

Brief Curriculum Vitae - Jason Brian Harper

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Professional Experience

- 2002 - Lecturer (2002-2007), Senior Lecturer (2007-2015) and Associate Professor (2016-),
School of Chemistry, University of New South Wales
(Visiting Positions at Queen's University, Belfast (2002/3), Australian National University
(2004), University of Melbourne (2004/5), Boston College (2009), Western Sydney University
(2021-), KTH Stockholm (2022-))
- 2000-2002 National Health and Medical Research Council C. J. Martin Postdoctoral Research Fellow,
University Chemical Laboratory, University of Cambridge (with Prof. Anthony J. Kirby)
- 2001 Associate Lecturer, The Open University in East Anglia

Education

- 2000 Ph.D., Australian National University (with Prof. Christopher J. Easton)
- 1996 B.Sc.(Hons), Australian National University
- 1995 B.Sc., University of Adelaide

Research Record

- Total publications: 142 (including 136 journal articles and 6 book chapters) – see final page.
- Total citations: 5300+ (Google Scholar)
- H-index: 40 (Google Scholar)
- Received >\$1M direct research funding and >\$1.5M infrastructure funding (ARC, UNSW)
- Supervised 24 Ph.D., 40 Honours and 30 undergraduate project students
[Twice awarded UNSW ARC Postgraduate Council Award for Excellence in Postgraduate Supervision.]
- Presented >80 Invited lectures; students have given >225 presentations (>50% orals)

Research Interests

- Understanding and predicting the outcome of processes in ionic liquids.
- Correlating structure, acidity and reactivity, particularly with respect to *N*-heterocyclic carbenes and polycyclic aromatic hydrocarbons.
- Developing novel methods, particularly using NMR spectroscopy, for following reaction outcomes.
- Applications of physical organic chemistry in the broader perspective – from tree rings to tribology!

Education and Curriculum Development

Curriculum design and leadership

- Lead and coordinated teaching changes through the pandemic era of 2020.
- Overarching responsibility for transition of School of Chemistry, UNSW, courses from semester to trimester teaching schedules. Involved both content curation across all levels and articulation for all courses in the major, along with managing client School requirements.
- Prepared School for accreditation through Royal Australian Chemical Institute, particularly noting change to threshold learning outcome model.

Experienced course developer and convenor

- Taught, developed, and convened courses from introductory to graduate level across, in general, discipline (organic, physical, analytical), service (engineering, food chemistry) and specialist (physical organic) courses.
- Continuously updated and modified courses to ensure currency. Developed new courses (average one every 2-3 years) as per requirements of School.
- Developed and formalised undergraduate research project courses as a pathway to honours and graduate programmes; part of a long term goal of incorporating research in undergraduate teaching.

Professional Activities

Leadership positions

- Deputy Head of School, School of Chemistry, UNSW (2021-); responsible for workload management and assisting the Head in areas such as appointments, financial matters, School policy, *etc.*
- Deputy Director (2011-2015) and Director (2015-2020) of Teaching, School of Chemistry, UNSW (received Dean of Science Education Excellence Award for the latter, 2020). Responsible for teaching allocation and management, including conversion from semester to trimester models, and pandemic response.
- Deputy Director (2011-2012) and Director (2013-2016). Faculty of Science Talented Students Programme, UNSW. Established new programme that saw the top 10% of each B.Sc. cohort engage with researchers from the first year of their degree.

Editorial Positions

- Editor, *Chemical Physics* (2022-)
- Serial Co-Editor, *Advances in Physical Organic Chemistry* (2022-)
- Advisory Board, *Organic and Biomolecular Chemistry* (2023-), *ChemPlusChem* (2020-) and *Targets in Heterocyclic Synthesis* (2015-)
- Guest Editor, *Physical Chemistry Chemical Physics* and *Organic and Biomolecular Chemistry* web based thematic issue (Non-Traditional Solvent Effects in Organic Reactions, 2021) and *Journal of Organic Chemistry* (Solvation effects in organic chemistry, 2022)

