Brian A. Day

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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

SKILLS

Programming Languages	Python (Numpy, Scipy, Pandas, Torch, ASE, RDKit, Flask, Django), Mathematica, JavaScript/TypeScript, MATLAB, Bash
Technologies	Compute Clusters, Git/Github/Gitlab, Jupyter Notebook, Google Collab, Docker, Kubernetes, AWS (EC2, EKS, S3, RDF, Aurora), Terraform
Scientific Software	Grand-canonical Monte Carlo (RASPA), Molecular Dynamics (LAMMPS), Density Functional Theory (CP2K), Chemical Process Modeling (Aspen Plus / Dynamics)
Visualization Software	Inkscape (Vector Graphics), Blender (3D Modelling), P5JS (Animations)

RESEARCH EXPERIENCE

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 gas adsorption simulations. Developed a genetic algorithm for the design of optimized gas sensing arrays from a large library of materials. Also developed analytical models and algorithms for the prediction of gas composition given a known sensor array output.
- Developed tool suite 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.
- Developed electrospun polymer separators for lithium-sulfur batteries to minimize poly-sulfide dissolution.
- Developed polymeric coating for controlling current density to improve coin cell testing, and investigated swelling due to solvent in the liquid electrolyte.

WORK EXPERIENCE

Simulations Plus, Inc. **Research Triangle Park, NC (Remote)**
Scientific Software Engineer *April 2024 – Current*

- Supported PK/PD modeling team in conducting virtual clinical trials by updating various model components, data analysis functions, model / data validation functions, and developing new plotting features.
- Developed a quasi-equilibrium-based binding primitive which significantly accelerated models with fast kinetics.

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

- 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 RESTful micro-services using Flask for Python, with Docker, Kubernetes, and AWS, for simulating peptide fragmentation and analyzing mass spectrometry data sets.
- Contributed to internal development frameworks, 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 newly uploaded files into the relational database.

TEACHING EXPERIENCE

Rowan University **Glassboro, NJ (Remote)**
Adjunct Faculty, Online Course Developer *Aug 2024 – Current*

- Online course developer for ChE 06586 - Advanced Engineering Thermodynamics, covering both classical and statistical 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

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]

PRESENTATIONS

Presenting Author (Oral):

4. **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)**
3. **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.
2. **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.
1. **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.

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.

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.

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)

BUSINESS WORKSHOPS, & COMPETITIONS

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)