Brian A. Day

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SKILLS

Programming Languages	Python (NumPy, SciPy, Pandas, Torch, Flask, Django, RDKit), JavaScript/TypeScript (Angular), Bash, MATLAB, Mathematica,
Technologies	Git/Github/GitLab, Docker, Kubernetes, AWS, Terraform
Scientific Software	Grand-canonical Monte Carlo (RASPA), Molecular Dynamics (LAMMPS, GROMACS), Density Functional Theory (CP2K), Chemical Process Modeling (Aspen Plus / Dynamics)

WORK & RESEARCH EXPERIENCE

Simulations Plus, Inc. — **Research Triangle Park, NC (Remote)**

Senior Scientific Software Engineer — *June 2025 - Current*

Scientific Software Engineer — *April 2024 – June 2025*

Scientific Domain: Quantitative Systems Pharmacology

Languages: Python, Typescript, Matlab — Technologies: Django, Angular, Docker, Azure

- Developed quantitative systems pharmacology (QSP) software, updating model components, analysis and validation functions, and various frontend features.
- Unified data analysis between backend and web plotting, which required on-demand recalculation due to custom patient filtering, ensuring consistent data quality when generating reports.
- Assisted with software development efforts for customer services projects, including the development of a Matlab-based GUI for manipulation of SimBiology models.
- Designed and implemented frontend features for streamlined navigation of large projects, including interactive job hierarchy diagrams and statistical overviews.
- Spearheaded a significant documentation overhaul, leading to reduced demand on developers for assisting with model debugging and accelerated the timeline for licensing software to customers.

Emerald Cloud Lab — **Austin, TX (Remote)**

Scientific Software Engineer — *Sept 2022 – Jan 2024*

Scientific Domain: Bioengineering (Proteomics)

Languages: Python, Mathematica — Technologies: Flask, Docker, Kubernetes, AWS

- Developed Mathematica code for scientific data analysis, following best practices for documentation and testing. Conducted frequent code reviews, wrote design documents, and addressed bugs during on-call shifts.
- Collaborated with scientists to develop tools for the design, analysis, and visualization of mass spectrometry-based proteomics experiments, resulting in more efficient use of equipment and faster research timelines.
- Developed and deployed RESTful micro-services using Flask for Python, with Docker, Kubernetes, and AWS, for simulation of peptide fragmentation and ETL and analysis of mass spectrometry data sets.
- Contributed to internal and public development frameworks, adding functionality for uploading, downloading, and streaming files from Amazon S3, with appropriate authorization and integration into the relational database.

University of Pittsburgh — **Pittsburgh, PA**

Graduate Student Researcher. — *May 2018 – July 2022*

Scientific Domain: Chemical Engineering / Materials Science

Languages: Python, Bash — Technologies: RASPA, LAMMPS, CP2K, HPC with Slurm

- Computational chemist researching metal-organic frameworks (MOFs) and their applications. Dissertation focused on the development of a gas sensing array (electronic nose) for breath-based disease detection.
- Conducted high-throughput grand-canonical Monte Carlo simulations, writing Bash and Python scripts to generate and manage jobs submission on slurm-managed HPC.

- Using Python, developed a genetic algorithm for the design of optimized gas sensing arrays from a large library of materials. Also developed models and algorithms for the prediction of gas composition from sensor array output.
- Building upon ASE for Python, developed tools for positioning, modifying, and visualizing molecules and crystalline materials, and generating input files for molecular dynamics simulations.
- Other research projects included predicting electrical conductivity in MOFs using density functional theory, elucidating mechanisms of liquid sensing platforms using molecular dynamics, and predicting ligand exchange reactions and topological conversions in MOFs using a molecular dynamics-based toy model.

