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## EDUCATION

- 2003-2008      **Harvard University, Department of Chemistry and Chemical Biology**  
Degree awarded: Ph.D., NDSEG, NSF, and Harvard Merit Pre-Doctoral Fellow  
Research Advisor: Professor Eric N. Jacobsen
- 2002-2003      **Stanford University, Department of Chemistry**  
NDSEG Pre-Doctoral Fellow  
Research Advisor: Professor Justin Du Bois
- 1998-2002      **Harvard University, Department of Chemistry and Chemical Biology**  
Degree awarded: A.B. and A.M. with Highest Honors, summa cum laude  
Research Advisor (2000-2002): Professor Eric N. Jacobsen

## PROFESSIONAL AND ACADEMIC EXPERIENCE

### A. Barton Hepburn Professor of Chemistry, Princeton University (July 2017 to present)

- Provide a team of 16 graduate students and postdoctoral scholars with leadership, personalized mentoring, scientific vision, financial support, and administrative guidance. I have set in place numerous mechanisms to promote creativity and encourage scientific breadth & depth in my co-workers, to foster a healthy, encouraging, and inclusive environment to pursue science, to mentor students on how to effectively communicate their work in written and oral form, and to enhance their professional development. Doyle lab members have gone on to careers in academia, process and medicinal chemistry, data science, and energy and materials science.
- Established a new research area at the interface of machine learning and synthetic chemistry with the goal of using ML to facilitate the discovery, optimization, and adoption of synthetic methodology.
- Elucidated the photophysics of organometallic Ni complexes relevant to cross coupling and metallaphotoredox catalysis (collaboration with Scholes lab). Identified Ni as an underexplored alternative to precious metal photocatalysts relevant to solar energy research and chemical synthesis.
- Discovered a new strategy for direct radical generation and C–O activation from alcohol and carboxylic feedstocks via photoredox catalysis with phosphine mediators (collaboration with Rovis lab).

### Senior Editor, Accounts of Chemical Research (November 2016 to present)

### Associate Professor of Chemistry, Princeton University (July 2013 to June 2017)

- Identified a new cross-coupling paradigm in which the combination of photoredox catalysis and nickel catalysis enables C(sp<sup>3</sup>)–C bond formation from simple and readily available organic molecules (collaboration with MacMillan lab). Independent studies by our group have established this activation mode as general for C–H functionalization under exceptionally mild conditions.
- Invented new methods for the introduction of <sup>18</sup>F into organic substrates that feature uncommonly mild, rapid, and operationally convenient procedures. The processes enable access to experimental and clinically-validated radiotracers by late-stage radiofluorination and have led to a number of collaborations with industrial and academic groups for the development of new PET tracers.
- Identified novel ligands for Ni catalysis that enable unprecedented reactivity or activity – phosphines featuring remote steric hindrance and the electron-deficient olefin ligand FroDO.

- Invented two new chemicals (one a fluorination reagent and the other a Ni pre-catalyst) that have been commercialized and have seen widespread adoption by the community including on kilo scale.
- Developed a collection of new synthetic methods for C(sp<sup>3</sup>)-C bond formation that afford access to valuable heterocycles and acyclic amines and ethers.

**Assistant Professor of Chemistry, Princeton University** (July 2008 to June 2013)

- Mentored 4 postdoctoral fellows, 12 graduate students, and 8 undergraduate researchers.
- Discovered the first asymmetric catalytic methods for nucleophilic fluorination, including cooperative catalytic systems for asymmetric ring opening of epoxides and aziridines, and two Pd-catalyzed protocols for enantio- and regioselective allylic fluorination.
- Identified catalytic cross-coupling reactions with styrenyl epoxides and aziridines as electrophiles. The methodologies feature unique ligand effects for nickel catalysis that enable regioselective Csp<sup>3</sup>-O and Csp<sup>3</sup>-N activation and mild C<sub>alkyl</sub>-C bond formation.
- Elucidated a new entry to alkyl cross coupling that involves oxidative interaction of a nickel catalyst with iminium and oxocarbenium electrophiles; this approach has led to the identification of enantioselective methods for the preparation of important chiral heterocyclic products.

**Summer Intern, Bristol-Myers Squibb, Discovery Chemistry** (Metabolic Diseases, May to August 2000)

## LECTURES

Over 130 invited lectures since 2009, including named lectureships in the US and abroad and plenary lectures at national & international conferences.

