

Professional Experience

Colorado State University, Department of Chemistry

- 2023 – Marshall Fixman and Branka Ladanyi Professor of Chemistry
2021 – Full Professor of Chemistry
2018 – 2021 Associate Professor: Colorado State University

University of Oxford, Department of Chemistry

- 2014 – 2017 Associate Professor in Organic Chemistry
2010 – 2014 University Lecturer in Organic Chemistry
2010 – 2017 Tutorial Fellow in Organic Chemistry: St Hilda's College, Oxford

Education & Training

UCLA, Department of Chemistry and Biochemistry

- 2009 – 2010 Fulbright UK-US Distinguished Postdoctoral Research Fellow
Research Advisor: Prof. K. N. Houk

University of Cambridge

- 2008 – 2009 St Catharine's College, Cambridge
Junior Research Fellow in Chemistry
2005 – 2008 PhD studies in the Department of Chemistry
Research advisor Prof. Jonathan M. Goodman
"Computational Studies of Boron Mediated C-C Bond Formation"
2000 – 2004 Trinity Hall, Cambridge
MA MSci Natural Sciences (Chemistry and Mathematics)
1st class degree, ranked top in the University
University Rafael Prize in Organic Chemistry; Trinity Hall prize in Natural Sciences

Awards & Honors

- 2023 Marshall Fixman and Branka Ladanyi Professor of Chemistry
2022 – 2024 Co-chair, Gordon Conference on Computational Chemistry
2019 Fellow of the Royal Society of Chemistry (FRSC)
2017 *Nature Journals* Outstanding Reviewer
2016 *Chem. Soc. Rev.* Emerging Investigator
2015 ACS COMP Division Outstanding Junior Faculty Award
2015 RSC Harrison-Meldola Memorial Medal
2015 Thieme Chemistry Journal Award
2014 Molecular Graphics and Modelling Society Silver Jubilee Award
2014 ACS Organic Division Young Academic Investigators Award
2009 – 2010 Distinguished Fulbright-AstraZeneca Research Scholarship
2009 – 2010 Royal Commission for the Exhibition of 1851 Science Research Fellowship
2008 UK Head Mentor, 40th International Chemistry Olympiad, Budapest, Hungary

Publications

- 164.** Fluorochemicals from fluor spar with a phosphate-enabled mechanochemical process bypassing HF. Patel, C.; André-Joyaux, E.; Leitch, J. A.; Martínez de Irujo-Labelde, J.; Ibba, F.; Struijs, J.; Ellwanger, M. A.; Paton, R. S.; Browne, D. L.; Pupo, G.; Aldridge, S.; Hayward, M. A.; Gouverneur, V. *Science* **2023**, *381*, 302–306.
- 163.** Harnessing triaryloxonium ions for aryne generation. Smith, O.; Hindson, M.; Sreenithya, A.; Tataru, V.;

