Brian A. Day

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Software Engineer with a background in computational chemistry and data science.

EDUCATION

Ph.D. Candidate 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

SKILLS

Programming Languages	Python (Flask, Numpy, Scipy, Pandas, TensorFlow), Mathematica, JavaScript/TypeScript, MATLAB, Bash
Technologies	Git, Github, Docker, Kubernetes, AWS, Amazon S3
Scientific Software	Grand-canonical Monte Carlo (RASPA), Molecular Dynamics (LAMMPS), Density Functional Theory (CP2K), Chemical Process Modeling (Aspen Plus / Dynamics)

WORK & RESEARCH EXPERIENCE

Emerald Cloud Lab **Austin, TX (Remote)**
Scientific Computing Engineer *Sept 2022 – Jan 2024*

- Developed Mathematica code for the analysis of scientific data, following best software practices for documentation and unit testing. Conducted frequent code reviews, wrote design documents, and addressed bugs during on-call shifts.
- Collaborated with research scientists to develop tools assisting with the design, analysis, and visualization of mass spectrometry-based proteomics experiments, resulting in more efficient use of laboratory equipment and faster research timelines.
- Developed REST API micro-services using Flask for Python, with Docker, Kubernetes, and AWS, for simulating peptide fragmentation and analyzing mass spectrometry data sets.
- Integrated new analysis, simulation, and visualizations functions into the front-end product.
- Developed and implemented a materials packing algorithm resulting in more efficient use of facility storage space and floor operator time.
- Contributed to internal development frameworks and tools, resulting in faster development times, and to the public software development kit, adding functionality for uploading, downloading, and streaming files from Amazon S3, with appropriate authorization, and integrating the uploaded files into the relational database.

University of Pittsburgh **Pittsburgh, PA**
Graduate Student Researcher – Wilmer Lab *May 2018 – July 2022*

- 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.
- Using Python, developed a genetic algorithm for the design of optimized gas sensing arrays from a large library of materials. Also developed analytical models and numeric algorithms for the prediction of gas composition given a known 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.

Graduate Student Researcher – Kumta Lab *January 2017 – May 2018*

- Developed nanostructured electrodes and coatings for lithium-metal batteries to control the deposition of lithium and formation of the solid electrolyte interphase.
- Developing electrospun polymer separators for lithium-sulfur batteries to minimize poly-sulfide dissolution.
- Develop polymeric coating for controlling current density to improve coin cell testing, and investigated swelling due to solvent in the liquid electrolyte.

Lehigh University **Bethlehem, PA**

Undergraduate Student Researcher – Snyder Lab *January 2015 – May 2016*

- Synthesized nanoporous carbon films through deposition of a glucose/silica nanoparticle solution, followed by carbonization, and subsequent etching of the silica
- Examined the effects of synthetic conditions and nitrogen doping on film ordering and behavior.

Undergraduate Student Researcher – Tuzla Lab *January 2014 - August 2014*

- Developed a computational model in MATLAB for comparing various energy storage technologies for use with concentrated solar power plants, focusing specifically on latent heat thermal energy storage using inorganic salts as the phase change materials.
- The model spanned hourly to yearly operations and the was used to determine economically efficient operating conditions.

Applied Separations Inc. **Allentown, PA**

Nanoparticle Synthesis using Supercritical Fluid Technologies *June 2015 - August 2015*

- Developed and refined laboratory equipment used to synthesize nanoparticles for biopharmaceutical research applications via the rapid expansion of a supercritical solution (RESS) of CO_2 through a fine-tipped nozzle.
- By varying process conditions, nozzle types, and collection methods, we developed an effective and highly reproducible procedure, resulting in a poster presentation at a local technology conference.