## AWARDS & HONORS

- RSC Fluorine Award (2019)
- 15<sup>th</sup> Hirata Prize (2019)
- BMS Unrestricted Grant in Synthetic Organic Chemistry (2016)
- Phi Lambda Upsilon National Fresenius Award (2014)
- Presidential Early Career Award for Scientists and Engineers (2014)
- Novartis Chemistry Lectureship (2014/2015)
- Bayer Excellence in Science Award (2013)
- Arthur C. Cope Scholar Award (2013)
- Camille-Dreyfus Teacher Scholar Award (2013)
- Thieme Chemistry Journals Award (2013)
- Amgen Young Investigator Award (2012)
- Alfred P. Sloan Foundation Fellowship (2012)
- NSF CAREER Award (2012-2017)
- Roche Early Excellence in Chemistry Award (2012)
- Eli Lilly Grantee Award (2012-2014)
- Boehringer Ingelheim New Investigator Award (2012)
- Merck Award for Selective Fluorination (2010-2012)
- ACS PRF Doctoral New Investigator Grant (2009)
- Sanofi Aventis New Faculty Award (2008)
- Eli Lilly New Faculty Award (2008)
- Harvard Merit Fellowship (2007)
- Sigma-Aldrich Graduate Student Innovation Award (2006)
- Christensen Prize for Outstanding Research Achievement (2005)
- National Science Foundation Pre-Doctoral Fellowship (2004-2007)

- National Defense Science and Engineering Pre-Doctoral Fellowship (2002-2004)
- Harvard College Certificate of Distinction in Teaching (2004)
- Phi Beta Kappa Junior Inductee (2001)
- Pfizer Undergraduate Summer Research Fellowship (2001)
- Harvard College Research Fellowship Award (2001)
- Harvard Detur Prize Recipient (1999)

## INDEPENDENT PUBLICATIONS

41. Estrada, J. G.; Ahneman, D. T.; Sheridan, R. P.; Dreher, S. D.; Doyle, A. G. **Response to Comment on "Predicting Reaction Performance in C–N Cross-Coupling Using Machine Learning"**. *Science* **2018**, *362*, eaat8763.
40. Stache, E. E.; Ertel, A. B.; Rovis, T.; Doyle, A. G. **Generation of Phosphoranyl Radicals via Photoredox Catalysis Enables Voltage-Independent Activation of Strong C–O Bonds**. *ACS Catalysis* **2018**, *8*, 11134–11139.
39. Ackerman, L. K. G.; Martinez Alvarado, J. I.; Doyle, A. G. **Direct C–C Bond Formation from Alkanes Using Ni-Photoredox Catalysis**. *J. Am. Chem. Soc.* **2018**, *140*, 14059–14063.
38. Nielsen, M. K.; Ahneman, D. T.; Riera, O.; Doyle, A. G. **Deoxyfluorination with Sulfonyl Fluorides: Navigating Reaction Space with Machine Learning**. *J. Am. Chem. Soc.* **2018**, *140*, 5004–5008.
37. Ahneman, D. T.; Estrada, J. G.; Lin, S.; Dreher, S. D.; Doyle, A. G. **Predicting Reaction Performance in C–N Cross-Coupling using Machine Learning**. *Science* **2018**, *360*, 186–190.
36. Shields, B. J.; Kudisch, B.; Scholes, G. D.; Doyle, A. G. **Long-Lived Charge Transfer States of Nickel(II) Aryl Halide Complexes Facilitate Bimolecular Photoinduced Electron Transfer**. *J. Am. Chem. Soc.* **2018**, *140*, 3035–3039.
35. Heinz, C.; Lutz, J. P.; Simmons, E. M.; Miller, M. M.; Ewing, W. R.; Doyle, A. G. **Ni-Catalyzed Carbon–Carbon Bond-Forming Reductive Amination**. *J. Am. Chem. Soc.* **2018**, *140*, 2292–2300.
34. Nielsen, M. K.; Shields, B. J.; Liu, J. Williams, M. J.; Zacuto, M. J.; Doyle, A. G. **Mild, Redox-Neutral Formylation of Aryl Chlorides via Photocatalytic Generation of Chlorine radicals**. *Angew. Chem. Int. Ed.* **2017**, *129*, 7297–7300.
33. Woods, B. P.; Orlandi, M.; Huang, C.-Y. Sigman, M. H.; Doyle, A. G. **Nickel-Catalyzed Enantioselective Reductive Cross-Coupling of Styrenyl Aziridines**. *J. Am. Chem. Soc.* **2017**, *139*, 5688–5691.
32. Stache, E. E.; Rovis, T.; Doyle, A. G. **Nickel-Photoredox Catalyzed Enantioselective Desymmetrization of Meso Cyclic Anhydrides**. *Angew. Chem. Int. Ed.* **2017**, *56*, 3679–3683.
31. Wu, K.; Doyle, A. G. **Parameterization of Phosphine Ligands Demonstrates Enhancement of Nickel Catalysis via Remote Steric Effects**. *Nature Chem.* **2017**, *9*, 779–784.
30. Shields, B. J.; Doyle, A. G. **Direct C(sp<sup>3</sup>)–H Cross Coupling Enabled by Catalytic Generation of Chlorine Radicals**. *J. Am. Chem. Soc.* **2016**, *138*, 12719–12722.

