

## Dr Robert Paton

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### Academic Positions

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2014 – present	Associate Professor in Organic Chemistry ( <i>with tenure</i> ) <ul style="list-style-type: none"><li>• Department of Chemistry, University of Oxford</li></ul>
2010 – 2014	University Lecturer in Organic Chemistry <ul style="list-style-type: none"><li>• Department of Chemistry, University of Oxford</li></ul>
2010 – present	Tutorial Fellow in Organic Chemistry <ul style="list-style-type: none"><li>• St Hilda's College, Oxford</li></ul>
2009 – 2012	Royal Commission for the Exhibition of 1851 Science Research Fellow
2009 – 2010	Fulbright UK-US Distinguished Research Scholar <ul style="list-style-type: none"><li>• University of California, Los Angeles with <i>Prof. K. N. Houk</i></li></ul>
2009	HPC-Europa Visiting Researcher, <ul style="list-style-type: none"><li>• ICIQ, Spain with Prof. Feliu Maseras</li></ul>
2007-2009	Junior Research Fellow ( <i>independent postdoctoral award</i> ) <ul style="list-style-type: none"><li>• St Catharine's College, Cambridge</li></ul>

### Education

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2005 – 2008	University of Cambridge, Department of Chemistry <ul style="list-style-type: none"><li>• PhD thesis supervised by <i>Prof. Jonathan M. Goodman</i>, "Computational Studies of Boron Mediated C-C Bond Formation"</li></ul>
2000 – 2004	Trinity Hall, University of Cambridge MA MSci Natural Sciences (Chemistry) 1st class degree, ranked top in the University University Rafael Prize in Organic Chemistry; Trinity Hall prize in Natural Sciences

### Awards and Honours

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2015	ACS COMP division Outstanding Junior Faculty Award
2015	RSC Harrison-Meldola Memorial Medal for " <i>pioneering work in using computation to understand reactivity and selectivity in organic and bio-organic chemistry allowing rational design in synthesis</i> "
2015	Thieme Chemistry Journal Awardee
2014	Silver Jubilee Award of the Molecular Graphics and Modelling Society for outstanding young researchers in the field
2014	Selected for ACS ORGN Division Young Academic Investigators Award Symposium, San Francisco
2014	Selected as the UK's representative for the EuChemS Young Investigator

Workshop, Cyprus

- 2013 Chemical Structure Association (CSA) Trust Grant for Early Career Researchers
- 2013 Selected by RSC to represent the UK at *Transatlantic Frontiers of Chemistry*, Kloster Seon, Germany
- 2009 Royal Commission of 1851 Science Research Fellowship – ca. 6 awarded yearly in the UK across all sciences
- 2009 Distinguished Fulbright–AstraZeneca Research Scholar – one awarded yearly in the UK across chemical and biological sciences
- 2008 UK's Head Mentor, 40th International Chemistry Olympiad, Budapest, Hungary
- 2008 Best Presentation, MGMS Young Modellers' Forum, London, UK
- 2007 Junior Research Fellowship, St Catharine's College, University of Cambridge
- 2006 ACS CINP Division Scholarship for Scientific Excellence, San Francisco, USA

## Publications

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### *Independent Career:*

- [73] "Structural and Stereoelectronic Insights into Oxygenase Catalyzed Formation of Ethylene from 2-Oxoglutarate" Zhang, Z.; Smart, T. J.; Choi, H.; Hardy, F.; Lohans, C. T.; Abboud, M. I.; Richardson, M. S. W.; Paton, R. S.; McDonough, M. A.; Schofield, C. J. *Proc. Nat. Acad. Sci.* **2017**, *accepted*.
- [72] "Enantioselective Silver and Amine Co-catalyzed Desymmetrizing Cycloisomerization of Alkyne-linked Cyclohexanones" Manzano, R.; Datta, S.; Paton\*, R. S.; Dixon, D. J. *Angew. Chem. Int. Ed.* **2017**, *accepted*.
- [71] "Phosphazene Catalyzed Addition to Electron-Deficient Alkynes: The Importance of Nonlinear Allenyl Intermediates upon Stereoselectivity" Simón, L.; Paton\*, R. S.; *J. Org. Chem.* **2017**, *article ASAP*.
- [70] "Dual Gold - Catalyzed Three - Component Reaction: Efficient Synthesis of Indene - Fused Esters, Acids, and Lactones through Gold Vinylidene Intermediates" Yu, C.; Ma, X.; Chen, B.; Tang, B.; Paton\*, R. S.; Zhang, G. *Eur. J. Org. Chem.* **2017**, *11*, 1561–1565.
- [69] "Divergent Photocyclization/1,4-Sigmatropic Rearrangements for the Synthesis of Sesquiterpenoid Derivatives" Gorobets, E.; Wong, N. E.; Paton, R. S.; Derksen, D. J. *Org. Lett.* **2017**, *19*, 484–487.
- [68] "Detailed Mechanistic Studies on Palladium-Catalyzed Selective C–H Olefination with Aliphatic Alkenes – A Significant Influence of Proton Shuttling" Deb, A.; Hazra, A.; Peng, Q.; Paton\*, R. S.; Maiti, D. *J. Am. Chem. Soc.* **2017**, *139*, 763–775.
- [67] "Correlating Reactivity and Selectivity to Cyclopentadienyl Ligand Properties in Rh(III)-Catalyzed C–H Activation Reactions — An Experimental and Computational Study" Piou, T.; Romanov-Michailidis, F.; Romanova-Michaelides, M.; Jackson, K. E.; Semakul, N.; Taggart, T. D.; Newell, B. S.; Rithner, C. D.; Paton\*, R. S.; Rovis, T. *J. Am. Chem. Soc.* **2017**, *39*, 1296–1310.
- [66] "Heptamethyl Indenyl (Ind\*) Enables Diastereoselective Benzamidation of Cyclopropenes via Rh(III)-Catalyzed C–H Activation", Semakul, N.; Jackson, K. E.; Paton\*, R. S. Rovis, T. *Chem. Sci.* **2017**, *8*, 1015–1020.
- [65] "Cation– $\pi$  interactions in CREBBP bromodomain inhibition: an electrostatic model for small-molecule binding affinity and selectivity" Cortopassi, W. A.; Kumar, K.; Paton\*, R. S. *Org. Biomol. Chem.* **2016**, *14*, 10926–10938.