Conference Organisation

- Co-chair, 23rd IUPAC Conference on Physical Organic Chemistry, Sydney, 2016
- Organising Committee, 6th Australasian Symposium on Ionic Liquids / 4th Asia-Pacific Symposium on Ionic Liquids, Sydney, 2014, and 10th Australasian Symposium on Ionic Liquids, Melbourne, 2022.
- Organising Committee, Conference on Ionic Liquids (COIL-10), Perth, 2025
- Treasurer (2003-), President (2020-2022), Southern Highlands Conference on Heterocyclic Chemistry

Standards and Representation

- Titular Member (2020-2023), Task Group Leader (2020-) and Associate Member (2018-2019), Division III (Organic), International Union of Pure and Applied Chemistry (IUPAC)
- Member, IUPAC Subcommittee on Structural and Mechanistic Chemistry (2017-)
- Member, National Accreditation Committee of the Royal Australian Chemical Institute (2015-)
- Fellow, Royal Australian Chemical Institute; Member, American Chemical Society; Member, Royal Society of Chemistry

Publications (last four years (2020-), most recent first, remainder available on request)

Journal Articles

- 136) Paporakis, S.; Liu, K. T.-C.; Brown, S.; Harper, J. B.; Martin, A. V.*; Greaves, T. L.*; “Thermal stability of protic ionic liquids”, *Journal of Physical Chemistry B*, submitted.
- 135) Doak, B. C.; Whitehouse, R. L.; Rimmer, K.; Williams, M.; Heras, B.; Caria, S.; Ilyichova, O.; Vazirani, M.; Mohanty, B.; Harper, J. B.; Scanlon, M. J.*; Simpson, J. S.: "Fluoromethylketone-fragment conjugates designed as covalent modifiers of EcDsbA are atypical substrate", *ChemMedChem*, **2024**, *in press*.
- 134) Hsieh, A. Y.; Haines, R. S.; Harper, J. B.*: “The effects of ionic liquids on the nucleofugality of bromide”, *Journal of Organic Chemistry*, **2024**, *in press*.
- 133) Hsieh, A. Y.; Haines, R. S.; Harper, J. B.*: “The effects of ionic liquids on the ethanolysis of a chloroaceneaphthene. Evaluation of the effectiveness of nucleofugality data to predict reaction outcome”, *RSC Advances*, **2023**, *13*, 21036-21043. doi: 10.1039/d3ra04302a