29. Gray, E. E.; Nielsen, M. K.; Choquette, K. A.; Kalow, J. A.; Graham, T. J. A.; Doyle, A. G. **Nucleophilic (Radio)Fluorination of  $\alpha$ -Diazocarbonyl Compounds Enabled by Copper-Catalyzed H-F Insertion.** *J. Am. Chem. Soc.* **2016**, *138*, 10802–10805.
28. Ahneman, D. T.; Doyle, A. G. **C-H Functionalization of Amines with Aryl Halides by Nickel-Photoredox Catalysis.** *Chem. Sci.* **2016**, *7*, 7002–7006.
27. Lutz, J. P.; Chau, S. T.; Doyle, A. G. **Nickel-Catalyzed Enantioselective Arylation of Pyridine.** *Chem. Sci.* **2016**, *7*, 7105–7109.
26. Joe, C. L.; Doyle, A. G. **Direct Acylation of C(sp<sup>3</sup>)-H Bonds Enabled by Nickel and Photoredox Catalysis.** *Angew. Chem. Int. Ed.* **2016** *55*, 4040–4043.
25. Nielsen, M. K.; Ugaz, C. R.; Li, W.; Doyle, A. G. **PyFluor: A Low-Cost, Stable, and Selective Deoxy-fluorination Reagent.** *J. Am. Chem. Soc.* **2015**, *137*, 9571–9574.
24. Arendt, K. M.; Doyle, A. G. **Dialkyl Ether Formation via Nickel-Catalyzed Cross Coupling of Acetals and Aryl Iodides.** *Angew. Chem. Int. Ed.* **2015**, *54*, 9876–9880.
23. Huang, C.-Y.; Doyle, A. G. **Electron-Deficient Olefin Ligands Enable Generation of Quaternary Carbons by Ni-Catalyzed Cross Coupling.** *J. Am. Chem. Soc.* **2015**, *137*, 5638–5641.
22. Shields, J. D.; Gray, E. E.; Doyle, A. G. **A Modular, Air-Stable Nickel Precatalyst.** *Org. Lett.* **2015**, *17*, 2166–2169.
21. Zuo, Z.; Ahneman, D.; Chu, L.; Terrett, J.; Doyle, A. G.; MacMillan, D. W. C. **Merging Photoredox with Nickel Catalysis: Coupling of  $\alpha$ -Carboxyl sp<sup>3</sup>-Carbons with Aryl Halides.** *Science* **2014**, *345*, 437–440.
20. Huang, C.-Y. (Dennis); Doyle, A. G. **The Chemistry of Transition Metals with Three-Membered Ring Heterocycles.** *Chem. Rev.* **2014**, *114*, 8153–8198.
19. Graham, T. J. A.; Lambert, R. F.; Ploessl, K.; Kung, H. F.; Doyle, A. G. **Enantioselective Radiosynthesis of Positron Emission Tomography (PET) Tracers Containing [<sup>18</sup>F]Fluorohydrins.** *J. Am. Chem. Soc.* **2014**, *136*, 5291–5294.
18. Katcher, M. H.; Norrby, P.-O.; Doyle, A. G. **Mechanistic Investigations of Palladium-Catalyzed Allylic Fluorination.** *Organometallics.* **2014**, *33*, 2121–2133.
17. Shields, J. D.; Ahneman, D. T.; Graham, T. J. A.; Doyle, A. G. **Enantioselective, Nickel-Catalyzed Suzuki Cross-Coupling of Quinolinium Ions.** *Org. Lett.* **2013**, *16*, 142–145.
16. Nielsen, D. K.; Huang, C.-Y. (Dennis); Doyle, A. G. **Directed Nickel-Catalyzed Negishi Cross Coupling of Alkyl Aziridines.** *J. Am. Chem. Soc.* **2013**, *135*, 13605–13609.
15. Braun, M.-G.; Doyle, A. G. **Palladium-Catalyzed Allylic C-H Fluorination.** *J. Am. Chem. Soc.* **2013**, *135*, 12990–12993.
14. Chau, S. T.; Lutz, J. P.; Wu, K.; Doyle, A. G. **Nickel-Catalyzed Enantioselective Arylation of Pyridinium Ions: Harnessing an Iminium Ion Activation Mode.** *Angew. Chem., Int. Ed.* **2013**, *52*, 9153–9156.