[64] "A Counterion-Directed Approach to the Diels-Alder Paradigm: Cascade Synthesis of Tricyclic Fused Cyclopropanes" Kiss, E.; Campbell, C. D.; Driver, R. W.; Jolliffe, J. D.; Lang, R.; Sergieiva, T.; Okovytyy, S.; Paton\*, R. S.; Smith, M. D. *Angew. Chem. Int. Ed.* **2016**, *55*, 13813–13817.

[63] "Computing Organic Stereoselectivity – from Concepts to Quantitative Calculations and Predictions" Peng, Q.; Duarte, F. Paton\*, R. S. *Chem. Soc. Rev.* **2016**, *45*, 6093–6107.

- Emerging Investigators Issue (chosen for front cover)

[62] "Synthesis of Malhamensilipin A Exploiting Iterative Epoxidation/Chlorination: Experimental and Computational Analysis of Epoxide-Derived Chloronium Ions" Saska, J.; Lewis, W.; Paton\*, R. S. Denton, R. *Chem. Sci.* **2016**, *7*, 7040–7049.

[61] "Mechanisms of histone-modifying and reading enzymes: the role of the protein environment from a computational perspective" Cortopassi, W. A.; Kumar, K.; Duarte, F.; Pimentel, A. S.; Paton\*, R. S. *J. Mol. Graph. Model.* **2016**, *67*, 69–84.

[60] "Catalytic Control in Cyclizations: from Computational Mechanistic Understanding to Selectivity Prediction" Peng, Q.; Paton\*, R. S. *Acc. Chem. Res.* **2016**, *49*, 1042–1051.

[59] "Furan production from light oxygenates in HZSM-5" Kim, S.; Evans, T. J.; Mukarakate, C.; Bu, L.; Beckham, G. T.; Nimlos, M. R.; Paton, R. S.; Robichaud, D. J. *ACS Sustain. Chem. Eng.* **2016**, *4*, 2615–2623.

[58] "Investigations on Recyclization and Hydrolysis in Avibactam Mediated Serine  $\beta$ -Lactamase Inhibition" Choi, H.; Paton, R. S.; Park, H.; Schofield, C. J. *Org. Biomol. Chem.* **2016**, *14*, 4116–4128.

[57] "Unraveling Innate Substrate Control in Site-Selective Palladium-Catalyzed C–H Heterocycle Functionalization" Choi, H.; Min, M.; Peng, Q.; Kang, D.; Paton\*, R. S.; Hong, S. *Chem. Sci.* **2016**, *7*, 3900–3909.

[56] "Development of a True Transition State Force Field (TTSFF) from Quantum Mechanical Calculations" Madarász, A.; Berta, D.; Paton, R. S.; *J. Chem. Theor. Comput.* **2016**, *12*, 1833–1844.

[55] "DFT study on the enantioselectivity of spiroacetalization catalysed by an imidodiphosphoric acid catalyst: how confinement works" Simón, L.; Paton\*, R. S.; *Org. Biomol. Chem.* **2016**, *14*, 3031–3039.

- Rated by reviewers as a *Hot Article* and featured on journal front cover

[54] "Computational Ligand Design in Enantio- and Diastereoselective Ynamide [5+2] Cycloisomerizations" Straker, R.; Peng, Q.; Mekareeya, A.; Paton\*, R. S.; Anderson, E. A. *Nature Commun.* **2015**, *7*, 10109.

[53] "Dioxygen binding in the active site of histone demethylase JMJD2A and the role of protein environment" Cortopassi, W. E.; Simion, R.; Hornsby, C. E.; Costa Franca, T. C.; Paton\*, R. S. *Chem. Eur. J.* **2015**, *21*, 18983–18992.

