.iams.sinica.edu.tw
Prof	Yuki	Kurashige	Kyoto University	Japan	kura@kuchem.kyoto-u.ac.jp
Mr	Ali	Kusay	The University of Sydney	Australia	akus8786@uni.sydney.edu.au
Prof	Luhua	Lai	Peking University	China	lhlai@pku.edu.cn
A/Prof	Jo	Lane	University of Waikato	New Zealand	jlane@waikato.ac.nz
Ms	Johanna	Langner	NCTU	Taiwan	johanna.langner@arcor.de
Prof	Yves	Lansac	University of Tours / DGIST	France	lansac@univ-tours.fr
Prof	Jin Yong	Lee	Sungkyunkwan University	South Korea	jinylee@skku.edu
Dr	Richmond	Lee	Singapore University of Technology and Design	Singapore	richmond_lee@sutd.edu.sg
Dr	Martina	Lessio	The University of Sydney	Australia	martina.lessio@sydney.edu.au

Prof	Jun	Li	Tsinghua University	China	junli@tsinghua.edu.cn
Prof	Shuhua	Li	Nanjing University	China	shuhua@nju.edu.cn
Prof	Carmay	Lim	Academia Sinica	Taiwan	carmay@gate.sinica.edu.tw
Mr	Jaechang	Lim	KAIST	South Korea	ljchang94@kaist.ac.kr
Dr	Taweetham	Limpanuparb	Mahidol University	Thailand	taweetham.lim@mahidol.edu
Miss	YC	Lin	Australian National University	Australia	u6352569@anu.edu.au
Prof	Fengyi	Liu	Shaanxi Normal University	China	fengyiliu@snnu.edu.cn
Prof	Jian	Liu	Peking University	China	jianliupku@pku.edu.cn
Prof	Wenjian	Liu	Shandong University	China	liuwj@sdu.edu.cn
Prof	Yajun	Liu	Beijing Normal University	China	yajun.liu@bnu.edu.cn
Dr	Yu	Liu	The University of New South Wales	Australia	z3386640@zmail.unsw.edu.au
Dr	Rabin	Lo	Czech Academy of Sciences	Czech Republic	rabindranath.lo@uochb.cas.cz
Mr	Dale	Lonsdale	The University of Melbourne	Australia	dlonsdale@student.unimelb.edu.au
Ms	Kaycee	Low	Monash University	Australia	kaycee.low@monash.edu
Prof	Haibo	Ma	Nanjing University	China	haibo@nju.edu.cn
Prof	Jing	Ma	Nanjing University	China	majing@nju.edu.cn
Mr	Zhifeng	Ma	Tokyo Metropolitan University	Japan	ma-zhifeng@ed.tmu.ac.jp
Mr	Hugo	MacDermott-Opeskin	Australian National University	Australia	hugomacdermott@gmail.com
Prof	Satoshi	Maeda	Hokkaido University	Japan	smaeda@eis.hokudai.ac.jp
Mr	Shyama Charan	Mandal	Indian Institute of Technology Indore	India	kssm04@gmail.com
Dr	Shree	Manna	Czech Academy of Sciences	Czech Republic	debashree.manna@uochb.cas.cz
Mr	Soumitra	Manna	Indian Institute of Technology (IIT) Kharagpur	India	mannas.973@gmail.com
Prof	Alan	Mark	The University of Queensland	Australia	a.e.mark@uq.edu.au
Mr	Samuel	Marlton	University of Wollongong	Australia	sjpm073@uowmail.edu.au
Mr	Tom	Mason	Monash University	Australia	thomas.mason1@monash.edu
A/Prof	Sarah	Masters	University of Canterbury	New Zealand	sarah.masters@canterbury.ac.nz
Prof	Toshiaki	Matsubara	Kanagawa University	Japan	matsubara@kanagawa-u.ac.jp
Dr	Laura	McKemmish	The University of New South Wales	Australia	l.mckemmish@unsw.edu.au
Mr	Simon	McKenzie	The University of Sydney	Australia	simonclaytonmckenzie@gmail.com