- Paton, R. S.; Burton, J. W.; Smith, M. D. *Nat. Synth.* **2023**, *accepted*.
- 162.** Iridium-Catalyzed Asymmetric Difunctionalization of C–C σ -Bonds Enabled by Ring Strained Boronate Complexes. Shen, H. C.; Popescu, M.V.; Wang, Z. S.; Lescure, L.; Noble, A.; Paton, R. S.; Aggarwal, V. K. *J. Am. Chem. Soc.* **2023**, *145*, 16508–16516.
- 161.** Exploring Cuneanes as Benzene Isosteres and Energetic Materials: Scope and Mechanistic Investigations into Regioselective Rear-rangements from Cubanes. Son, J.Y.; Aikonen, S.; Morgan, N.; Harmata, A. S.; Sabatini, J. J.; Sausa, R.C.; Byrd, E. F. C.; Ess, D. H.; Paton, R. S.; Stephenson, C. R. J. *J. Am. Chem. Soc.* **2023**, *145*, 16355–16364.
- 160.** Pd-Catalyzed Asymmetric Amination of Enamines: Expedient Synthesis of Structurally Diverse N–C Atropisomers. Zhang, P.; Guo, C. Q.; Yao, W.; Lu, C. J.; Li, Y.; Paton, R. S.; Liu, R. R. *ACS Catal.* **2023**, *13*, 7680–7690.
- 159.** Experimental and computational studies of the production of 1,3-butadiene from bio-2,3-butanediol using silica-supported H_3PO_4 derivatives. Alegre-Requena, J. V.; Hafenstine, G. R.; Huo, X.; Guan, Y.; Stunkel, J.; Baddour, F. G.; Unocic, K. A.; Klein, B. C.; Davis, R. E.; Paton, R. S.; Vardon, D. R.; Kim, S. *Chem. Eng. J.* **2023**, *466*, 143346.
- 158.** Regiodivergent Nucleophilic Fluorination under Hydrogen Bonding Catalysis: A Computational and Experimental Study. Horwitz, M. A.; Dürr, A. B.; Afratis, K.; Chen, Z.; Soika, J.; Christensen, K. E.; Fushimi, M.; Paton, R. S.; Gouverneur, V. *J. Am. Chem. Soc.* **2023**, *145*, 9708–9717.
- 157.** Metal-free arylation of benzothiophenes at C4 by activation as their benzothiophene S-oxides. Bisht, R.; Popescu, M. V.; He, Z.; Ibrahim, A. M.; Crisenza, G. E. M.; Paton, R. S.; Procter, D. J. *Angew. Chem Int. Ed.* **2023**, e202302418.
- 156.** AQME: Automated Quantum Mechanical Environments for Researchers and Educators. Alegre-Requena, J. V.; Sowndarya, S. S. V.; Alturaifi, T.; Pérez-Soto, R.; Paton, R. S. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2023**, DOI: 10.1002/wcms.1663.
- 155.** Control of stereogenic oxygen in a helically chiral oxonium ion. Smith, O.; Popescu, M. V.; Hindson, M.; Paton, R. S.; Burton, J.; Smith, M. *Nature* **2022**, *615*, 430–435.
- 154.** Catalytic enantioselective 6π photocyclization of acrylanilides. Jones, B.; Solon, P.; Popescu, M. V.; Du, J.-Y.; Paton, R. S.; Smith, M. *J. Am. Chem. Soc.* **2022**, *145*, 171–178.
- 153.** Halogenation of the 3-position of pyridines through Zincke imine intermediates. Boyle, B. T.; Levy, J. N.; de Lescure, L.; Paton, R. S.; McNally, A. *Science* **2022**, *378*, 773–779.
- 152.** Site-Selective Photocatalytic Functionalization of Peptides and Proteins at Selenocysteine. Dowman, L. J.; Kulkarni, S. S.; Alegre-Requena, J. V.; Giltrap, A. M.; Norman, A. R.; Sharma, A.; Gallegos, L. C.; Welegedara, A. P.; Watson, E. E.; Van Raad, D.; Huhmann, S.; Proschogo, N.; Patel, K.; Larance, M.; Becker, C. F. W.; Mackay, J. P.; Lakhwani, G.; Huber, T.; Paton, R. S.; Payne, R. J. *Nat. Commun.* **2022**, *13*, 6885.
- 151.** Mechanistic Studies on (3 + 2) Cycloaddition Reactions of Azides to Nitroolefins: A Computational and Kinetic Study. Kawamura, M. Y.; Alegre-Requena, J. V.; Barbosa, T. M.; Tormena, C. F.; Paton, R. S.; Ferreira, M. A. B. *Chem. Eur. J.* **2022**, *28*, e202202294.
- 150.** Umpolung Synthesis of Pyridyl Ethers via Bi(V)-Mediated O-Arylation of Pyridones. Ruffell, K.; Gallegos, L. C.; Ling, K. B.; Paton, R. S.; Ball, L. T. *Angew. Chem. Int. Ed.* **2022**, *61*, e2022128.
- 149.** Multi-objective goal-directed optimization of de novo stable organic radicals for aqueous redox flow batteries. Sowndarya, S. S. V.; Law, J.; Tripp, C.; Duplyakin, D.; Skordilis, E.; Biagioni, D.; Paton, R. S.; St. John, P. C. *Nat. Mach. Intell.* **2022**, *7*, 720–730.
- 148.** Expanding chemical space by para-C–H arylation of arenes. Maiti, S.; Li, Y.; Sasmal, S.; Guin, S.; Bhattacharya, T.; Lahiri, G.K.; Paton, R. S.; Maiti, D. *Nat. Commun.* **2022**, *13*, 3963.
- 147.** Mechanistic Studies Yield Improved Protocols for Base-Catalyzed anti-Markovnikov Alcohol Addition Reactions. Luo, C.; Alegre-Requena, J. V.; Sujansky, S. J.; Pajk, S.; Gallegos, L. C.; Paton, R. S.; Bandar, J. S. J.