- Rated by reviewers as a *Hot Paper* and featured on journal front cover

[52] " $\alpha$ - and  $\alpha'$ -Lithiation–Electrophile trapping of *N*-thiopivaloyl and *N*-*t*-butoxythiocarbonyl  $\alpha$ -substituted Azetidines: rationalisation of the regiodivergence using NMR and computation" Jackson, K. E.; Mortimer, C. L.; Odell, B.; McKenna, J. M.; Claridge, T. D. W.; Paton\*, R. S.; Hodgson, D. M. *J. Org. Chem.* **2015**, *80*, 9838–9846.

- Selected as a JOC Featured Article

[51] "Substrate-Controlled Asymmetric Total Syntheses of Microcladallenes A, B, and C Based on the

*Proposed Structures*” Sohn, T.-I.; Kim, D.; Paton, R. S. *Chem. Eur. J.* **2015**, *21*, 15988–15997.

- Rated by reviewers as a *Hot Paper* and featured on journal inside cover

[50] “*Role of Hydrogen Bonding Acceptors in Organo-Enamine Catalysis*” Han, J.; Zhichao Lu, Z.; Flach, A. L.; Paton\*, R. S.; Hammond, G. B.; Xu, B. *Chem. Eur. J.* **2015**, *21*, 11687–11691.

[49] “*Coordination Diversity in Hydrogen-Bonded Homoleptic Fluoride–Alcohol Complexes Modulates Reactivity*” Engle, K. M.; Pfeifer, L.; Pidgeon, G. W.; Giuffredi, G. T.; Thompson, A. L.; Paton, R. S.; Brown, J. M.; Gouverneur, V. *Chem. Sci.* **2015**, *6*, 5293–5302.

[48] “*Origins of asymmetric phosphazene organocatalysis: computations reveal a common mechanism for nitro- and phospho-aldol additions*” Simon, L.; Paton\*, R. S. *J. Org. Chem.* **2015**, *80*, 2756–2766.

[47] “*Ethanol Dehydration in HZSM-5 studied by Density Functional Theory: Evidence for a Concerted Processes*” Kim, S.; Robichaud, D. J.; Beckham, G. T.; Paton, R. S.; Nimlos, M. R. *J. Phys. Chem. A* **2015**, *119*, 3604–3614.

[46] “*Enantioselective Desymmetrization of Prochiral Cyclohexanones via Organocatalytic Intramolecular Michael Additions to  $\alpha,\beta$ -Unsaturated Esters*” Gammack-Yamagata, A. D.; Datta, S.; Jackson, K. E.; Stegbauer, L.; Paton\*, R. S.; Dixon, D. J. *Angew. Chem. Int. Ed.* **2015**, *127*, 4981–4985.

- Highlighted in *Synfacts*

[45] “*Thermal and Photochemical Mechanisms for Cyclobutane Formation in Bielschowskysin Biosynthesis*” Tang, B.; Simion, R.; Paton\*, R. S. *Synlett* **2015**, *26*, 501–507.

- Invited submission for Young Investigators Special Issue

[44] “*Small molecule inhibitors of bromodomain–acetyl-lysine interactions*” Brand, M.; Measures, A.; Wilson, B.; Cortopassi, W. A.; Alexander, R.; Hoss, M.; Hewings, D. S.; Paton, R. S.; Conway, S. J. *ACS Chem. Bio.* **2015**, *10*, 22–39.

[43] “*Catalytic Enantioselective Synthesis of Indanes via Cation-Directed 5-Endo-Trig Cyclization*” Johnston, C. P.; Kothari, A.; Sergeieva, T.; Okovytyy, S. I.; Jackson, K. E.; Paton\*, R. S.; Smith, M. D. *Nature Chem.* **2015**, *7*, 171–177.

- Subject of a *Synform* Feature Article and *ChemInform* Editor’s Choice

[42] “*A series of potent CREBBP bromodomain ligands reveals an induced fit pocket stabilized by a cation- $\pi$  interaction*” Rooney, T. P. C.; Filippakopoulos, P.; Fedorov, O.; Picaud, S.; Cortopassi, W.; Hay, D. A.; Martin, S.; Tumber, A.; Rogers, C. M.; Philpott, M.; Wang, M.; Thompson, A. L.; Heightman, T. D.; Pryde, D. C.; Cook, A.; Paton, R. S.; Müller-Knapp, S.; Knapp, S.; Brennan, P. E.; Conway, S. J. *Angew. Chem. Int. Ed.* **2014**, *126*, 26, 6240–6244.

[41] “*Cation-directed synthesis of pyrroloindolines and pyridoindolines via a hydrogen bond assisted isocyanide cyclization cascade*” Knipe, P. C.; Gredičak, M.; Cernijenko, A.; Paton\*, R. S.; Smith, M. D. *Chem. Eur. J.* **2014**, *11*, 3005–3009.

[40] “*Dissecting non-covalent interactions in oxazaborolidinium catalyzed cycloadditions of maleimides*” Paton\*, R. S.; *Org. Biomol. Chem.* **2014**, *12*, 1717–1720.

[39] “*Natural product biosynthesis: It’s all downhill from here*” Hornsby, C. E.; Paton\*, R. S. *Nature Chem.* **2014**, *6*, 88–89.

[38] “*Intramolecular Diels–Alder Reactions of Cycloalkenones: Stereoselectivity, Lewis Acid Influence, and Halogenation Effects*” Pham, H.; Paton\*, R. S.; Ross, A. G.; Danishefsky, S. J.; Houk, K. N. *J. Am. Chem. Soc.*

2014, 136, 2397–2403.