TEACHING EXPERIENCE

Teaching Assistantships

- CHE 314 – Product Design (University of Pittsburgh, Fall 2019)
- CHE 100 – Introduction to Chemical Engineering (University of Pittsburgh, Fall 2018)
- CHE 400 – Reactor Engineering & Design (University of Pittsburgh, Summer 2018)
- ENGR 011 – Introduction to Engineering (University of Pittsburgh, Fall 2017)
- CHE 210 – Chemical Engineering Thermodynamics (Lehigh University, Spring 2015)

Guest Lectures

- “Edit Mode: Shaping Objects in Blender” for Blender Workshop (University of Pittsburgh, Summer 2022)
- “Health-E-Nose: Intro to Product Design” for ChE 613 - Process Design (University of Pittsburgh, Spring 2021)
- “Visualization Crash Course” for CHE 314 - Product Design (University of Pittsburgh, Fall 2020)
- “Visualization Crash Course” for CHE 314 - Product Design (University of Pittsburgh, Fall 2019)

Mentoring Experience

- Nicholas Ahualii, Undergraduate Student Researcher (Summer 2021 - Spring 2022)
- Spencer Conway, Undergraduate Student Researcher (Summer - Fall 2021)
- Christian Molfetto, Undergraduate Student Researcher (Summer - Fall 2021)
- Spencer Smith, Undergraduate Student Researcher (Fall 2019)

PUBLICATIONS

Google Scholar

Published:

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 Sensors*, 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]

In Preparation:

- **B. A. Day*,** Y. Han*, N. L. Rosi, and C. E. Wilmer, Ligand Exchange Induced Dynamic Topological Conversions in Mesoporous bio-MOFs Family. (*indicates equal contribution)
- **B. A. Day,** N. I. Ahualli, and C. E. Wilmer, Multiplexed E-Noses: Improving Sensitivity through Multiple Pressure Sampling

PRESENTATIONS

Presenting Author (Oral):

5. **B. A. Day** and C. E. Wilmer, "Computational Design of MOF-based Electronic Noses for Disease Detection by Breath", AIChE Pandemic Advance Capabilities and Engineering: Solutions in the Aftermath of COVID-19, Virtual, November 18, 2021. **(Invited Talk)**
4. **B. A. Day** and C. E. Wilmer, "Computational Design of MOF-based Electronic Noses for Disease Detection by Breath", AIChE Annual Meeting, Boston, MA, USA, November 8, 2021.
3. **B. A. Day** and C. E. Wilmer, "Computational Design of MOF-based Electronic Noses for Disease Detection by Breath", University of Pittsburgh's ΩXE Departmental Research Day, University of Pittsburgh, Pittsburgh, PA, USA, August 26, 2021.
2. **B. A. Day** and C. E. Wilmer," Examining Electrical Conductivity in Metal-Organic Frameworks Through Marcus Theory", Pitt-CMU Simulators Meeting, University of Pittsburgh, Pittsburgh, PA, USA, May 15, 2019.
1. P. J. Hanumantha, **B. A. Day**, M. K. Datta, P. M. Shanthi, B. Gattu, and P. N. Kumta, "Engineered Porous Foam Electrodes-New Approaches to Dendrite-Free Anodes for Li-Metal Batteries", 232nd ECS National Conference, National Harbor, MD, USA, October 4, 2017.

Presenting Author (Poster):

3. **B. A. Day** and C. E. Wilmer, "Computational Design of a MOF-Based Electronic Nose for Exhaled Breath Analysis", Midwest Thermodynamics and Statistical Mechanics Conference [Wed-based], University of Wisconsin-Madison, Madison, WI, USA, June 14, 2021.
2. **B. A. Day** and C. E. Wilmer, "Computational Design of MOF-based Electronic Noses: Pursuing Complex Gas Mixtures and Large-Scale Screening", Pittsburgh Quantum Institute Poser Session [Wed-based], Pittsburgh, PA, USA, April 17, 2020.
1. **B. A. Day** and C. E. Wilmer, "Computational Design of MOF-based Electronic Noses: Pursuing Complex Gas Mixtures and Large-Scale Screening", University of Pittsburgh's ΩXE Departmental Research Day, University of Pittsburgh, Pittsburgh, PA, USA, February 14, 2020.