Am. Chem. Soc. **2022**, *144*, 9586–9596.

146. ¹⁸F-Difluorocarbene for Positron Emission Tomography. Sap, J. B. S.; Meyer, C. F.; Ford, J.; Straathof, N. J. W.; Dürr, A. B.; Lelos, M. J.; Paisey, S. J.; Mollner, T. A.; Hell, S. A.; Trabanco, A.; Genicot, C.; am Ende, C. W.; Paton, R. S.; Tredwell, M.; Gouverneur, V. *Nature* **2022**, *606*, 102–108.

145. Asymmetric Azidation under Hydrogen Bonding Phase-Transfer Catalysis: A Combined Experimental and Computational Study. Wang, J.; Horwitz, M.; Dürr, A.; Ibba, F.; Pupo, G.; Gao, Y.; Ricci, P.; Christensen, K.; Pathak, T.; Claridge, T. W.; Lloyd-Jones, G.; Paton, R. S.; Gouverneur, V. *J. Am. Chem. Soc.* **2022**, *144*, 4572–4584.

144. Reading and Erasing of the Phosphonium Analogue of Trimethyllysine by Epigenetic Proteins. Kamps, J. J. A. G.; Belle, R.; Poater, J.; Kumar, K.; Pieters, B. J. G. E.; Salah, E.; Brown, T.; Claridge, T. D. W.; Paton, R. S.; Bickelhaupt, F. M.; Kawamura, A.; Schofield, C. J.; Mecinović, J. *Commun. Chem.* **2022**, *5*, 27.

143. Modeling catalysis in allosteric enzymes: Capturing conformational consequences. Klem, H.; McCullagh, M.; Paton, R. S. *Top. Catal.* **2022**, *65*, 165–186.

142. Homologation of Electron-Rich Benzyl Bromide Derivatives via Diazo C–C Bond Insertion. Modak, A.; Alegre-Requena, J. V.; Lescure, L.; Rynders, K. J.; Paton, R. S.; Race, N. *J. Am. Chem. Soc.* **2021**, *144*, 86–92.

141. A Quantitative Metric for Organic Radical Persistence Using Thermodynamic and Kinetic Features. Sowndarya, S. S. V.; St. John, P. C.; Paton, R. S. *Chem. Sci.* **2021**, *12*, 13158–13166.

140. Reactions of NO₃ with Aromatic Aldehydes: Gas phase Kinetics and Insights into the Mechanism of the reaction. Ren, Y.; Zhou, L.; Mellouki, A.; Daele, V.; Idir, M.; Brown, S.; Rusic, B.; Paton, R. S.; Ravishankara, A. R. *Atmos. Chem. Phys.* **2021**, *21*, 13537–13551.

139. Real-time Prediction of ¹H and ¹³C Chemical Shifts with DFT accuracy using a 3D Graph Neural Network. Guan, Y.; Sowndarya, S. S. V.; Gallegos, L. C.; St. John, P. C.; Paton, R. S. *Chem. Sci.* **2021**, *12*, 12012–12026.

138. Controlling Intramolecular Interactions in the Design of Selective, High-Affinity, Ligands for the CREBBP Bromodomain. Brand, M.; Clayton, J.; Moroglu, M.; Schiedel, M.; Picaud, S.; Bluck, J. P.; Skwarska, A.; Chan, A. K. N.; Laurin, C. M. C.; Scoriah, A. R.; See, L.; Rooney, T. P. C.; Fedorov, O.; Perell, G.; Cortopassi, W. A.; Christensen, K. E.; Cooper, R. I.; Paton, R. S.; Pomerantz, W. C. K.; Biggin, P. C.; Hammond, E. M.; Filippakopoulos, P.; Conway, S. J. *J. Med. Chem.* **2021**, *64*, 10102–10123.

137. Phosphorus-mediated sp²–sp³ couplings for C–H fluoroalkylation of azines. Zhang, X.; Nottingham, K. G.; Patel, C.; Alegre-Requena, J. V.; Levy, J. N.; Paton, R. S.; McNally, A. *Nature* **2021**, *594*, 217–222.