- 132) Morris, D. C.; Morris, A. R.; Price, W. S.; Prescott, S. W.*; Harper, J. B.*: “Diffusion measurements to understand dynamics and structuring in solutions involving a homologous series of ionic liquids”, *ChemPhysChem*, **2023**, e202300015. doi: 10.1002/cphc.202300015
- 131) Rohlmann, P.; Black, J. J.; Watanabe, S.; Leckner, J.; Shimpi, M. R.; Rutland, M. W.*; Harper, J. B.*; Glavatskih, S.*: “Tribochemistry of imidazolium and phosphonium bis(oxalato)borate ionic liquids: understanding the differences”, *Tribology International*, **2023**, *181*, 108263. doi: 10.1016/j.triboint.2023.108263
- 130) Barnett, C. D.*; Cole, M. L.; Harper, J. B.*: “The core difference between a mesoionic and a normal *N*-heterocyclic carbene”, *ACS Omega*, **2022**, *7*, 34657-34664. doi: 10.1021/acsomega.2c04682
- 129) Chen, J.; Harper, J. B.; Ho, J.*: “Improving the Accuracy of QM/MM Models with Polarised Fragment Charges”, *Journal of Chemical Theory and Computation*, **2022**, *18*, 5607-5617. doi: 10.1021/acs.jctc.2c00491
- 128) Hagen, M. L.; Harper, J. B.; Croft, A. K.*: “Recent Advances in Use of Ionic liquids as Solvents for Protein-based Materials and Chemistry”, *Current Opinion in Green and Sustainable Chemistry*, **2022**, *36*, 100637. doi: 10.1016/j.cogsc.2022.100637
- 127) Doak, B. C.; Whitehouse, R. L.; Rimmer, K.; Williams, M.; Heras, B.; Caria, S.; Ilyichova, O.; Vazirani, M.; Mohanty, B.; Harper, J. B.; Scanlon, M. J.*; Simpson, J. S.: "Fluoromethylketone-fragment conjugates designed as covalent modifiers of *EcDsbA* are atypical substrate", *ChemRxiv*, doi: 10.26434/chemrxiv-2022-2621h
- 126) Barnett, C.*; Harper, J. B.* ; Cole, M. L.: “Correlating electronic properties of *N*-heterocyclic carbenes with structure, and the implications of using different probes”, *ChemistrySelect*, **2022**, *7*, e202104348. doi: 10.1002/slct.202104348
- 125) Coney, M. D.; Morris, D. C.; Gilbert, A.; Prescott, S. W.; Haines, R. S.; Harper, J. B.*: “Effects of ionic liquids on the nucleofugality of chloride”, *Journal of Organic Chemistry*, **2022**, *87*, 1767-1779. doi: 10.1021/acs.joc.1c02043
- 124) Wang, J. E.; Gilbert, A.; Harper, J. B.*; Kim, D. J.: “Understanding the failure mechanism of rechargeable aluminum batteries: Metal anode perspective through X-ray tomography”, *Advanced Energy and Sustainability Research*, **2022**, *3*, 2100164. doi: 10.1002/aesr.202100164
- 123) Munavirov, B.; Black, J. J.; Shah, F. U.; Leckner, J.; Rutland, M. W.*; Harper, J. B.*; Glavatskih, S.*: "The effect of anion architecture on the lubrication chemistry of phosphonium orthoborate ionic liquids", *Scientific Reports*, **2021**, *11*, 24021. doi: 10.1038/s41598-021-02763-5.
- 122) Barnett, C.*; Cole, M. L.; Harper, J. B.*: “Steric properties of *N*-heterocyclic carbenes affect the performance of electronic probes”, *European Journal of Inorganic Chemistry*, **2021**, *47*, 4954-4958. doi: 10.1002/ejic.202100796
- 121) Chen, J.; Kato, J.; Harper, J. B.; Shao, Y.; Ho, J.*: “On the Accuracy of QM/MM Models. A Systematic Study of Intramolecular Proton Transfer Reactions of Amino Acids in Water” *Journal of Physical Chemistry B*, **2021**, *125*, 9304-9316. doi: 10.1021/acs.jpcc.1c04876.
- 120) Barnett, C.*; Cole, M. L.; Harper, J. B.*: “A dual NMR probe approach to understanding the electronic properties of *N*-heterocyclic carbenes”, *Chemistry – Methods*, **2021**, *1*, 374-381. doi: 10.1002/cmtd.202100043.¹
- 119) Rohlmann, P.; Watanabe, S.; Shimpi, M.; Leckner, J.; Rutland, M. W.; Harper, J. B.; Glavatskih, S.*: “Boundary lubricity of phosphonium bisoxalato borate ionic liquids”, *Tribology International*, **2021**, *161*, 107075. doi: 10.1016/j.triboint.2021.107075.
- 118) Gilbert, A.; Haines, R. S.; Harper, J. B.*: “The effects of using an ionic liquid as a solvent for a reaction that proceeds through a phenonium ion”, *Journal of Physical Organic Chemistry*, **2021**, *34*, e4217. [COVER ARTICLE] doi: 10.1002/poc.4217.³
- 117) Morris, D. C.; Prescott, S. W.*; Harper, J. B.*: “Rapid relaxation NMR measurements to predict rate coefficients in ionic liquid mixtures. An examination of reaction outcome changes in a homologous series of ionic liquids”, *Physical Chemistry Chemical Physics*, **2021**, *23*, 9878-9888. doi: 10.1039/d0cp06066f.