AWARDS & HONORS

Conferences:

- University of Pittsburgh's ΩXE Departmental Research Day – 2nd Place Oral Presentation Award, (Pittsburgh, PA, August 26, 2021]
- Pittsburgh Quantum Institute Poster Session Travel Award Winner (Pittsburgh, PA [Web-based], April 17, 2020)

Business Competitions:

B. A. Day "Health-E-Nose"

- TiE Global Pitch Competition, **Awarded: Top 12 - $1,250, Social Impact Award - $1,250** (2021-2022 Season)
- TiE Pittsburgh Pitch Fest, **Awarded: 1st Place, Entry into TiE Global Pitch Competition** (Pittsburgh, PA, March 30, 2022)
- Product Data and Management Alliance Pitch Competition, **Awarded: 1st Place, $2,500, Free Consulting Services** (Pittsburgh, PA, November 11, 2021)

B. A. Day and B. Segel, "Health-E-Nose"

- Randall Family Big Idea Competition, **Awarded: 2nd Place, $15,000** (University of Pittsburgh, February 26 – April 9, 2021)
- Pitt Big Idea Blitz, **Awarded: 1st Place, $1000** (University of Pittsburgh, February 12-13, 2021)
- Pitt Big Idea Blast, **Awarded: 1st Place, Entry into final round of Randall Family Big Idea Competition** (University of Pittsburgh, October 30-31, 2020)

B. A. Day, A. I. Baimoldina, A. C. Greene, A. L. Schilling, and K. B. Sezginel, "WeHaul Healthcare"

- IBM BlueHack, **Awarded: 2nd Place, $1250 (**University of Pittsburgh, October 25-26, 2019)

CONFERENCES, WORKSHOPS, & COMPETITIONS

Academic Conferences:

- American Institute of Chemical Engineering Annual Meeting (Boston, MA, November 7-19, 2021)
- Midwest Thermodynamics and Statistical Mechanics Conference (University of Wisconsin-Madison, June 14-17, 2021)
- Pittsburgh Quantum Institute Poster Session (Pittsburgh, PA, April 17, 2020)
- Pitt-CMU Simulators Meeting (Carnegie Mellon University, May 15, 2019)
- American Institute of Chemical Engineering Annual Meeting (Pittsburgh, PA, October 28 – November 2, 2018)
- Midwest Thermodynamics and Statistical Mechanics Conference (University of Pittsburgh, June 10-12, 2018)
- Pitt-CMU Simulators Meeting (Carnegie Mellon University, May 22, 2018)
- Electrochemical Energy Symposium (Carnegie Mellon University, November 2-3, 2017)
- 232nd Electrochemical Society National Conference (National Harbor, MD, October 1-5, 2017)

Academic Workshops:

- Python for Scientific Computing and TensorFlow for AI by Dr. Steven Lynch (Web-based Workshop, June 7-11, 2021)
- Northwestern University RASPA Workshop (Northwestern University, July 10-13, 2018)
- Academic Writing from the Readers Perspective by Dr. George G. Gopen (University of Pittsburgh, November 30, 2016)

Business Workshops & Competitions:

- Pitt Ventures First Gear (University of Pittsburgh, May 12, 2022 - June 30, 2022)
- Product Development and Management Association (PDMA) Pitch Competition (Carnegie Mellon University, November 11, 2021)
- 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)
- Randall Family Big Idea Competition (University of Pittsburgh, February 26 – April 9, 2021)
- Pitt Big Idea Blitz (University of Pittsburgh, February 12-13, 2021)
- Pitt Big Idea Blast, (University of Pittsburgh, October 30-31, 2020)
- The Money Table (Carnegie Mellon University, November 15-16, 2019)
- IBM BlueHack, (University of Pittsburgh, October 25-26, 2019)