136. Asymmetric Total Synthesis and Determination of the Absolute Configuration of (+)-Srilankenyne via Sequence-sensitive Halogenations Guided by Conformational Analysis. Jang, H.; Kwak, S. Y.; Lee, D.; Alegre-Requena, J. V.; Kim, H.; Paton, R. S.; Kim, D. *Org. Lett.* **2021**, *23*, 1321–1326.

135. Mechanistic Investigation of Rh(I)-Catalyzed Asymmetric Suzuki-Miyaura Coupling with Racemic Allyl Halides. van Dijk, L.; Ardkhean, R.; Sidera, M.; Karabiyikoglu, S.; Sari, O.; Claridge, T. D. W.; Paton, R. S.; Fletcher, S. P. *Nat. Catal.* **2021**, *4*, 284–292.

134. Importance of Engineered and Learned Molecular Representations in Predicting Organic Reactivity, Selectivity, and Chemical Properties. Gallegos, L. C.; Luchini, G.; St. John, P. C.; Kim, S.; Paton, R. S. *Acc. Chem. Res.* **2021**, *54*, 827–836.

133. Visible light mediated heterocycle functionalization via a geometrically interrupted 2+2 cycloaddition. Popescu, M. V.; Mekereeya, A.; Alegre-Requena, J. V.; Paton, R. S.; Smith, M. D. *Angew Chem. Int. Ed.* **2020**, *59*, 23020–23024.

132. Stereoretention in styrene heterodimerisation promoted by one-electron oxidants. Zhang, X.; Paton, R. S. *Chem. Sci.* **2020**, *11*, 9309–9324.

131. Elucidating the chemical pathways responsible for the sooting tendency of 1 and 2-phenylethanol. Etz, B. D.; Fioroni, G. M.; Messerly, R. A.; Rahimi, M. J.; St. John, P. C.; Robichaud, D. J.; Christensen, E. D.; Beekley, B. P.; McEnally, C. S.; Pfefferle, L. D.; Xuan, Y.; Vyas, S.; Paton, R. S.; McCormick, R. L.; Kim, S. *Combust. Inst.* **2020**,