- 116) Greaves, T. L.*; Schaffarczyk McHale, K. S.; Burkart-Radke, R. F.; Harper, J. B.*; Le, T.*: "Machine learning approaches to understand and predict rate constants for organic processes in mixtures containing ionic liquids", *Physical Chemistry Chemical Physics*, **2021**, *23*, 2742-2752. doi: 10.1039/d0cp04227g.
- 115) Sandler, I.; Harper, J. B.; Ho, J.*: "Explanation of Substituent Effects on Enolization of β -Diketones and β -Ketoesters", *Journal of Chemical Education*, **2021**, *98*, 1043-1048. doi: 10.1021/acs.jchemed.0c01076.
- 114) Schindl, A.; Hawker, R. R.; Schaffarczyk McHale, K. S.; Liu, K. T.-C.; Morris, D. C.; Hsieh, A. Y.; Gilbert, A.; Prescott, S. W.; Haines, R. S.; Croft, A. K.*; Harper, J. B.*; Jäger, C. M.*: "Controlling the outcome of S_N2 reactions in ionic liquids: From rational data set design to predictive linear regression models", *Physical Chemistry Chemical Physics*, **2020**, *22*, 23009-23018. [SELECTED AS A HOT ARTICLE] doi: 10.1039/d0cp04224b.
- 113) Liu, K. T.-C.; Haines, R. S.; Harper, J. B.*: "The effect of bisimidazolium based ionic liquids on a bimolecular substitution process. Are two head(group)s better than one?", *Organic and Biomolecular Chemistry*, **2020**, *18*, 7388-7395. doi: 10.1039/d0ob01500h.
- 112) Gilbert, A.; Haines, R. S.; Harper, J. B.*: "Controlling the reactions of 1-bromogalactose acetate in methanol using ionic liquids as co-solvents", *Organic and Biomolecular Chemistry*, **2020**, *18*, 5442-5452. doi: 10.1039/d0ob01198c.
- 111) Konstandaras, N.; Dunn, M. H.; Luis, E. T.; Cole, M. L.; Harper, J. B.*: "The pK_a values of *N*-aryl imidazolium salts, their higher homologues, and formamidinium salts in dimethyl sulfoxide", *Organic and Biomolecular Chemistry*, **2020**, *18*, 1910-1917. doi: 10.1039/d0ob00036a.
- 110) Mallo, N.; Tron, A.; Andréasson, J.; Harper, J. B.; Jacob, L. S. D.; McClenaghan, N. D.; Jonusauskas, G.; Beves, J. E.*: "Hydrogen-bonding donor-acceptor Stenhouse adducts", *ChemPhotoChem*, **2020**, *4*, 407-412. doi: 10.1002/cptc.201900295.
- 109) Blake, S. A. P.*; Palmer, J. G.; Björklund, J.; Harper, J. B.; Tierney, C. S. M.: "Palaeoclimate potential of New Zealand *Manoao colensoi* (silver pine) tree rings using Blue-Intensity", *Dendrochronologia*, **2020**, *60*, Article 125644. doi: 10.1016/j.dendro.2020.125664.
- 108) Konstandaras, N.; Dunn, M. H.; Guerry, M. S.; Barnett, C. D.; Cole, M. L.; Harper, J. B.*: "The impact of cation structure upon the acidity of triazolium salts in dimethyl sulfoxide", *Organic and Biomolecular Chemistry*, **2020**, *18*, 66-75. doi: 10.1039/c9ob02258a.

Book Chapters

- 6) Harper, J. B.* Schaffarczyk McHale, K. S.: "Pyridines and their benzo derivatives: Structure" in *Comprehensive Heterocyclic Chemistry IV*, D. StC. Black, J. Cossy and C. V. Stevens, Eds.; Elsevier: Oxford, 2021; Vol. 7, pp 1-26. doi: 10.1016/B978-0-12-818655-8.00068-8 doi: 10.1016/B978-0-12-818655-8.00068-8.

Conference Proceedings

- 3) Leckner, J.*; Reddy, A. B.; Black, J. J.; Harper, J. B.; Glavatskih, S.: "Bevel gear grease case study continued – mechanism revealed", in *Proceedings of National Lubricating Greases Institute (NLGI) 90th Annual Meeting*, June 4-7, 2023, San Diego, California.

Other contributions

- 3) Burrows, C. J.*; Harper, J. B.*; Sander, W.; Tantillo, D. J.: "Solvation Effects in Organic Chemistry", *Journal of Organic Chemistry*, **2022**, *87*, 1599-1601. doi: 10.1021/acs.joc.1c03148
- 2) Harper, J. B.*; Kirchner, B.*; Pavez, P.*; Welton, T.*: "Non-traditional solvent effects in organic reactions", *Physical Chemistry Chemical Physics*, **2021**, *23*, 26028-26029. doi: 10.1039/d1cp90187g