[37] “*Ligand Bite Angle-dependent Palladium-catalyzed Cyclization of Propargylic Carbonates to 2-Alkynyl Azacycles or Cyclic Dienamides*” Daniels, D. S. B.; Jones, A. S.; Thompson, A. L.; Paton\*, R. S.; Anderson, E. A. *Angew. Chem. Int. Ed.* **2014**, 53, 1915–1920.

[36] “*Quantum mechanical calculations suggest that lytic polysaccharide monoxygenases employ a copper-oxygen rebound mechanism*” Kim, S.; Sandgren, M.; Paton\*, R. S.; Beckham G. T. *Proc. Nat. Acad. Sci.* **2014**, 111, 149–154.

[35] “*A mechanistic investigation of acid-catalyzed cleavage of aryl-ether linkages: Implications for lignin depolymerization in acidic environments*” Sturgeon, M. R.; Kim, S.; Lawrence, K.; Paton, R. S.; Chmely, S. C.; Nimlos, M. R.; Foust, T. D.; Beckham G. T. *ACS Sustain. Chem. Eng.* **2014**, 2, 472–485.

[34] “*Asymmetric Total Synthesis of (+)-Bermudenynol, a C15 Laurencia Metabolite with a Vinyl Chloride-Containing Oxocene Skeleton, via Intramolecular Amide Enolate Alkylation*” Kim, G.; Sohn, T.-I.; Kim, D.; Paton, R. S. *Angew. Chem. Int. Ed.* **2014**, 53, 272–276.

- Highlighted in *Synfacts*

[33] “*Diels-Alder Reactivities of Strained and Unstrained Cycloalkenes with Normal and Inverse-Electron-Demand Dienes: Activation Barriers and Distortion/Interaction Analysis*” Liu, F.; Paton, R. S.; Kim, S.; Liang, Y.; Houk, K. N. *J. Am. Chem. Soc.* **2013**, 135, 15642–15649.

[32] “*Mechanistic investigations on the enantioselective Conia-ene reaction catalyzed by cinchona-derived amino urea pre-catalysts and Cu(I)*” Sladojevich, F.; Fuentes de Arriba, A. L.; Yang, T.; Ferrali, A.; Paton\*, R. S.; Dixon, D. J. *Chem. Eur. J.* **2013**, 19, 14286–14295.

[31] “*Structure Reassignment of Laurefurenynes A and B by Computation and Total Synthesis*” Shepherd, D. J.; Broadwith, P. A.; Dyson, B. S.; Paton\*, R. S.; Burton, J. W. *Chem. Eur. J.* **2013**, 19, 12644–12648.

- Featured on the Computational Chemistry Highlights blog

[30] “*Rapid Cross Metathesis for Protein Modifications via Chemical Access to Se-Allyl Selenocysteine in Proteins*” Lin, Y. A.; Boutureira, O.; Lercher, L.; Bhushan, B.; Paton, R. S.; Davis, B. G. *J. Am. Chem. Soc.* **2013**, 135, 12156–12159.

[29] “*Computational Organic Chemistry*” Jackson, K.; Jaffar, S.; Paton\*, R. S. *Annu. Rep. Prog. Chem., Sect. B*, **2013**, 109, 235–255.

[28] “*Mechanistic Study of a Ru-Xantphos Catalyst for Tandem Alcohol Dehydrogenation and Reductive Aryl-Ether Cleavage*” Chmely, S. C.; Kim, S. C.; Ciesielski, P. N.; Jiménez-Osés, G.; Paton\*, R. S.; Beckham, G. T. *ACS Catalysis* **2013**, 3, 963–974.

[27] “*Enhanced Reactivity in Dioxirane C-H Oxidations via Strain Release: A Computational and Experimental Study*” Zhou, L.; Paton\*, R. S.; Eschenmoser, A.; Newhouse, T. R.; Baran, P. S.; Houk, K. N. *J. Org. Chem.* **2013**, 78, 4037–4048.

[26] “*C-Alkylation of Chiral Tropane- and Homotropene-Derived Enamines*” Hodgson, D. M.; Charlton, A.; Paton\*, R. S.; Thompson, A. S. *J. Org. Chem.* **2013**, 8, 1508–1518.

[25] “*Synthesis of Cyclic  $\alpha$ -Aminophosphonates through Copper Catalyzed Enamine Activation*” Han, J.; Paton, R. S.; Xu, B.; Hammond, G. B. *Synthesis* **2013**, 45, 463–470.

[24] “*Concise Substrate-Controlled Asymmetric Total Syntheses of Dioxabicyclic Marine Natural Products with 2,10-Dioxabicyclo-[7.3.0]dodecene and 2,9-Dioxabicyclo[6.3.0]undecene Skeletons*” Kim, M. J.; Sohn,

T.-I.; Kim, D.; Paton, R. S.; *J. Am. Chem. Soc.* **2012**, *34*, 20178–20188.

[23] “Dinuclear Palladium Complexes – Precursors or Catalysts?” Paton\*, R. S.; Brown, J. M. *Angew. Chem. Int. Ed.* **2012**, *51*, 10448–10450.