Mr	Ben	McKinnon	University of Wollongong	Australia	bm125@uowmail.edu.au
Mr	Ben	McLean	The University of Newcastle	Australia	ben.d.mclean@uon.edu.au
Mr	Michael	McTigue	Australian National University	Australia	u6083745@anu.edu.au
Dr	Nastaran	Meftahi	RMIT University	Australia	nastaran.meftahi@rmit.edu.au
Ms	Nisha	Mehta	The University of Melbourne	Australia	nisham@student.unimelb.edu.au
Ms	Nana	Misawa	Nagoya University	Japan	misawa@ncube.human.nagoya-u.ac.jp
Mr	Vipin Kumar	Mishra	Indian Institute of Technology Kharagpur	India	vipinpandit13@gmail.com

Dr	Elaaf	Mohamed	Australian National University	Australia	elaaf.mohamed@anu.edu.au
Dr	Muhammad Alif	Mohammad Latif	Universiti Putra	Malaysia	aliflatif@upm.edu.my
Mr	Andrew	Molino	La Trobe University	Australia	a.molino@latrobe.edu.au
Miss	Debora	Monego	The University of Sydney	Australia	dmon2404@uni.sydney.edu.au
Dr	Damian	Moran	Macquarie University	Australia	damian.moran@mq.edu.au
Mr	Parishudda Babu	Movva	The University of Newcastle	Australia	c3272878@uon.edu.au
Prof	Debashis	Mukherjee	S N Bose National Centre for Basic Sciences, Kolkata	India	pcdemu@gmail.com
Mr	Sebastian	Muraru	Universitatea Politehnica Bucuresti	Romania	sebmuraru@gmail.com
Dr	Vinuthaa	Murthy	Charles Darwin University	Australia	vinuthaa.murthy@cdu.edu.au
Mr	Hitoshi	Nabata	Hokkaido University	Japan	nabata@eis.hokudai.ac.jp
Prof	Masataka	Nagaoka	Nagoya University	Japan	mnagaoka@i.nagoya-u.ac.jp
Dr	Shigeru	Nagase	Fukui Institute	Japan	nagase@ims.ac.jp
Prof	Hiromi	Nakai	Waseda University	Japan	nakai@waseda.jp
Dr	Takahito	Nakajima	RIKEN	Japan	nakajima@riken.jp
Dr	Hiroyuki	Nakashima	Quantum Chemistry Research Institute	Japan	h.nakashima@qcri.or.jp
Dr	Supawadee	Namuangruk	NANOTEC	Thailand	supawadee@nanotec.or.th
Dr	Ricky	Nellas	University of the Philippines Diliman	Philippines	rbnellas@up.edu.ph
Miss	Anh Tram	Nguyen	La Trobe University	Australia	tramanh.nguyen@latrobe.edu.au
Dr	Yoshio	Nishimoto	Kyoto University	Japan	nishimoto.yoshio@fukui.kyoto-u.ac.jp
Mr	Soichiro	Nishio	Kyoto University	Japan	nishio@theoc.kuchem.kyoto-u.ac.jp
Dr	Benjamin	Noble	Australian National University	Australia	benjamin.noble@anu.edu.au
Prof	Koichi	Ohno	IQCE	Japan	ohnok@iqce.jp
Dr	Masaki	Okoshi	Research Organization for Information Science and Technology	Japan	m_okoshi@me.com
A/Prof	Megan	O'Mara	Australian National University	Australia	megan.omara@anu.edu.au
Dr	Junichi	Ono	Waseda University	Japan	jono@aoni.waseda.jp
Dr	Cihan	Ozen	Hokkaido University	Japan	ozenc@icredd.hokudai.ac.jp
A/Prof	Alister	Page	The University of Newcastle	Australia	alister.page@newcastle.edu.au
Prof	Sourav	Pal	IISER Kolkata	India	s.pal@iiserkol.ac.in
Dr	Manikandan	Paranjothy	Indian Institute of Technology Jodhpur	India	pmanikandan@iitj.ac.in
Prof	Vudhichai	Parasuk	Chulalongkorn University	Thailand	vudhichai.p@chula.ac.th