- 130.** Quantum chemical calculations for over 200,000 organic radical species and 40,000 associated closed-shell molecules. St John, P. C.; Guan, Y.; Kim, Y.; Etz, B. D.; Kim, S.; Paton, R. S. *Scientific Data* **2020**, *7*, 244.
- 129.** GoodVibes: automated thermochemistry for heterogeneous computational chemistry data. Luchini, G.; Alegre-Requena, J. V.; Funes-Ardoiz, I.; Paton, R. S. *F1000Research* **2020**, *9*, 291.
- 128.** Hydrogen Bonding Phase-Transfer Catalysis with Ionic Reactants: Enantioselective Synthesis of γ -Fluoroamines. Roagna, G.; Ascough, D. M. H.; Ibba, F.; Fontana, A.; Christensen, K. E.; Misale, A.; Trabanco, A. A.; Paton, R. S.; Pupo, G.; Gouverneur, V. *J. Am. Chem. Soc.* **2020**, *142*, 14045–14051.
- 127.** BIMP Catalyzed 1,3-Prototropic Shift for the Highly Enantioselective Synthesis of Conjugated Cyclohexenones. Golec, J. C.; Carter, E. M.; Ward, J. W.; Whittingham, W. G.; Simón, L.; Paton, R. S.; Dixon, D. *J. Angew. Chem. Int. Ed.* **2020**, *59*, 17417–17422.
- 126.** Enantiomerically enriched tetrahydropyridine allyl chlorides. Karabiyikoglu S. I.; Brethomé, A. V.; Palacin, T.; Paton, R. S.; Fletcher, S. P. *Chem. Sci.* **2020**, *11*, 4125–4130.
- 125.** Mechanism of biomolecular recognition of trimethyllysine by the fluorinated aromatic cage of KDM5A PHD3 finger. Pieters, B. J. G. E.; Wuts, M. H. M.; Poater, J.; Kumar, K.; White, P. B.; Kamps, J. J. A. G.; Sherman, W.; Pruijn, G. J. M.; Paton, R. S.; Beuming, T.; Bickelhaupt, F. M.; Mecinović, J. *Commun. Chem.* **2020**, *3*, 69.
- 124.** Comparison of Molecular Recognition of Trimethyllysine and Trimethylthialysine by Epigenetic Reader Proteins. Hintzen, J. C. J.; Poater, J.; Kumar, K.; Al Temimi, A. H. K.; Pieters, B. J. G. E.; Paton, R. S.; Bickelhaupt, F. M.; Mecinović, J. *Molecules* **2020**, *25*, 1918.
- 123.** Selective Halogenation Using Designed Phosphine Reagents. Levy, J. N.; Alegre-Requena, J. V.; Liu, R.; Paton, R. S.; McNally, A. *J. Am. Chem. Soc.* **2020**, *142*, 11295–11305
- 122.** Prediction of homolytic bond dissociation enthalpies for organic molecules at near chemical accuracy with sub-second computational cost. St John, P. C.; Guan, Y.; Kim, Y.; Kim, S.; Paton, R. S. *Nat. Commun.* **2020**, *11*, 2328.
- 121.** Fungal-derived brevianamide assembly by a stereoselective semipinacolase. Ye, Y.; Du, L.; Zhang, X.; Newmister, S. A.; McCauley, M.; Alegre-Requena, J. V.; Zhang, W.; Mu, S.; Minami, A.; Fraley, A. E.; Adrover-Castellano, M. L.; Carney, N.; Shende, V. K.; Oikawa, H.; Kato, H.; Tsukamoto, S.; Paton, R. S.; Williams, R. M.; Sherman, D. H.; Li, S. *Nat. Catal.* **2020**, *3*, 497–506.
- 120.** An Alkyne Linchpin Strategy for Drug: Pharmacophore Conjugation: Experimental and Computational Realization of a meta-Selective Inverse Sonogashira Coupling. Porey, S.; Zhang, X.; Bhowmick, S.; Singh, V. K.; Guin, S.; Paton, R. S.; Maiti, D. *J. Am. Chem. Soc.* **2020**, *142*, 3762–3774.
- 119.** Effects of substituents X and Y on the NMR chemical shifts of 2-(4-X phenyl)-5-Y pyrimidines. Yuan, H.; Chen, P.-W.; Li, M.-Y.; Zhang, Y.; Peng, Z.-W.; Liu, W.; Paton, R. S.; Cao, C. *J. Mol. Struct.* **2020**, *1204*, 127489.
- 118.** Unconventional Reactivity of Ethynylbenziodoxolone (EBX) Reagents and Thiols: Scope and Mechanism. Liu, B.; Alegre-Requena, J. V.; Paton, R. S.; Miyake, G. *Chem. Eur. J.* **2020**, *26*, 2386–2394.
- 117.** Synthesis, Characterization, and Reactivity of Complex Tricyclic Oxonium Ions, Proposed Intermediates in Natural Product Biosynthesis. Chan, H. S. S.; Nguyen, Q. N. N.; Paton, R. S.; Burton, J. W. *J. Am. Chem. Soc.* **2019**, *141*, 15951–15962.
- 116.** A Pyridine-Pyridine Cross-Coupling Reaction via Dearomatized Radical Intermediates. Koniarczyk, J. L.; Greenwood, J. W.; Alegre-Requena, J. V.; Paton, R. S.; McNally, A. *Angew. Chem. Int. Ed.* **2019**, *58*, 14882–14886.