[22] “Enzymatic Catalysis of Anti-Baldwin Ring-Closure in Polyether Biosynthesis” Hotta, K.; Chen, X.; Paton, R. S.; Minami, A.; Li, H. Swaminathan, K. T.; Mathews, I. I.; Watanabe, K.; Oikawa, H.; Houk, K. N.; Kim, C. Y. *Nature* **2012**, *483*, 355–358.

- Highlighted by *C&EN* and *ScienceDaily*, given the highest recommendation by *Faculty of 1000*.

[21] “An Efficient Computational Model to Predict the Synthetic Utility of Heterocyclic Arynes” Goetz, A. E.; Bronner, S. M.; Cisneros, J.; Melamed, J.; Paton\*, R. S.; Houk, K. N.; Garg, N. K. *Angew. Chem. Int. Ed.* **2012**, *51*, 2758–2762.

[20] “Unusual Base-Induced Rearrangement of *exo*-9-Oxabicyclo[4.2.1]non-7-ene Oxide to *exo*-8-Hydroxybicyclo[3.3.0]octan-2-one” Hodgson, D. M.; Stent, M. A. H.; Paton, R. S.; Wilson, F. X. *Heterocycles (Albert Padwa Birthday Issue)* **2012**, *84*, 625–635.

[19] “Computational Study of Bond Dissociation Enthalpies for a Large Range of Native and Modified Lignins” Kim, S.; Chmely, S. C.; Nimlos, M. R.; Bomble, Y. J.; Foust, T. D.; Paton, R. S.; Beckham, G. T. *J. Phys. Chem. Lett.* **2011**, *2*, 2846–2852.

[18] “A stereoselective total synthesis of ( $\pm$ )-tormesol” Kim, H.; Bae, H.; Kim, S.; Kim, D.; Lee, D.; Paton, R. S. *Tetrahedron (Gilbert Stork Special Issue)* **2011**, *67*, 10017–10025.

[17] “Experimental Diels–Alder Reactivities of Cycloalkenones and Cyclic Dienes Explained Through Transition State Distortion Energies” Paton\*, R. S.; Kim, S.; Ross, A. G.; Danishefsky, S. J.; Houk, K. N. *Angew. Chem. Int. Ed.* **2011**, *50*, 10366–10368.

#### **PhD and Postdoctoral Studies:**

[16] “Gold-Catalyzed Intramolecular Oxygen Transfer Reactions of 2-Alkynyl-1,5-Diketones or 2-Alkynyl-5-Ketoesters. Scope, Expansion and Mechanistic Investigations on A Novel [4+2] Cycloaddition” Liu, L.; Malhotra, D.; Jin, Z.; Paton, R. S.; Houk, K. N.; Hammond, G. B. *Chem. Eur. J.* **2011**, *17*, 10690–10699.

[15] “Unraveling the Mechanism of Cascade Reactions of Zincke Aldehydes” Paton, R. S.; Steinhardt, S. E.; Vanderwal, C. D.; Houk, K. N. *J. Am. Chem. Soc.* **2011**, *133*, 3895–3905.

[14] “Indolyne Experimental and Computational Studies: Synthetic Applications and Origins of Selectivities of Nucleophilic Additions” Im, G.-Y. J.; Bronner, S. M.; Goetz, A. E.; Paton, R. S.; Cheong, P.-H. Y.; Houk, K. N. Garg, N. K. *J. Am. Chem. Soc.* **2010**, *132*, 17933–17944.

[13] “The [4+2], not [2+2], Mechanism Occurs in the Gold-Catalyzed Intramolecular Oxygen Transfer Reaction of 2-Alkynyl-1,5-Diketones” Liu, L.-P.; Malhotra, D.; Paton, R. S.; Houk, K. N.; Hammond, G. B. *Angew. Chem. Int. Ed.* **2010**, *49*, 9132–9135.

[12] “Origins of Stereoselectivity in the *trans*-Diels–Alder Paradigm” Paton, R. S.; Mackey, J. L.; Kim, W.H.; Lee, J. H.; Danishefsky, S. J.; Houk, K. N. *J. Am. Chem. Soc.* **2010**, *132*, 9335–9340.

[11] “Indolyne and Aryne Distortions and Nucleophilic Regioselectivities” Cheong, P. H. Y.; Paton, R. S.; Bronner, S. M.; Im, G. Y.; Garg, N. K.; Houk, K. N. *J. Am. Chem. Soc.* **2010**, *132*, 1267–1269.

- Subject of a feature article in RSC Magazine, Chemistry World

[10] “Origins of Regioselectivity of Diels–Alder Reactions for the Synthesis of Bisanthraquinone Antibiotic BE-43472BA” Hayden, A. E.; Paton, R. S.; Becker, J.; Lim, Y. H.; Nicolaou, K. C.; Houk, K. N. *J. Org. Chem.* **2010**, *75*,

922–928.

[9] “Gold(I)-Catalyzed Intermolecular Hydroalkoxylation of Allenes: a DFT Study” Paton, R. S.; Maseras, F. *Org. Lett.* **2009**, *11*, 2237–2240.