13. Kalow, J. A.; Doyle, A. G. **Enantioselective Fluoride Ring Opening of Aziridines Enabled by Cooperative Lewis Acid Catalysis.** *Tetrahedron*, **2013**, *69*, 5702–5709.
12. Braun, M.-G.; Katcher, M. H.; Doyle, A. G. **Carbofluorination via a Palladium-Catalyzed Cascade Reaction.** *Chemical Science*, **2013**, *4*, 1216–1220.
11. Sylvester, K. T.; Wu, K.; Doyle, A. G. **Mechanistic Investigations of the Nickel-Catalyzed Suzuki Reaction of *N,O*-Acetals: Evidence for Boronic Acid-Assisted Oxidative Addition and an Iminium Activation Pathway.** *J. Am. Chem. Soc.* **2012**, *134*, 16967–16970.
10. Kalow, J. A.; Schmitt, D. E.; Doyle, A. G. **Synthesis of  $\beta$ -Fluoroamines by Lewis Base-Catalyzed Hydrofluorination of Aziridines.** *J. Org. Chem.* **2012**, *77*, 4177–4183.
9. Huang, C.-Y. (Dennis); Doyle, A. G. **Nickel-Catalyzed Negishi Alkylations of Styrenyl Aziridines.** *J. Am. Chem. Soc.* **2012**, *134*, 9541–9544.
8. Graham, T. J. A.; Doyle, A. G. **Nickel-Catalyzed Cross Coupling of Chromene Acetals and Boronic Acids.** *Org. Lett.* **2012**, *14*, 1616–1619.
7. Katcher, M. H.; Sha, A.; Doyle, A. G. **Regio- and Enantioselective Fluorination of Acyclic Allylic Halides.** *J. Am. Chem. Soc.* **2011**, *133*, 15902–15905.
6. Kalow, J. A.; Doyle, A. G. **Mechanistic Investigations of Cooperative Catalysis in the Enantioselective Fluorination of Epoxides.** *J. Am. Chem. Soc.* **2011**, *133*, 16001–16012.
5. Nielsen, D. K.; Doyle, A. G. **Nickel-Catalyzed Cross Coupling of Styrenyl Epoxides with Boronic Acids.** *Angew. Chem., Int. Ed.* **2011**, *50*, 6056–6059.
4. Graham, T. J. A.; Doyle, A. G. **Transition Metal-Catalyzed Cross Coupling with *N*-Acyliiminium Ions Derived from Quinolines and Isoquinolines.** *Chem. Sci.* **2011**, *2*, 980–984.
3. Shaw, T. W.; Kalow, J. A.; Doyle, A. G. **Fluoride Ring-Opening Kinetic Resolution of Terminal Epoxides: Preparation of (*S*)-2-Fluoro-1-Phenylethanol.** *Org. Syn.* **2012**, *89*, 9–18.
2. Katcher, M. H.; Doyle, A. G. **Palladium-Catalyzed Asymmetric Synthesis of Allylic Fluorides.** *J. Am. Chem. Soc.* **2010**, *132*, 17402–17404.
1. Kalow, J. A.; Doyle, A. G. **Enantioselective Ring-Opening of Epoxides by Fluoride Anion Promoted by a Cooperative Dual Catalyst System.** *J. Am. Chem. Soc.* **2010**, *132*, 3268–3269.