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- 113.** Retooling Asymmetric Conjugate Additions for Sterically Demanding Substrates with an Iterative Data-Driven Approach. Brethomé, A. V.; Paton, R. S.; Fletcher, S. P. *ACS Catal.* **2019**, *9*, 7179–7187.
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- 111.** Iterative Arylation of Amino Acids and Aliphatic Amines via δ -C(sp³)-H Activation: Experimental and Computational Exploration. Guin, S.; Dolui, P.; Zhang, X.; Paul, S.; Singh, V. K.; Pradhan, S.; Chandrashekar, H. B.; Anjana, S. S.; Paton, R. S.; Maiti, D. *Angew. Chem. Int. Ed.* **2019**, *131*, 5689–5694.
- 110.** Hydrogen Bonding Phase-Transfer Catalysis with Potassium Fluoride: Enantioselective Synthesis of β -Fluoroamines. Pupo, G.; Vicini, A. C. Ascough, D. M. H.; Ibba, F.; Christensen, K. E.; Thompson, A. L.; Brown, J. M.; Paton, R. S.; Gouverneur, V. *J. Am. Chem. Soc.* **2019**, *141*, 2878–2883.
- 109.** Biosynthesis of Providencin: Understanding Photochemical Cyclobutane Formation with Density Functional Theory. Tang, B.; Paton, R. S. *Org. Lett.* **2019**, *21*, 1243–1247.
- 108.** Conformational Effects on Physical–Organic Descriptors – the Case of Sterimol Steric Parameters. Brethomé, A. V.; Fletcher, S. P.; Paton, R. S. *ACS Catalysis* **2019**, *9*, 2313–2323.
- 107.** Hydrogen bond enabled dynamic kinetic resolution of axially chiral amides mediated by a chiral counterion. Fugard, A.; Lahdenperä, A.; Mekareeya, A.; Tan, J.; Paton, R. S.; Smith, M. D. *Angew. Chem. Int. Ed.* **2019**, *58*, 2795–2798.
- 106.** Enantioselective rhodium-catalysed insertion of trifluorodiaoethanes into tin hydrides. Hyde, S.; Veliks, J.; Ascough, D. M. H.; Szpera, R.; Paton, R. S.; Gouverneur, V. *Tetrahedron* **2019**, *75*, 17–25.
- 105.** Data-mining the diaryl (thio) urea conformational landscape: Understanding the contrasting behavior of ureas and thioureas with quantum chemistry. Luchini, G.; Ascough, D. M. H.; Alegre-Requena, J. V.; Gouverneur, V.; Paton, R. S. *Tetrahedron* **2019**, *75*, 697–702.
- 104.** Frontier Molecular Orbital Effects Control the Hole-Catalyzed Racemization of Atropisomeric Biaryls. Tan, J.; Paton, R. S. *Chem. Sci.* **2019**, *10*, 2285–2289.
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- 102.** Non-Hydrolytic β -Lactam Antibiotic Fragmentation by L, D-Transpeptidases and Serine β -Lactamase Cysteine Variants. Lohans, C. T.; Chan, H. T. H.; Malla, T. R. Kumar, K.; Kamps, J. J. A. G.; McArdle, D. J. B.; van Groesen, E.; de Munnik, M.; Tooke, C. L.; Spencer, J.; Paton, R. S. Brem, J.; Schofield, C. J. *Angew. Chem. Int. Ed.* **2019**, *131*, 2012–2016.
- 101.** Heterobiaryl synthesis by contractive C–C coupling via P(V) intermediates. Hilton, M. C.; Zhang, X.; Boyle, B. T.; Alegre-Requena, J. V.; Paton, R. S.; McNally, A. *Science* **2018**, *62*, 799–804.
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- 99.** Selectivity in Transition Metal-catalyzed Cyclizations: Insights from Experiment and Theory. Anderson, E. A.; Paton, R. S. *CHIMIA* **2018**, *72*, 614–620.
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- 97.** Experimental and theoretical insight into the soot tendencies of the methylcyclohexene isomers. Kim, S.; Fiorinia, M. Park, J.-W.; Robichaud, D. J.; Dhruvajyoti, D. D.; St. John, P. C.; Lu, T.; McEnally, C.; Pfeifferle, L. D.; Paton, R. S.; Foust, T. D.; McCormick, R. L. *Proc. Combust. Inst.* **2018**, *37*, 1083–1090.
- 96.** Post-Translational Site-selective Protein α -Deuteration Protein Backbone Modification and Use as a Tool for Protein Mechanism. Galan, S. R. G.; Wickens, J. R.; Dadova, J.; Ng, W.-L.; Zhang, X.; Simion, R. A.; Quinlan, R.;

