

BENJAMIN J. SHIELDS

Research Scientist



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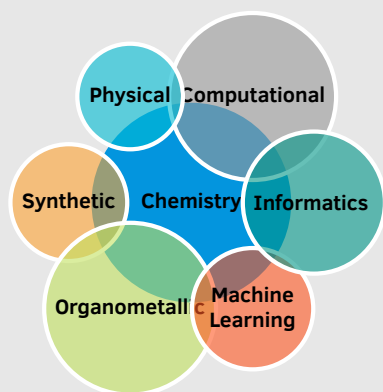
/in/benjamin-shields



b-shields

Technical Skills

Overview



Programming/Development

Experience →

Code: Python • Mathematica

HPC: Bash • Cloud • GPU

Typesetting: Markdown • \LaTeX

Education

Ph.D., Chemistry

Princeton University

2016 - 2019 | Princeton, NJ

M.A., Chemistry (distinction)

Princeton University

2014 - 2016 | Princeton, NJ

B.S., Chemistry (highest honors)

University of North Carolina Asheville

2010 - 2014 | Asheville, NC

B.A., Applied Math (highest honors)

University of North Carolina Asheville

2010 - 2014 | Asheville, NC

Experience

July 2019 - Present Postdoctoral Researcher

Adams & Doyle Labs, Princeton University

- **Focus:** developing an integrated Bayesian framework for reaction optimization and knowledge transfer in chemical synthesis.
- **Projects:** Bayesian reaction optimization, online game to benchmark ML against human decisions, automated high-throughput quantum chemistry, chemical feature engineering, mechanistic inference via explanatory modeling.
- **Tools:** Jupyter Lab, pandas, numpy, Gaussian, Open-Babel, RD-Kit, PyTorch, GPyTorch, GpyOpt, scikit-learn, pyclustering, keras, R, shiny, Mathematica.

June 2015 - June 2019 Graduate Research Assistant

Doyle Lab, Princeton University

- **Focus:** development and understanding of novel methods for the preparation of small molecules. Worked in teams towards larger research program goals such as writing journal articles and submitting grant applications.
- **Projects:** C-H functionalization via Ni photochemistry, computational photophysics and ultrafast spectroscopy of Ni complexes, navigating chemical reactivity via machine learning.
- **Tools:** Gaussian, Open-Babel, scikit-learn, Mathematica, Schlenk, glovebox, HTE, TA, XAS, NMR, NIR, UV, MS.

Aug 2014 - May 2015 Graduate Teaching Assistant

Princeton University

- Instructor for General Chemistry and Organic Chemistry.
- Weekly lectures, grading, and writing problems for homework and exams.

Research Highlights

Machine Learning & Chemical Synthesis: My research in this area seeks to realize hybrid chemical-ML approaches to synthetic chemistry. Subjects of current interest include: synergistic reaction design and discovery, Bayesian optimization of chemical reactions, interpreting hybrid physical-ML models, and translation of knowledge between applications via transfer learning. **Representative Publication:** Shields, Benjamin J.; Stevens, Jason; Li, Jun; Parasram, Marvin; Damani, Farhan; Martinez Alvarado, Jesus; Janey, Jacob; Adams, Ryan; Doyle, Abigail G. "Bayesian Reaction Optimization as A Tool for Chemical Synthesis", *Manuscript Submitted*, **2020**.

Organometallic Photophysics & Spectroscopy: Transition metal complexes play critical roles as photocatalysts for solar-to-electrical energy conversion and chemical synthesis. My research in this area utilizes organometallic chemistry, quantum mechanical modeling, and ultrafast spectroscopy to understand and improve photocatalytic systems. **Representative Publication:** Shields, Benjamin J.; Kudisch, Bryan; Scholes, Gregory, D.; Doyle, Abigail 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.

Synthetic Photochemistry & Methods Development: Photochemistry utilizes energy in the form of light to drive unique and otherwise unfavorable chemical reactions. The objective of this work is to develop broadly useful photosynthetic methods for small molecule synthesis. **Representative Publication:** Shields, Benjamin J.; Doyle, Abigail G. "Direct C(sp³)-H Cross Coupling Enabled by Catalytic Generation of Chlorine Radicals" *J. Am. Chem. Soc.*, **2016**, *138*, 12719–12722.

Select Presentations

"Bayesian reaction optimization", *Center for Computer Assisted Synthesis*, **2020**.

"Machine learning in methods development", *Green Chemistry & Engineering*, **2019**.

"Photochemistry of nickel complexes", *BMS Fellowship Symposium*, **2018**.