TEACHING EXPERIENCE

Rowan University **Glassboro, NJ (Remote)**

Adjunct Faculty, Online Course Developer *Aug 2024 – Current*

- Online course developer for ChE 06586 - Advanced Engineering Thermodynamics
- Topics include 1st and 2nd Law, Thermodynamic Calculus, Equilibrium and Stability, Pure Component and Mixture Properties, Phase and Reaction Equilibrium, Statistical Analysis of Ideal Gas, Imperfect Gases, Intro to Computational Chemistry, Polymer and Lattice Statistics, and Fermi-Dirac and Bose-Einstein Statistics

BUSINESS DEVELOPMENT EXPERIENCE

Competitions & Awards:

- TiE Global Pitch Competition, **Top 12 & Social Impact Award** (2021-2022 Season)
- TiE Pittsburgh Pitch Fest, **1st Place (**Pittsburgh, PA, March 30, 2022)
- Product Data and Management Alliance Pitch Competition, **1st Place** (Pittsburgh, PA, November 11, 2021)
- Randall Family Big Idea Competition, **2nd Place** (University of Pittsburgh, February 26 – April 9, 2021)
- Pitt Big Idea Blitz, **1st Place** (University of Pittsburgh, February 12-13, 2021)
- Pitt Big Idea Blast, **1st Place** (University of Pittsburgh, October 30-31, 2020)
- IBM BlueHack, **2nd Place (**University of Pittsburgh, October 25-26, 2019)

Workshops & Accelerators:

- Pitt Ventures First Gear (University of Pittsburgh, May 12, 2022 - June 30, 2022)
- Big Idea Center's Forge Student Accelerator (Pitt Innovation Institute, August 30, 2021 – May 2, 2022)
- Blast Furnace Student Accelerator (Pitt Innovation Institute, May 18 – July 15, 2021)
- The Money Table (Carnegie Mellon University, November 15-16, 2019)

EDUCATION

Ph.D. in Chemical Engineering **2016-2022**

University of Pittsburgh, Swanson School of Engineering

Advisor: Christopher E. Wilmer

Dissertation: Computational Design of MOF-based Electronic Noses for Disease Detection by Breath

B.S. in Chemical Engineering **2012-2016**

Lehigh University, P.C. Rossin College of Engineering & Applied Science

PUBLICATIONS

Google Scholar

6. **B. A. Day,** N. I. Ahualli, and C. E. Wilmer, Multipressure sampling for improving the performance of MOF-based electronic noses, *ACS Sens.*, 9, 3531–3539 (2024). [https://doi.org/10.1021/acssensors.4c00199]
5. Z. Zeng, M. Islamov, Y. He, **B. A. Day,** N. L. Rosi, C. E. Wilmer, and A. Star, Size-Based Norfentanyl Detection with SWCNT@UiI-MOF Composites, *ACS Appl. Mater. Interfaces*, 16, 1, 1361–1369 (2023). [https://doi.org/10.1021/acsami.3c17503]
4. P. Qin, **B. A. Day**, S. Okur, C. Li, A. Chandresh, C. E. Wilmer, and L. Heinke, VOC-mixture sensing with a MOF-Film Sensor Array: Detection and Discrimination of Xylene Isomers and Its Ternary blends, *ACS Sens.*, 7, 6, 1666–1675 (2022). [https://doi.org/10.1021/acssensors.2c00301]

3. **B. A. Day** and C.E. Wilmer, Computational Design of MOF-based Electronic Noses for Dilute Gas Species Detection: Application to Kidney Disease Detection, *ACS Sensors*, 6, 12, 4425–4434, (2021). [https://doi.org/10.1021/acssensors.1c01808]
2. D. L. White, **B. A. Day,** Z. Zeng, Z. M. Schulte, N. R. Borland, N. L. Rosi, C. E. Wilmer, and A. Star, Size Discrimination of Carbohydrates via Conductive Carbon Nanotube @ Metal Organic Framework Composites, *J. Am. Chem. Soc.*, 143, 21, 8022-8033, (2021). [https://doi.org/10.1021/jacs.1c01673]
1. **B. A. Day** and C. E. Wilmer, Genetic Algorithm Design of MOF-based Sensor Arrays for CO_2-in-Air Sensing, *Sensors*, 20, 3, 924, (2020). [https://doi.org/10.3390/s20030924]

PATENTS

1. **B. A. Day** and C. E. Wilmer, Multi-Pressure Sampling for Improving the Performance of Electronic Noses Using Gas Adsorbing Sensing Elements. PCT/US2023/070839. Filed July 24, 2023.