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Invited Lectures

100. September 2024: European Conference on Organic Free Radicals, Manchester, UK
99. July 2024: Organic Reactions and Processes Gordon Research Conference, Bryant University
98. November 2023: University of North Carolina at Chapel Hill
97. November 2023: Chemistry Graduate Student Association Invited Lecturer, Northeastern University
97. October 2023: Whitman College
96. October 2023: Vanderbilt University
95. August 2023: Data Science for Catalysis: Automated-Synthesis, Process Optimization & Catalyst Discovery, ACS National Meeting, San Francisco, CA
94. July 2023: International Conference on Chemical Bonding, Kauai
93. July 2023: Accelerating Reaction Discovery, Telluride
92. June 2023: 23rd Tetrahedron Symposium, Gothenburg, Sweden
91. March 2023: Theoretical and Experimental Approaches to Catalyst Development, ACS National Meeting, Indianapolis
90. December 2022: Syngenta Catalysis Network Lecture 2022
89. December 2022: ISQBS 2022, Ibaraki University, Japan

88. December 2022: University of Pittsburgh
87. November 2022: Carnegie Mellon University
86. August 2022: Roitberg Symposium, ACS National Meeting, Chicago
85. August 2022: Houk Symposium, UCLA
84. July 2022: [Gordon Conference on Stereochemistry](#)
83. July 2022: [Gordon Conference on Computational Chemistry](#)
82. July 2022: [WATOC](#)
81. May 2022: Daejeon, Daejeon, South Korea
80. May 2022: PKNU, Busan, South Korea
79. May 2022: Department of Chemistry, Stanford University
78. April 2022: Molecule Maker Lab Institute (MMLI)
77. April 2022: 36th Annual Symposium of the Rocky Mountain Catalysis Society, Colorado School of Mines
76. March 2022: From Theory to Therapy: New Developments in Quantum Mechanical Calculations for Driving Best Chemistry in Academia and Industry, ACS National Meeting, San Diego
75. March 2022: Presidential Workshop: Everything Chemists Always Wanted To Know About Machine Learning, ACS National Meeting, San Diego
74. January 2022: [15th Winter Conference on Medicinal & Bioorganic Chemistry](#), Steamboat Springs
73. December 2021: Department of Chemistry, Montana State University
72. October 2021: Department of Chemistry, Lawrence University
71. October 2021: Department of Chemistry, California Polytechnic State University
70. September 2021: Department of Chemistry, Truman State University
69. August 2021: IUPAC World Chemistry Congress, Montreal, Canada
68. July 2021: [VISTA Symposium on Artificial-Intelligence and Data-Science assisted Synthesis](#)
67. May 2021: International Consortium for Innovation and Quality in Pharmaceutical Development
66. April 2021: Houk International Alumni Meeting
65. November 2020: Genentech
64. August 2020: GSK
63. June 2020: 24th Annual ACS Green Chemistry & Engineering Conference
62. May 2020: Canadian Chemistry Conference and Exhibition (CCCE), Winnipeg
61. February 2020: Department of Chemistry and Biochemistry, University of Missouri – St. Louis
60. November 2019: Department of Chemistry, University of Denver
59. November 2019: Frontiers in Physical Organic Chemistry, Southwest & Rocky Mountain Regional ACS Meeting, El Paso
58. November 2019: Department of Chemistry, Princeton University, NJ
57. October 2019: Department of Chemistry and Biochemistry, UCLA, CA
56. September 2019: Machine Learning and Informatics for Chemistry and Materials, Telluride, CO
55. September 2019: Mechanistic Homogeneous Catalysis – A Meeting between Theory and Experiment, Stockholm, Sweden
54. July 2019: [ISTCP X](#), Tromsø, Norway
53. January 2019: University of Vienna, Austria
52. November 2018: University of Colorado, Denver, USA
51. July 2018: Hanyang University, Seoul, South Korea
50. July 2018: Pukyong National University, South Korea
49. June 2018: [Computational Catalysis for Sustainable Chemistry](#), ICIQ, Tarragona, Spain
48. June 2018: [37th Reaction Mechanisms Conference](#), University of British Columbia, Canada
47. May 2018: [2nd International Symposium on Organic Reaction Mechanism](#), Peking University, Shenzhen Graduate School, China
46. April 2018: [Predictive Catalysis](#) 2018, Girona, Spain
45. March 2018: Complutense University of Madrid, Spain