A/Prof	Katya	Pas	Monash University	Australia	katya.pas@monash.edu
Dr	Parameswaran	Pattiyil	National Institute of Technology Calicut	India	param@nitc.ac.in
Prof	Ankan	Paul	Indian Association for the Cultivation of Science	India	rcap@iacs.res.in
Mrs	Ishara	Peiris	La Trobe University	Australia	58pikpeiris@gmail.com
Dr	Manolo	Per	CSIRO Data61	Australia	manolo.per@data61.csiro.au
Prof	Mario	Piris	University of the Basque Country	Basque	mario.piris@ehu.eus

Dr	Dave	Priyakumar	IIIT Hyderabad	India	deva@iiit.ac.in
Prof	Addy	Pross	Ben Gurion University	Israel	addy.pross@gmail.com
Mr	Josh	Pryor	University of New England	Australia	jpryor5@myune.edu.au
Prof	Leo	Radom	The University of Sydney	Australia	radom@chem.usyd.edu.au
Prof	Krishnan	Raghavachari	Indiana University	USA	kraghava@indiana.edu
Dr	Manussada	Ratanasak	Hokkaido University	Japan	manussada@cat.hokudai.ac.jp
Mr	Madhuranga	Rathnayake	The University of Sydney	Australia	prat8656@uni.sydney.edu.au
Prof	Jeff	Reimers	Shanghai University and UTS	Australia	jeffrey.reimers@uts.edu.au
Mr	Michael	Robinson	Monash University	Australia	michael.robinson1@monash.edu
Mr	Fergus	Rogers	Australian National University	Australia	u5356225@anu.edu.au
Dr	Tanglaw	Roman	The University of Queensland	Australia	tanglaw@romanmail.net
Miss	Ras Baizureen	Roseli	The University of Queensland	Australia	r.roseli@uqconnect.edu.au
Dr	Ivan	Rostov	NCI	Australia	ivan.rostov@anu.edu.au
Mr	Keiran	Rowell	The University of New South Wales	Australia	k.rowell@unsw.edu.au
Mr	Charlie	Ruffman	University of Otago	New Zealand	charlieruffman@gmail.com
Dr	Thanyada	Rungrotmongkol	Chulalongkorn University	Thailand	t.rungrotmongkol@gmail.com
Dr	Masaaki	Saitow	Nagoya University	Japan	masa.saitow@chem.nagoya-u.ac.jp
Dr/Prof	Shigeyoshi	Sakaki	Kyoto University	Japan	sakaki.shigeyoshi.47e@st.kyoto-u.ac.jp
Dr	Matthew	Sale	The University of Sydney	Australia	msal4559@sydney.edu.au
Prof	WMC	Sameera	Hokkaido University	Japan	wmcsameera@lowtem.hokudai.ac.jp
Miss	Isolde	Sandler	The University of New South Wales	Australia	i.sandler@student.unsw.edu.au
Prof	Hirofumi	Sato	Kyoto University	Japan	hirofumi@moleng.kyoto-u.ac.jp
Prof	Henry	Schaefer	University of Georgia	USA	ccq@uga.edu
Prof	Timothy	Schmidt	The University of New South Wales	Australia	timothy.schmidt@unsw.edu.au
Prof	Peter	Schwerdtfeger	Massey University	New Zealand	p.a.schwerdtfeger@massey.ac.nz
Prof	Gustavo	Scuseria	Rice University	USA	guscus@rice.edu
Ms	Zoe	Seeger	Monash University	Australia	zoe.seeger@monash.edu
Dr	Junji	Seino	Waseda University	Japan	j.seino@aoni.waseda.jp
Mr	Takafumi	Shiraogawa	The Graduate University for Advanced Studies	Japan	shiraogawa@ims.ac.jp
Prof	Zhigang	Shuai	Tsinghua University	China	zgshuai@tsinghua.edu.cn
Prof	Eunji	Sim	Yonsei University	South Korea	esim@yonsei.ac.kr
