Jack D. Sundberg

Materials Chemist, Data Scientist, & Software Developer

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ABOUT

Materials chemist and data scientist with specialties in materials discovery, ab-initio simulations, and database architectures. As I've progressed through academic research, I've worked primarily in experimental laboratories, and during my PhD research, I discovered a passion for guiding research with computational analyses and for creating materials science software that emphasize beginner-friendly guides and use. Looking forward, I hope to take my broad range of experiences and apply what I've learned to new and unfamiliar fields – driving the development of tools for data-driven research and beyond!

EDUCATION & EXPERIENCE

PhD Candidate in Materials Chemistry 2017-Present

University of North Carolina (Chapel Hill, NC)

Materials Discovery Research w. Prof. Scott Warren

Details: Performed a combination of experimental and computational research, which included building a custom chemical vapor deposition system that enabled synthesis of ultra-reductive materials. Thesis focuses on computational studies and software development, where my predictions led to the proposal and completion of several experimental projects. In addition, my work culminated in the development of Simmate (link), which is a workflow & database framework for materials science that initiated collaborations with several academic and national labs – such as the Materials Project and OPTIMADE organizations.

BS in General Chemistry 2013-2017

Denison University (Granville, OH)

Organic Synthesis Research w. Prof. Jordan Fantini

Cumulative GPA: **3.84** | Major GPA: **3.84**

Details: Full-time research during the summers of 2015 & 2016. Credit-hour based research during Spring & Fall semesters of 2015-2017. Became fully independent and proficient in wet synthesis under inert conditions and in purification/characterization of products.

Senior Thesis: "Synthesis of tetrasulfonated calix[4]arenes designed for carbon-nanotube grafting and acetylcholine sensing" (pdf)

Aquatic Center & Swim Coach 2010-2014

The Khakwa Club (Erie, PA)

Concessions ('10-11) ⇨ Lifeguard ('12-14) ⇨ Assistant Swim Coach ('13-14)

Details: Progressed through roles of increasing responsibility and certification. Demonstrated leadership skills while being 1 of 4 assistant coaches for a team of ~150 swimmers (aged 6 through 17 years old).

AWARDS

- NSF Graduate Research Fellowship **2019** *Doctoral Research Fellowship*
- Woodland Prize **2017** *Award for Excellence in Chemistry Research*
- E. Stanley Mellick Scholarship **2016** *Award for Excellence in Physical Sciences*
- Denison Founders Scholarship **2014** *Undergraduate Merit Scholarship*
- K.I. Brown Scholarship **2013** *Undergraduate Merit Scholarship*

HOBBIES

Chess	Swimming	Breweries	Boardgames	Graphic Design
Pickup Sports	Wake Surfing	Home-made Cocktails	Open-source Software	3D Modeling & Art

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PUBLICATIONS

Simmate: a framework for materials science

J.D. Sundberg, S.S. Benjamin, L.M. McRae, S.C. Warren
Under review at the Journal of Open-Source Software **2022** (link)

High-Throughput Discovery of Fluoride-ion Conductors via a Decoupled, Dynamic, and Iterative (DDI) Framework

J.D. Sundberg, D.L. Druffel, L.M. McRae, M.G. Lanetti, J.T. Pawlik, S.C. Warren
NPJ Computational Materials **2022** (link)
Featured by Chemistry World and Chemistry Views

Sc_2C, a 2D Semiconducting Electride

L.M. McRae, R.C. Radomsky, J.T. Pawlik, D.L. Druffel, J.D. Sundberg, M.G. Lanetti, C. Donley, K. White, and S.C. Warren
JACS **2022** (link) (& ChemRxiv **2021**)
Featured by C&EN

First-Principles Prediction of Electrochemical Electron–Anion Exchange: Ion Insertion without Redox

D.L. Druffel, J.T. Pawlik, J.D. Sundberg, L.M. McRae, M.G. Lanetti, and S.C. Warren
Journal of Physical Chemistry Letters **2020** (link)
Featured by Chemistry World

Synthesis and Electronic Structure of a 3D Crystalline Stack of MXene-Like Sheets

D.L. Druffel, M.G. Lanetti, J.D. Sundberg, J.T. Pawlik, M.S. Stark, C.L. Donley, L.M. McRae, K.M. Scott, and S.C. Warren
Chemistry of Materials **2019** (link)

Bonding in 2D Donor–Acceptor Heterostructures

A.H. Woomer, D.L. Druffel, J.D. Sundberg, J.T. Pawlik, and S.C. Warren.
Journal of American Chemical Society **2019** (link)

SKILLS OVERVIEW

Computational Chemistry

Core libraries: PyMatGen, ASE
Simulations: VASP, Materials Studio (CASTEP), LAMMPS
Evolutionary Algorithms: USPEX, CALYPSO
Machine Learning: MatMiner, DeepMD, Scikit-learn
Workflow Management: Atomate, Fireworks, Custodian
APIs: OPTIMADE, Materials Project, COD, AFLOW, OQMD, JARVIS

Experimental Chemistry

Synthesis: >1000°C furnaces, CVD, ALD, Arc Melting, Quartz Welding, Schlenk lines, Chromatography
Characterization: XRD, Raman, SEM, AFM, TEM, NMR, IR, MassSpec
Extras: Mass-flow, Vacuum, & Pressure control systems (built custom CVD system)

General Software Stack

Coding Languages: Python, SQL, Bash, HTML/CSS
Data Analysis + utilities: pandas, dask, numpy, numba, matplotlib, plotly
CLI: click, argparse, python-fire
ETL Workflows: Prefect, Fireworks, AirFlow
Website Frameworks: Django, Flask+Jinja+SQLAlchemy
Databases: SQLite, Postgres, MongoDB
APIs: Django-REST Framework, Graphene (graphql)
Front-end CSS & 3D: Bootstrap, Three.js, Verge3D
3D Modeling: Blender, VTK
CI: pytest, black, coverage, GitHub Actions

** I recommend visiting my Simmate repository, which showcases the use of many skills and packages listed above **

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