44. February 2018: Colorado School of Mines, Golden, USA
43. June 2017: [11th EUCO-TCC](#), Barcelona, Spain
42. June 2017: [Challenges in Computational Homogeneous Catalysis](#), Stockholm, Sweden
41. April 2017: [V ENEQUI](#), University of Coimbra, Portugal
40. February 2017: University of Cologne, Germany
39. October 2016: University of Liverpool, UK
38. August 2016: KAIST, South Korea
37. July 2016: [IX International School On Organometallic Chemistry](#), San Sebastian, Spain
36. June 2016: ECS 2016, University of Strathclyde, UK
35. June 2016: [RCOM9](#), Marseilles, France
34. June 2016: RSC Awards Symposium, Queens University Belfast, UK
33. April 2016: Hans Suschitzky Symposium, University of Salford, UK
32. March 2016: RSC South East Regional Meeting, University of East Anglia, UK
31. March 2016: UK-Japanese Symposium on Asymmetric Catalysis, University of Manchester, UK
30. February 2016: Department of Chemistry, University of Cambridge, UK
29. February 2016: Department of Condensed Matter Physics, University of Cambridge, UK
28. February 2016: Federal University of São Carlos, Brazil
27. December 2015: Department of Chemistry, Warwick University, UK
26. December 2015: Department of Chemistry, Heriot-Watt University, UK
25. November 2015: Department of Chemistry, University of Oxford, UK
24. October 2015: University of Geneva, Switzerland
23. October 2015: Department of Chemistry, POSTECH, Pohang, South Korea
22. September 2015: [International Symposium on Synthesis and Catalysis](#), Evora, Portugal
21. August 2015: Colorado State University, USA
20. July 2015: NSCCS Computational Workshop for Synthetic Chemists, Imperial College London, UK
19. May 2015: University of Helsinki, Finland
18. March 2015: [Computational Molecular Science](#), Warwick, UK
17. February 2015: ICIQ, Tarragona, Spain
16. February 2015: Imperial College London, UK
15. February 2015: RWTH Aachen, Germany
14. August 2014: [ACS Organic Division Young Investigators Award Symposium](#), San Francisco, USA
13. February 2014: RSC South-West Regional Meeting – Oxford, UK
12. December 2013: University of California, Los Angeles, USA
11. October 2013: University College London, UK
10. August 2013: [Transatlantic Frontiers of Chemistry](#) – Kloster Seeon, Germany
9. July 2013: [Asia-Pacific Conference of Theoretical/Computational Chemistry](#) – Gyeongju, South Korea
8. April 2013: [UK Young Chemists 2013](#) – Imperial College London, UK
7. March 2013: Seoul National University, South Korea
6. February 2013: University of Bristol, UK
5. January 2013: LCC University of Toulouse, France
4. June 2012: Quantum Mechanics and Molecular Dynamics of Chemical and Biological Reactivity, UCLA, USA
3. March 2012: University of Birmingham, UK
2. January 2011: University of Nottingham, UK
1. January 2011: United States Food and Drug Administration – Irvine, USA

Service

- Editorial Advisory Board member for *Trends in Chemistry*, *Tetrahedron Chemistry*, *Journal of Molecular Graphics and Modelling*, *Heteroatom Chemistry*; *Chemistry – Methods*, *Magnetic Resonance in Chemistry*.
- ACS National Award Selection Committee (2024-2026 award cycle)

- ACS COMP Division Awards Co-chair
- 2022-2024: Co-chair – Gordon Conference on Computational Chemistry
- 2019 – present: Co-chair: Telluride annual Workshop “Machine Learning and Informatics for Chemistry and Materials”
- ACS COMP Division Alternate Councillor
- *Ad Hoc* Review Panel Member for NSF, NIH, DFG
- *Nature Journals* Outstanding Reviewer (2017) *Publons* top reviewers in Chemistry, 99th percentile 2017-2019.
- External PhD examiner at the Universities of Oxford, Cambridge, Helsinki and Heriot-Watt.

Current Research Support (Paton’s allocation at CSU shown)

- 09/01/2023 – 08/31/2023 NIH R01 GM151533-01 \$1,247,328
- 12/01/2022 – 11/31/2023 NSF Molecular Maker Lab Institute - \$75,000
- 09/01/2022 – 08/31/2027 NSF CCI Phase II: NSF Center for Computer Assisted Synthesis - \$1,100,000
- 09/01/2022 – 08/31/2023 Collaboration Agreement (NREL) - \$55,000
- 04/01/2022 – 03/31/2025 NSF Collaborative Research: Electrochemical Ni-Catalyzed Reductive Biaryl Coupling: Mechanistic Studies to Enable Chemical Synthesis (NSF CAT) - \$180,000
- 03/01/2022 – 09/28/2023 Collaboration Agreement (GlaxoSmithKline) - \$100,000
- 09/01/2020 – 08/31/2023 Mechanism, Selectivity and Reaction Dynamics in Hydrogen Atom Transfer (ACS-PRF New Directions Grant) - \$110,000
- 06/01/2020 – 05/31/2023 Discovering Modular Catalysts for Asymmetric Synthesis with Computation (NSF CAT) - \$420,786,000)