[8] “Hydrogen Bonding and Pi-Stacking: How Reliable are Force Fields? A Critical Evaluation of Force Field Descriptions of Non-Bonded Interactions” Paton, R. S.; Goodman, J. M. *J. Chem. Inf. Model.* **2009**, *49*, 944–955.

- One of the ten most downloaded *JCIM* articles in 2009/2010, and highlighted by the Curious Wavefunction blog.

[7] “Mechanistic Insights into the Catalytic Asymmetric Allylboration of Ketones: Bronsted or Lewis Acid Activation?” Paton, R. S.; Goodman, J. M.; Pellegrinet, S. C. *Org. Lett.* **2009**, *11*, 37–40.

[6] “A DFT Study of the Asymmetric Alkenylation of Enones Catalyzed by Binaphthols” Paton, R. S.; Goodman, J. M.; Pellegrinet, S. C. *J. Org. Chem.* **2008**, *73*, 5078–5089.

[5] “Stereostructure Assignment of Flexible Five-Membered Rings by GIAO 13C NMR Calculations: Prediction of the Stereochemistry of Elatinyne” Smith, S. G.; Paton, R. S.; Burton, J. W.; Goodman, J. M. *J. Org. Chem.* **2008**, *73*, 4053–4062.

[4] “1,5-Anti Stereocontrol in the Boron-Mediated Aldol Reactions of  $\beta$ -Alkoxy Methyl Ketones: the Role of the Formyl Hydrogen Bond” Paton, R. S.; Goodman, J. M. *J. Org. Chem.* **2008**, *73*, 1253–1263.

[3] “Exploration of the Accessible Chemical Space of Acyclic Alkanes” Paton, R. S.; Goodman, J. M. *J. Chem. Inf. Model.* **2007**, *47*, 2124–2132.

[2] “Enantioselectivity in the boron aldol reactions of methyl ketones” Goodman, J. M.; Paton, R. S. *Chem. Commun.* **2007**, 2124–2126.

[1] “Understanding the Origins of Remote Asymmetric Induction in the Boron Aldol Reactions of  $\beta$ -Alkoxy Methyl Ketones” Paton, R. S.; Goodman, J. M. *Org. Lett.* **2006**, *8*, 4299–4302.

#### **Books and Book Chapters:**

“Computational Design of New Protein Catalysts” Kiss, G.; Johnson, S. A.; Nosrati, G.; Çelebi-Ölçüm, N.; Kim, S.; Paton, R. S.; Houk, K. N. in *Modeling of Molecular Properties* (ed P. Comba), Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany **2011**, chapter 16.

“Theoretical Studies of Asymmetric Gold Catalysis” Paton, R. S.; Maseras, F. in *Science and Supercomputing in Europe 2008*, pp. 140–142.

“Chemistry Olympiad Support Booklet” Copley, P.; Hersey, T.; McCaw, C.; Paton, R. S.; Scott, K.; Worrall, A.; Wothers, P.; Woodley, E. *Royal Society of Chemistry 2008*, ISBN: 978-1-84755-866-4.

#### **Invited Talks**

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04.04.2018	Keynote speaker: Predictive Catalysis, Girona Seminar 2018, Spain
15.06.2017	Invited Speaker: 11 <sup>th</sup> EUCCO-TCC, Barcelona, Spain
07.06.2017	Challenges in Computational Homogeneous Catalysis, Stockholm, Sweden
07.04.2017	Plenary speaker: V ENEQUI, University of Coimbra, Portugal
22.02.2017	University of Cologne, Carnival Science Session, Germany

26.10.2016 Department of Chemistry, University of Liverpool

05.08.2016 KAIST, South Korea

06.07.2016 **Plenary speaker:** International School Marcial Moreno Mañas 2016, San Sebastian, Spain

23.06.2016 **Plenary speaker:** RSC Early Career Symposium 2016, University of Strathclyde

08.06.2016 RCOM9, Marseilles, France

25.05.2016 RSC Awards Symposium, Queens University Belfast

29.04.2016 RSC Award Lecture: 3<sup>rd</sup> Hans Suschitzky Symposium, University of Salford

23.03.2016 **Plenary speaker:** RSC South East Symposium, University of East Anglia

14.03.2016 UK-Japanese Symposium on Asymmetric Catalysis, University of Manchester

25.02.2016 Department of Condensed Matter Physics, University of Cambridge

25.01.2016 Brazilian Summer School in Chemistry, Federal University of São Carlos, Brazil

07.12.2015 Department of Chemistry, Warwick University

02.12.2015 RSC Award Lecture: Department of Chemistry, Heriot-Watt University

05.11.2015 Department of Chemistry, University of Oxford

29.10.2015 Department of Chemistry, University of Geneva, Switzerland

08.10.2015 Department of Chemistry, POSTECH, Pohang, South Korea

03.09.2015 **Plenary speaker:** *International Symposium on Synthesis and Catalysis*, Evora, Portugal