## PROFESSIONAL ACTIVITIES

### Outside Service

- Senior Editor, Accounts of Chemical Research (Nov 2016–present)
- Chirality 2018 organizer
- ACS National Award Selection Committee
- Editorial Advisory Board member for *ACS Central Science*, *Organic Letters* (term completed), and

#### *Advanced Synthesis & Catalysis (2014-present)*

- Study section, SBCA, SBCB - NIGMS
- Grant reviewer for National Science Foundation (2012-present)
- Grant reviewer for American Chemical Society Petroleum Research Fund (2009-present)
- Co-organizer of the 42<sup>nd</sup> National Organic Chemistry Symposium (2010-2011)
- Session chair for ACS National Meetings & Gordon Research Conferences (2009-present)
- Organized and performed chemistry demonstrations for children at Trenton Science Museum's Super Science Saturday (2011-present)
- Faculty mentor for Mercer County Community College honors chemistry program
- Outside reader and examiner for graduate students in the Chemistry Department at Columbia University
- Reviewer for ACS, Wiley, Elsevier, Nature Publishing Group, Science, and Royal Society of Chemistry journals
- Member of the American Chemical Society (2002-present)

#### *Princeton University Service*

- Director of Graduate Studies (2017-present)
- Member of the Graduate Work Committee (2008-present)
- Member of the Staffing and Long Range Planning Committee (2014-present)
- Initiated new Student Invited Lecture Series (SILS) in collaboration with the Chemistry Graduate Student Organization (2009-present)
- Panelist, Tigers with Cubs (2015)
- Member, Women in STEM Working Group at Princeton (2014-present)
- Member, Committee of Committees (2013-2015)
- Chair of the Organic Chemistry Seminar Series (2008-2013)
- Chair of the Organic Graduate Admissions Committee (2008-2013)
- Member of the Junior Faculty Search Committee (2008-2015); chair in 2015
- Member of the Instrumentation Committee (2010-2018)
- Member of the Chemistry Diversity Committee (2014-present)
- Created new graduate course "Chem 536," which has been offered as part of Princeton University's Industrial Affiliates Program (2009-present)
- Grader for incoming Chemistry graduate student's organic placement exam (2008-2011)
- Faculty panel member for Princeton's incoming women in science, engineering, and mathematics (2009-present)
- Roundtable discussion facilitator for Princeton's undergraduate chemistry club dinner series (2011-present)
- Grader for undergraduate organic prize exams (2010-present)
- Reader and external grader for organic undergraduate senior theses (2010-present)

#### **COLLABORATORS**

- Professor Gregory Scholes (Princeton University)
- Professor Tomislav Rovis (Columbia University)
- Professor Ryan Adams (Department of Computer Science, Princeton University)
- Professor Matt Sigman (Department of Chemistry, University of Utah)
- Professor Hank Kung (Department of Radiology, University of Pennsylvania)
- Professor David MacMillan (Princeton University)
- Dr. Eric Hostetler (Translational Imaging Biomarkers, Merck Research Laboratories)
- Drs. Sam Bonacorsi, David Donnelly, Erin Cole, Eric Simmons, Michael Miller, and Rick Ewing (Bristol-Myers Squibb)

- Drs. Spencer Dreher, Robert Sheridan, Tom Lyons, Heather Johnson (Merck Research Laboratories)
- Professor Per-Ola Norrby (Astra-Zeneca)
- Dr. Michael Zacuto (Celgene)

## TEACHING EXPERIENCE

*Chemistry 532: Mechanistic and Physical Organic Chemistry (graduate-level)*

*Chemistry 303: Organic Chemistry I (undergraduate-level)*

*Chemistry 536: Methods for Complex Organic Synthesis (upper-level)*

*Chemistry 521: Organometallic Chemistry*

*Chemistry 530: Synthetic Organic Chemistry (graduate-level)*

## OUTREACH ACTIVITIES

- Trenton Science Museum, Super Science Saturday (Spring 2011–2015)
- Faculty mentor for Mercer County Community College Honors Chemistry Program (2012)
- Faculty panel member for Princeton's incoming women in science, engineering, and mathematics (2009-present)
- Roundtable discussion facilitator for Princeton's undergraduate chemistry club dinner series (2011-present)