BENJAMIN J. SHIELDS

Research Scientist

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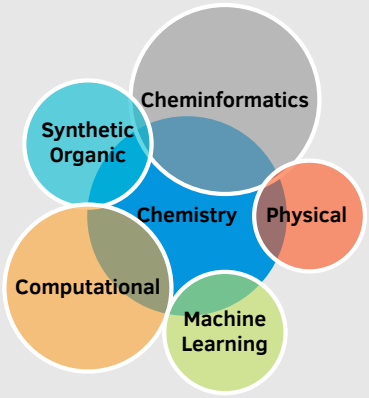
b-shields

Technical Skills

Overview



Programming/Development

Experience

Code: Python • Bash • Wolfram

ML: scikit-learn • PyTorch • GPyTorch

CIX: RDKit • OpenEye • OpenBabel

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

Jan 2021 - Present — **Principal Scientist** — CADD, Bristol Myers Squibb

- **Focus**: Developing software, ML/informatics methods, and models for drug discovery. Working closely with interdisciplinary teams to identify hits and optimize leads across multiple modalities and therapeutic areas.
- **Projects**: ML infrasructure development, uncertainty estimation, molecular Bayesian optimization, virtual screening, large-scale enumeration and generative design, sequence modeling, synthetic accessiblity scoring, ADMET modeling.

July 2019 - Jan 2021 — **Postdoctoral Researcher** — Adams & Doyle Labs, Princeton University

- **Focus**: Developed a Bayesian optimization framework for chemical reaction optimization.
- **Projects**: Bayesian reaction optimization, online game to benchmark ML against human decisions, chemical feature engineering and explanitory modeling.

Aug 2014 - June 2019 — **Graduate Research/Teaching Assistant** — Doyle Lab, Princeton University

- **Focus**: Development and understanding of novel methods for the preparation of small molecules.
- **Projects**: C-H functionalization, photophysics and ultrafast spectroscopy of Ni complexes, navigating chemical reactivity via ML.

Research Highlights

Machine Learning & Drug Discovery: My research in this area seeks to tackle challenging problems in drug discovery using machine learning, automation, physical modeling, and iterative design. Subjects of current interest include: Bayesian chemical structure optimization, unertainty estimation, large-scale virtual screening, generative design, matched molecular pair analysis, and automated retrosynthesis. **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", *Nature*, **2021**, *590*, 89–96.

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(sp^3)–H Cross Coupling Enabled by Catalytic Generation of Chlorine Radicals" *J. Am. Chem. Soc.*, **2016**, *138*, 12719–12722.

Select Presentations & Awards

"Leadership Award in Synthetic and Medicinal Chemistry", *BMS*, **2023**.
"Bayesian optimization as an approach to drug development", *MABC*, **2021**.
"Bayesian reaction optimization", *Center for Computer Assisted Synthesis*, **2020**.
"Machine learning in methods development", *Green Chemistry & Engineering*, **2019**.