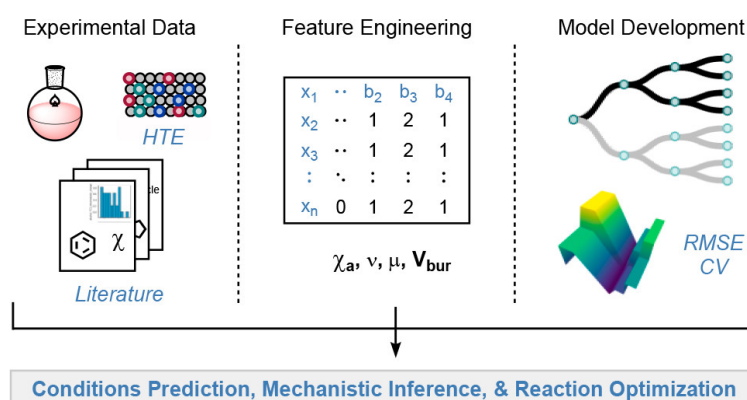


Enabling Chemical Synthesis via Machine Learning

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The Doyle lab conducts research at the interface of organic, organometallic, physical organic, and computational chemistry. Our goal is to address unsolved problems in organic synthesis through the development of catalysts, catalytic reactions, and synthetic methods. We apply mechanistic and computer-assisted techniques to the analysis of these reactions in order to uncover general principles that can guide the design of improved ligands, catalysts and the discovery of new reactions. These studies have also included the development of machine learning tools for reaction optimization, prediction and mechanistic inference. This lecture will describe our integrated efforts to develop, assess, and deploy machine learning tools in reaction and catalyst design.



References

1. “**Predicting Reaction Yields via Supervised Learning.**” Żurański, A. M.; Martinez Alvarado, J. I.; Shields, B. J.; Doyle, A. G. *Acc. Chem. Res* **2021**, *54*, 1856-1865. [DOI: 10.1021/acs.accounts.0c00770](https://doi.org/10.1021/acs.accounts.0c00770)
2. “**Bayesian reaction optimization as a tool for chemical synthesis.**” Shields, B. J.; Stevens, J.; Li, J.; Parasram, M.; Damani, F.; Martinez Alvarado, J. I.; Janey, J. M.; Adams, R. P.; Doyle, A. G. *Nature* **2021**, *590*, 89-96. [DOI: 10.1038/s41586-021-03213-y](https://doi.org/10.1038/s41586-021-03213-y)
3. “**Univariate classification of phosphine ligation state and reactivity in cross-coupling catalysis.**” Newman-Stonebraker, S. H.; Smith, S. R.; Borowski, J. E.; Peters, E.; Gensch, T.; Johnson, H. C.; Sigman, M. S.; Doyle, A. G. *Science* **2021**, *374*, 301-308. [DOI: 10.1126/science.ajb4213](https://doi.org/10.1126/science.ajb4213)

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A. EDUCATION & TRAINING

- 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

B. PROFESSIONAL APPOINTMENTS

Saul Winstein Endowed Chair in Organic Chemistry, UCLA (July 2021 to present)

A. Barton Hepburn Professor of Chemistry, Princeton University (July 2017 to June 2021)

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

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

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

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

C. HONORS & AWARDS

- OMCOS award (2023)
- Finalist of the 2022 Blavatnik National Awards for Young Scientists
- Bessel Award (2022)
- EJ Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator (2022)
- The Camille and Henry Dreyfus Foundation Machine Learning in the Chemical Sciences and Engineering Award (2021)
- American Chemical Society Fellow (2020)
- RSC Fluorine Award (2019)
- 15th 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)