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Foreword

RACI Awards 2017–19

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Another year has passed, and it is time to celebrate the medals, prizes, and lectureships awarded by the Royal Australian Chemical Institute (RACI) from 2017 to 2019. *Aust. J. Chem*. is pleased to publish this special issue authored by some of the award winners, who represent a broad cross-section of Australian chemistry.

Lars Goerigk (The University of Melbourne), winner of the 2017 RACI Physical Chemistry Division Lectureship, contributes an account with Nisha Mehta on 'A Trip to the Density Functional Theory (DFT) Zoo: Warnings and Recommendations for the User'. As the authors state, DFT calculations are very popular, but that does not imply accuracy! DFT is a confusing field for many users, and the purpose of the account is to provide a succinct overview and recommendations for the potential users.[1]

Irene Yarovsky (RMIT University, Melbourne) was the 2017 Physical Chemistry Division Medallist. Her account, co-authored with N. Todorova on the subject of the 'Enigma of Amyloid Forming Proteins: Insights from Molecular Simulations', investigates the effects of mutations and environment on the structure and aggregation propensity of several types of amyloidogenic peptides and proteins, including apolipoprotein C-II, insulin, amylin, and amyloid-β, using theoretical modelling as well as experimental studies in collaboration with several research groups.[2]

Curt Wentrup (The University of Queensland) was awarded the 2018 Leighton Memorial Medal for service to chemistry. He contributes an autobiographical account on high-energy molecules based on sulfur and/or nitrogen, which started with amateur rocket propellants at the age of 13 and progressed to the highly sensitive compounds nitrogen trichloride and fulminating gold. Further research on the inorganic and organic fulminates and the isomeric cyanates led to detailed investigations of reactive intermediates generated by flash vacuum pyrolysis or photolysis; in particular, nitrenes and carbenes derived from azides, diazo compounds, triazoles, and tetrazoles and characterised in low temperature matrices.[3]

Georgina Such (The University of Melbourne) received the Polymer Division's 2018 David Sangster Polymer Science and Technology Achievement Award. In an account with Angus P. R. Johnston on 'Understanding Cell Interactions Using Modular Nanoparticle Libraries', the potential of nanoparticle systems to deliver novel therapeutics, such as proteins, DNA or small molecules is outlined. The article discusses how nanoparticle structure can be tuned to optimise biological interactions and in particular to control cell targeting and trafficking within a cell.[4]

Neeraj Sharma (University of New South Wales) received the 2018 Rennie Memorial Medal and contributes a paper with Jimmy Wu on alkali-metal modified, layered lithium transition metal oxides of the types used in lithium ion batteries, viz. $Li(Ni_{0.33}Mn_{0.33}Co_{0.33})O_2$. It is shown that the larger alkali atoms do not dope onto the Li sites, but instead are likely to be distributed on the surface of the particles.[5]

Amir Karton (The University of Western Australia) is the recipient of the 2019 Physical Chemistry Division's Lectureship. His paper on the thermochemistry of guanine tautomers uses high-level CCSD(T) composite *ab initio* methods to obtain accurate tautomerisation energies for 14 guanine tautomers. The highly accurate W1-F12 computational method found that the five most stable guanine tautomers exist within an energy range of less than 1 kcal mol^{-1} in the gas phase.[6]

Jason Dutton (La Trobe University) received the Organometallic Chemistry Award for 2018. His paper on the elimination of ethene from 1,2-diiodoethane induced by N-heterocyclic carbenes (NHCs) reveals a new type of reaction between NHCs and alkyl halides, whereby the reaction of 1,2-diiodoethane with the NHCs unexpectedly generated a 2-iodoimidazolium salt and

