

## RACI and AAS Awards 2018–2020

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We are pleased to present a new collection of papers authored by the recipients of awards, citations, and medals of the Royal Australian Chemical Society and the Australian Academy of Science.

Lars Goerigk and co-author Marcos Casanova-Paéz (University of Melbourne) start out with an account, ‘The Trip to the Density Functional Theory Zoo Continues: Making a Case for Time-Dependent Double Hybrids for Excited-State Problems’,<sup>[1]</sup> which is written for the general users of time-dependent (TD) density functional theory (DFT). It is written in a way that also makes it useful for scientists who have little prior knowledge in the area. As such, it contains an overview of conventional TD-DFT approaches and advice on their use in organic chemistry based on the authors’ own experience. More importantly, the authors provide an in-depth review of TD double-hybrid functionals, where their group has been the main driver in recent years. This method provides unprecedented robustness for a variety of electronic excitation events and does not suffer from the production of artificial ghost-states, which often occur in other DFT approaches.

Jonathan Baell, from the Monash Institute of Pharmaceutical Science, contributes ‘Personal Accounts of Australian Drug Discovery at the Public–Private Interface’,<sup>[2]</sup> starting with his Honours work at the University of Tasmania under the supervision of John Bremner and Elaine Browne and followed by PhD studies with Peter Andrews and Paul Alewood at the then Victorian College of Pharmacy. This is a highly readable account of how it was to be a PhD student in the days of much freer management. It is also a highly interesting account of the development of pharmaceutical chemistry in Australia – a process that is still ongoing and hopefully will continue for a long time.

Joanne Jamie (Macquarie University) presents an account on the ‘Macquarie–Yaegl Partnership: Community Capability Strengthening Through Western and Indigenous Science’.<sup>[3]</sup> The Macquarie–Yaegl partnership commenced as a bush

medicine research project. It has been the catalyst for positive cultural change and educational outcomes to the benefit of Australian aboriginal people. Jamie emphasises that it is possible for chemists to collaborate with the indigenous communities and achieve satisfying research as well as societal benefits. The program promotes the scientific education of Australian aboriginal youth.

Paul V. Bernhardt and co-workers Jessica K. Bilyj and Jeffrey R. Harmer (University of Queensland)<sup>[4]</sup> report on ‘Copper Complexes of Benzoylacetone bis-Thiosemicarbazones: Metal and Ligand Based Redox Reactivity’. These complexes exhibit complex and unusual chemistry, which includes the stabilisation of Cu<sup>III</sup> in a dimeric product of ligand oxidation. UV-vis and EPR spectroscopies, cyclic voltammetry, and X-ray structure analysis are reported. The data indicate a symmetrical 5-6-5 chelate ring binding mode in these Cu complexes.

Frances Separovic (University of Melbourne) and co-workers Frederick Backler, Marc Antoine Sani, Vladislav Vasilyev, and Feng Wang at Swinburne University of Technology and ANU report a study on the ‘NMR Chemical Shift and Methylation of 4-Nitroimidazole: Experiment and Theory’. Although nitroimidazoles are pharmaceutically important, detailed NMR studies have surprisingly not been available previously. Now, comprehensive <sup>13</sup>C and <sup>15</sup>N NMR data for the solid state and solution are reported for two 4-nitroimidazoles. The experimental results are analysed with the aid of DFT calculations.<sup>[5]</sup>

Graeme Moad and colleagues Caroline Bray, Guoxin Li, Almar Postma, Lisa T. Strover, and Jade Wang at CSIRO Manufacturing, Clayton, describe the ‘Initiation of RAFT Polymerization: Electrochemically-Initiated RAFT Polymerization in Emulsion (Emulsion eRAFT), and Direct PhotoRAFT Polymerization of Liquid Crystalline Monomers’,<sup>[6]</sup> namely the electrochemically initiated emulsion RAFT (eRAFT) polymerisation process, which provides rapid polymerisation of styrene at ambient temperature without the use of surfactants, and the



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), a junior position at the Université de Lausanne, and a professorship at the Universität Marburg, he returned to Australia in 1985 as Professor and Chair of Organic Chemistry and Head of the Organic Chemistry Section at the University of Queensland. Now an emeritus professor, he is a Fellow of the Australian Academy of Science, and a recipient of the Centenary Medal of the Australian Commonwealth, the David Craig Medal of the Australian Academy of Science, the Arthur J. Birch and Leighton Medals of the RACI, and a Dr. h.c. from the Université de Pau, France. He works in the area of historical chemistry as well as reactive intermediates, flash vacuum pyrolysis, photochemistry, and computational chemistry.

direct photoinitiated RAFT polymerisation, which provides an effective route to high purity side chain liquid crystalline polymers at high monomer conversion with low molar mass dispersity. The optimisation of polymerisation conditions benefited from numerical simulations. Interestingly, the authors note that there have been few commercial success stories associated with RAFT, but since the first RAFT patents are now expiring, an upsurge in commercial applications may be forthcoming.

Bernard L. Flynn and Shuqi Chen at the Monash Institute of Pharmaceutical Sciences present a research paper on ‘Iodocyclisation of Electronically Resistant Alkynes: Synthesis of 2-Carboxy(and sulfoxy)-3-iodobenzo[*b*]thiophenes’.<sup>[7]</sup> The intramolecular iodocyclisation of alkynes bearing tethered nucleophiles was found to be a highly effective method for the construction of novel heterocyclic compounds. The so-called ‘umpolung’-alkynes are electronically predisposed towards addition reactions rather than cyclisations. This problem was overcome in the construction of 2-carboxy- and 2-sulfoxy-3-iodobenzo[*b*]thiophenes (but not the corresponding benzo[*b*]

furans and indoles) in *5-endo-dig* iodocyclisations of such alkynes. Further iodocyclisations generating lactones and pyridines are also described.

### Conflicts of Interest

The author declares no conflicts of interest.

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