27.08.2015 Department of Chemistry, Colorado State University, USA

16.07.2015 NSCCS Workshop for Synthetic Chemists, Imperial College London

21.05.2015 Department of Chemistry, University of Helsinki, Finland

15.03.2015 Computational Molecular Science 2015, University of Warwick

27.02.2015 Department of Chemistry, Chemical Institute of Catalonia (ICIQ), Spain

24.02.2015 Department of Chemistry, Imperial College London

04.02.2015 Department of Chemistry, RWTH Aachen, Germany

18.08.2014 EucheMs Organic Division Young Investigator Workshop, Cyprus

10.08.2014 ACS Organic Division Young Investigators Award Symposium, San Francisco, USA

27.02.2014 RSC South-West Regional Meeting, University of Oxford

16.12.2014 Department of Chemistry, UCLA, USA

09.10.2013 Department of Chemistry, University College London

09.08.2013 GDCh Transatlantic Frontiers of Chemistry Meeting 2013, Kloster Seeon, Germany.

26.04.2013 Young Chemists Meeting 2013, Imperial College London

26.03.2013 Department of Chemistry, Seoul National University, South Korea

10.07.2013 Asia-Pacific Conference of Theoretical/Computational Chemistry (APCTCC 6), Korea



26.02.2013 Centre for Computational Chemistry, University of Bristol  
16.01.2013 Centre for Coordination Chemistry (LCC), University of Toulouse, France  
22.06.2012 ICQC Satellite Meeting, UCLA, USA  
20.03.2012 Department of Chemistry, University of Birmingham  
26.01.2011 Department of Chemistry, University of Nottingham

## Research Funding

**2017–2019** “Computational dynamics studies of drug metabolism by P450 enzymes” as PI (European Commission, £160,541)

**2017** Renewal of “Computational Models for the Prediction of Catalyst Performance in Ethylene Polymerisation with Zirconocene Complexes” as PI (SCG, £126,000)

**2016–2020** “Automated Prediction of Organic Thermochemistry” as PI: a four-year funded PhD studentship (AWE, £80,000)

**2016–2017** “Organocatalytic Carbon Dioxide Harvesting: Computational Investigations into Mechanism and Scope” as PI (SCG, £9,000)

**2015–2016** “Computational Models for the Prediction of Catalyst Performance in Ethylene Polymerisation with Zirconocene Complexes” as PI (SCG, £126,000)

**2015–2017** “Plagiarizing Proteins: In Silico Evolution of Catalysts for Selective Chemical Synthesis” as PI (Royal Society, £66,000)

**2015** “Catalysis in Confined Spaces: Modeling Organic Nanoreactors” as PI (SCG, £9,000)

**2015** “Ligand Design for Asymmetric Catalysis” as Co-I with Prof. E. Anderson as PI (SCG, £9,000)

**2014–2016** “Optimizing Selectivity in C-H Functionalization Through Computational Design” as PI (European Commission, £160,541)

**2013** “Chemical Structure Association Trust Grant for Early Career Researchers” as PI (\$1,796)

**2012** “Optimizing Selectivity in Heterocycle C-H Functionalization Through Computational Design” as PI (Royal Society, £10,088)

**2012** “Equipment grant for early-career researchers” as PI (EPSRC, £4,761)

**2011** “Computer Accelerated Catalyst Design” as PI (John Fell OUP Research Fund, £26,570)

**2011–2014** “Optimizing Selectivity in Heterocycle C-H Functionalization Through Computational Design” as PI (AstraZeneca £27,000)

## Teaching

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I design and deliver undergraduate and graduate courses at Oxford. I am a graduate supervisor for three centres for doctoral training (CDTs) – Theory and Modelling in Chemical Sciences (TMCS), Synthesis for Biology and Medicine (SBM) and Systems Approaches to Biomedical Science (SABS).

2016: I gave a 10-hour lecture course “*Computational Organic Chemistry*” at the Brazilian Summer School on Chemistry.

2014-present: DFT and Mechanism – two day hands-on workshop for cohort of 20 graduate students

2014-present: Electronic Structure Theory: DFT and TD-DFT – graduate lecture course and problem class for cohort of 18 graduate students

2014-present: Foundation Mathematics – graduate lecture course and problem classes for cohort of 18 students

2011-present: Orbitals and Mechanism – undergraduate course for 300 students

2010-2013: Organic Spectroscopy – undergraduate course for 190 students

2010-present: In addition to lecturing Oxford positions are combined with college Tutorial Fellowships. I am responsible for teaching (6 hours per week) organic chemistry to groups of two or three students.

## Research Supervision

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### *PhD students supervised:*

2017- present	Xinglong Zhang, Jacqueline Tan
2016 – present	Alex Brethomé, David Ascough
2015 – present	Kiran Kumar
2014 – present	Ruchuta Ardkhean (with Prof. S. Fletcher), Hannah Patel (with Prof. G. Morris)
2013 – 2017	Wilian Cortopassi
2012 – 2016	Kelvin Jackson, Robert Simion
2011 – 2015	Sami Jaffar

### *Masters theses supervised:*

2016 – 2017	Jan-Niklas Boyn, Connor Brogan
2015 – 2016	Will Hak, Matthew Raybould, Shinny Woo
2014 – 2015	Callum Arnold, Michael Kennedy, Susan Leung (jointly with Prof. Darren Dixon), Sophie Mathew-Jones
2013 – 2014	Alex Anthony, Charlie Hornsby, Alan Wise
2012 – 2013	Alex Curran, Katie Hansel, Rosie Lang
2011 – 2012	Kelvin Jackson, Christoph Schnedermann, Erin Shepherd