Curt Wentrup was educated at the University of Copenhagen (Cand. Scient. 1966 with K. A. Jensen; D.Sc. 1976) and the Australian National University (Ph.D. 1969 with W. D. Crow). After post-doctoral periods with Hans Dahn (Lausanne), W. M. Jones (Gainesville, FL) and Maitland Jones, Jr (Princeton, NJ), he held academic positions at the Université de Lausanne, Switzerland, and a professorship at the Universität Marburg, Germany (1976–85), before returning to Australia in 1985 as Professor and Chair of Organic Chemistry and Head of the Organic Chemistry Section at the University of Queensland, where he is now Emeritus Professor. He is a Fellow of the Australian Academy of Science, a recipient of the Centenary Medal of the Australian Commonwealth (2003), the David Craig Medal of the Australian Academy of Science (2014), the A. J. Birch Medal (2014) and the Leighton Medal (2018) of the Royal Australian Chemical Institute, and an honorary doctorate from the Université de Pau, France (2014). He collaborates intensely with research groups in France, Germany, Japan, and China on experimental and theoretical investigations of reactive intermediates using flash vacuum pyrolysis, matrix isolation, and matrix photochemistry.

ethylene. Halogen bonding was found to be the source of this novel interaction.[7]

Yuning Hong (La Trobe University) was awarded the Rita Cornforth Lectureship 2018, which consists of a medal and a travel award. She presents a paper motivated by the need to produce selective biosensors for use in portable devices for personal health monitoring. A simple biosensing strategy based on the combination of a cationic AIEgen, TPE-2+, with aptamer for specific protein detection is reported. Here, the target protein displaces the dye molecules on the dye-aptamer complex, resulting in changes in a fluorescence signal.[8]

Michelle Coote (Australian National University) received the Physical Chemistry Division Medal for 2019. In a paper with Nicholas S. Hill, she reports time-dependent DFT calculations on an acetophenone-type photoinitiator, in which three strategies for red-shifting are compared, viz. the use of internal electric fields, Lewis acids, and increasing conjugation. Internal electric fields were shown to provide the best target for manipulation of specific excited states.[9]

Simone Ciampi (Curtin University) was awarded the A. M. Bond Medal in electrochemistry for 2017. In a paper with Jinyang Zhang, he describes the position of solid carbon dioxide in the triboelectric series. The background for this research is based on the fact that releasing solid carbon dioxide from a fire extinguisher causes a strong build-up of static electricity on the plastic discharge horn, sometimes resulting in an electric shock. Using Faraday pail measurements, it is shown that non-conductive polymers gain a net static charge when brought in and out of contact with dry ice, and the results suggest a position of solid CO_2 between PMMA and PVC in the triboelectric series.[10]

Brendan Wilkinson (University of New England) received the 2017 Beckwith Lectureship of the Organic Division. His paper reports on the glass transition behaviour, membrane permeability, and ice recrystallisation inhibition of octyl (thio)glycosides. The membrane permeability revealed cellular uptake relevant to the inhibition of intracellular ice formation, thereby presenting a promising lead for further biophysical and cryopreservation studies.[11]

Angie Jarrad was awarded the Graham Johnston Best Thesis Award 2018 for her PhD dissertation at The University of Queensland. Currently an Alexander von Humboldt Fellow at the Helmholtz Centre for Infection Research in Germany, she contributes a Focus article on ATP-firefly bioluminescence-based detection of ATP. Adenosine triphosphate-bioluminescence occurs through a multistep reaction between firefly luciferase, ATP, a magnesium salt, and oxygen. Briefly, luciferyl adenylate is first formed from luciferin and Mg^{2+}-ATP. The luciferyl adenylate is then oxidised with molecular oxygen to form a dioxetanone. Cleavage of the dioxetanone with CO_2 elimination produces an electronically excited state of oxyluciferin, and the return of this state to the ground state occurs with emission of visible light.[12]

Angus Olding (University of Tasmania) received the Masson Memorial Scholarship for 2018, which is awarded to young researchers to allow them to continue their research studies. In a focus article with Curtis C. Ho, recent applications of the versatile Zhdankin oxidising reagent (1 azido-1,2-benziodoxol-3(1*H*)-one) in organic synthesis, including azidotrifluoromethoxylations, aminoazidations, and C–H azidations, are summarised. Use in photoredox reactions allows the generation of radicals under particularly mild conditions. The reagent is frequently employed in tandem with a metal catalyst like copper or iron. It is expected that the reagent will continue to find new applications.[13]

Conflicts of Interest

The author declares no conflicts of interest.

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