Mrs	Catherine	Simpson	Australian National University	Australia	catherine.simpson@anu.edu.au
Mr	Abhishek	Singh	Monash University	Australia	abhishek.singh@monash.edu
Miss	Sukriti	Singh	Indian Institute of Technology Bombay	India	sukriti243@gmail.com
Prof	Brian	Smith	La Trobe University	Australia	brian.smith@latrobe.edu.au
Prof	Sean	Smith	NCI	Australia	sean.smith@anu.edu.au
Dr	Alessandro	Soncini	University of Melbourne	Australia	asoncini@unimelb.edu.au

Dr	Aloysius	Soon	Yonsei University	South Korea	aloysius.soon@yonsei.ac.kr
A/Prof	Michelle	Spencer	RMIT University	Australia	michelle.spencer@rmit.edu.au
Dr	Peifeng	Su	Xiamen University	China	supi@xmu.edu.cn
Dr	Irene	Suarez-Martinez	Curtin University	Australia	I.Suarez-Martinez@curtin.edu.au
Prof	Jaeyoung	Sung	Center for Chemical Dynamics in Living Cells	South Korea	jaeyoung@cau.ac.kr
Prof	Raghavan B	Sunoj	Indian Institute of Technology Bombay	India	sunoj@chem.iitb.ac.in
Dr	Kimichi	Suzuki	Hokkaido University	Japan	ki_suzuki@eis.hokudai.ac.jp
Dr	Yuichi	Suzuki	Nagoya University	Japan	suzuki@ncube.human.nagoya-u.ac.jp
Miss	Anna	Syme	The University of New South Wales	Australia	anna.maree.syme@gmail.com
Prof	Masanori	Tachikawa	Yokohama City University	Japan	tachi@yokohama-cu.ac.jp
Dr	Hui-Chung	Tai	Institute of Biomedical Sciences, Academia Sinica	Taiwan	huichung.tai@gmail.com
Dr	Makito	Takagi	Yokohama City University	Japan	mtakagi@yokohama-cu.ac.jp
Prof	Tatsuya	Takagi	Osaka University	Japan	ttakagi@phs.osaka-u.ac.jp
Dr	Kaito	Takahashi	IAMS Academia Sinica	Taiwan	kt@gate.sinica.edu.tw
Prof	Kazuo	Takatsuka	Kyoto University	Japan	kaztak@fukui.kyoto-u.ac.jp
Mr	Masato	Takenaka	Hokkaido University	Japan	s02122020x@eis.hokudai.ac.jp
Prof	Tetsuya	Taketsugu	Hokkaido University	Japan	take@sci.hokudai.ac.jp
Dr	Margaret	Tan	Singapore University of Technology and Design	Singapore	margaret_tan@sutd.edu.sg
Mr	Patrick	Taylor	RMIT University	Australia	s3484746@student.rmit.edu.au
Prof	Seiichiro	Ten-no	Kobe University	Japan	tenno@garnet.kobe-u.ac.jp
Dr	Nevena	Todorova	RMIT University	Australia	nevena.todorova@rmit.edu.au
Dr	Takashi	Tsuchimochi	Kobe University	Japan	tsuchimochi@gmail.com
Mr	Yoshiaki	Tsunekawa	Hokkaido University	Japan	yoshi-tsune-j23@eis.hokudai.ac.jp
Mx	Ash	Turner	University of Wollongong	Australia	at076@uowmail.edu.au
Dr	Liviu	Ungur	National University of Singapore	Singapore	chmlu@nus.edu.sg
Mr	Hiroki	Uratani	Waseda University	Japan	uratani@suou.waseda.jp
Dr	Vladislav	Vassiliev	NCI	Australia	vvv900@nci.org.au
Mr	Rahul	Verma	Indian Institute of Technology Kanpur	India	vrahul@iitk.ac.in
Mr	Luigi	Villani	La Trobe University	Australia	llvillani@students.latrobe.edu.au
Miss	Simone	Waite	The University of Newcastle	Australia	simone.waite@uon.edu.au
Dr	Mark	Waller	Pending.AI	Australia	mark@pending.ai
Prof	Tiff	Walsh	Deakin University	Australia	tiffany.walsh@deakin.edu.au