### *Postdoctoral researchers mentored:*

2016 – present	Dr Kelvin Jackson – now working in computational finance, city of London
2015 – present	Dr Fernanda Duarte – now Assistant Professor at Edinburgh University
2014 – present	Dr Qian Peng – now Assistant Professor at Nankai University, China
2014	Dr Adam Madarasz - now at the University of Budapest
2012 – 2014	Dr Bencan Tang - now Assistant Professor at the University of Nottingham, Ningbo, China

### *Hosted research visits:*

- 2015 Ignacio Funes (PhD student with Feliu Maseras, ICIQ, Spain); Almudena Couce (PhD student with Gregori Ujaque, University of Barcelona, Spain); Connor Brogan (undergraduate research)
- 2014 Sergiy Okovytyy and Tetiana Sergeiva (visiting academic and PhD student from University of Dnipropetrovsk, Ukraine)
- 2013 Sam Hall (NVIDIA-sponsored undergraduate research project)
- 2012 Wenbo Xie (Oxford-University of Georgia, Athens student exchange program)

### *PhD examinations by viva-voce:*

- 2017 Martin Peeks (supervisor Prof Harry Anderson, University of Oxford)
- 2016 Kevin Carr (supervisor Prof. Stuart MacGregor, Heriot-Watt University)
- 2015 Anthony Bradley (supervisor Dr Brian Marsden, University of Oxford)
- 2015 Mikko Muuronen (supervisor Prof Juho Helaja, University of Helsinki, Finland)
- 2014 Igor Boczarow (supervisor Prof Harry Anderson, University of Oxford)
- 2011 Muhsen Al-Ibadi (supervisor Prof John McGrady, University of Oxford)

## Commissions of Trust

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2015: Editorial board member for *Journal of Molecular Graphics and Modelling*

2015-present: Selection panel member for St Hilda's College Junior Research Fellowships.

2014: Editorial board member for *Frontiers in Chemistry*

2013 – present: External specialist Assessor to the Research Fellowship appointments panel for University of Cambridge colleges (Corpus Christi, Churchill College, Kings College, Trinity Hall)

2010 - 2012: Academic Committee member, Society of Chemical Industry Young Chemists Panel

Reviewer for journals including *ACS Catalysis*; *Angewandte Chemie*; *Chem. Commun.*; *Chem. Eur. J.*; *Chem. Sci.*; *Org. Lett.*; *J. Am. Chem. Soc.*; *J. Org. Chem.*; *J. Phys. Chem.*; *Molecules*, *Nature*; *Nature Chem.*; *Nature Commun.*; *Org. Biomol. Chem.*; *Tetrahedron*; *Tetrahedron Lett.*; *Tetrahedron Asymm.*; *WIREs Comp. Mol. Sci.* and grant applications to the *Leverhulme Trust*, the *Royal Society*, the BBSRC research council and Flanders: Research Foundation, Belgium.

## Administration

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**University Examining:** setting of public examinations sat by all undergraduate Chemists including resits; marking and grading all papers; attending Examination Board meetings; signing off the class lists.

2016-2017: 1B organic chemistry examiner (ca. 200 candidates)

2015-2016: 1A organic chemistry examiner (ca. 200 candidates)

2013-14: Preliminary organic chemistry examiner (ca. 200 candidates); resits (ca. 5 candidates)

2012-13: Preliminary organic chemistry examiner (ca. 200 candidates); resits (ca. 5 candidates)

**Admissions Interviewing:** admissions to undergraduate places at Oxford are decided by interview – this involves 3-4 days each year interviewing candidates; I also interview 1 day each year for graduate training

programs (Systems Approaches to Biomedical Sciences, Synthesis for Biology and Medicine)

#### Committee Membership:

- 2017–present: Department of Chemistry Outreach Committee
- 2015–present: Department of Chemistry Consultative Committee
- 2014–present: St Hilda’s College IT committee
- 2014–present: St Hilda’s College Academic Disciplinary Committee
- 2012–2014: St Hilda’s College College Library Committee
- 2011 – 2013: Department of Chemistry, Organizer of Organic Colloquia
- 2011 – 2013: Department of Chemistry, Organiser of the Symposium of Final Year PhD Talks
- 2010 – 2012: Department of Chemistry Staff-Student Consultative Committee
- 2010–present: St Hilda’s College College Governing Body
- 2010–present: St Hilda’s College College Academic Committee

#### Engagement

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2015: Visited high schools in inner London to conduct chemistry workshops introducing students to IR spectroscopy and career routes for chemists.

2014: Gave career talks for graduate and postdoctoral scientists in Oxford; I was also featured in a recent careers piece in *Chemistry World*.

2014–present: Chemistry tutor for residential courses aimed at increasing participation in higher-education. I have lectured to high-school students from schools under-represented in higher education: 70% of students attending obtained offers from Oxford/Cambridge/Imperial. I have written a book on Chemistry problems distributed by the RSC throughout UK schools, and was head-mentor for the UK at the International Chemistry Olympiad.