Prof	Binju	Wang	Xiamen University	China	wangbinju2018@xmu.edu.cn
Dr	Chun-I	Wang	Academia Sinica	Taiwan	bradciwang@gmail.com
Prof	Feng	Wang	Swinburne University of Technology	Australia	fwang@swin.edu.au
Ms	Lily	Wang	Australian National University	Australia	lily.wang@anu.edu.au
Miss	Dominique	Wappett	The University of Melbourne	Australia	dwappett@student.unimelb.edu.au
Prof	Stacey	Wetmore	University of Lethbridge	Canada	stacey.wetmore@uleth.ca
Miss	Nicole	Wheatley	The University of Queensland	Australia	nicole.wheatley@uq.edu.au

Dr	Asaph	Widmer-Cooper	The University of Sydney	Australia	asaph.widmer-cooper@sydney.edu.au
A/Prof	David	Wilson	La Trobe University	Australia	david.wilson@latrobe.edu.au
Dr	Katie	Wilson	Australian National University	Australia	katie.wilson@anu.edu.au
Prof	Henryk A	Witek	National Chiao Tung University	Taiwan	hwitek@mail.nctu.edu.tw
Prof	Richard	Wong	National University of Singapore	Singapore	chmwmw@nus.edu.sg
Mr	Jared	Wood	The University of Sydney	Australia	jared.wood@sydney.edu.au
Prof	Wei	Wu	Xiamen University	China	weiwu@xmu.edu.cn
Prof	Yun-Dong	Wu	Peking University Shenzhen Graduate School	China	wuyd@pkusz.edu.cn
Mr	Luke	Wylie	Monash University	Australia	luke.wylie1@monash.edu
Mr	Longkun	Xu	Australian National University	Australia	Longkun.Xu@anu.edu.au
Prof	Xin	Xu	Fudan University	China	xxchem@fudan.edu.cn
Prof	Satoshi	Yabushita	Keio University	Japan	yabusita@chem.keio.ac.jp
Prof	Hideo	Yamakado	Wakayama University	Japan	yamakado@sys.wakayama-u.ac.jp
Dr	Kentaro	Yamamoto	Kyoto University	Japan	kyamamoto@fukui.kyoto-u.ac.jp
Prof	Hsiao-Ching	Yang	Fu Jen Catholic University	Taiwan	yanghc@gmail.com
Mr	Likun	Yang	Shanghai University	China	likun_yang@foxmail.com
Dr	Soujanya	Yarasi	CSIR-IICT	India	yarasi68@gmail.com
Dr	Takeshi	Yoshikawa	Waseda University	Japan	t.yoshikawa@aoni.waseda.jp
Prof	Kazunari	Yoshizawa	Kyushu University	Japan	kazunari@ms.ifoc.kyushu-u.ac.jp
Prof	Chin-Hui	Yu	National Tsing Hua University	Taiwan	chyu@mx.nthu.edu.tw
Dr	Haibo	Yu	University of Wollongong	Australia	hyu@uow.edu.au
Prof	Jen-Shiang Kenny	Yu	National Chiao Tung University	Taiwan	jsyu@mail.nctu.edu.tw
Dr	Jingxian	Yu	The University of Adelaide	Australia	jingxian.yu@adelaide.edu.au
Dr	Lijuan	Yu	Australian National University	Australia	lijuan.yu@anu.edu.au
Dr	Qinghong	Yuan	The University of Queensland	Australia	qinghong.yuan@uq.edu.au
Miss	Linxing	Zhang	Peking University Shenzhen Graduate School	China	zhanglinxing@pku.edu.cn
Prof	Jijun	Zhao	Dalian University of Technology	China	zhaojj@dlut.edu.cn
Prof	Yan	Zhao	Wuhan University Technology	China	yan2000@whut.edu.cn
Prof	Yi	Zhao	Xiamen University	China	yizhao@xmu.edu.cn
Dr	Xiuwen	Zhou	The University of Queensland	Australia	x.zhou6@uq.edu.au
Ms	Judy	Zhu	The University of Sydney	Australia	wzhu6669@uni.sydney.edu.au