

Brian A. Day

(215) 850-1896 | 22bday@gmail.com | <https://birdday.github.io>

EDUCATION

Ph.D. Candidate in Chemical Engineering	2016-2022
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University of Pittsburgh, Swanson School of Engineering

Advisor: Christopher E. Wilmer

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

B.S. in Chemical Engineering	2012-2016
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Lehigh University, P.C. Rossin College of Engineering & Applied Science

RESEARCH EXPERIENCE

University of Pittsburgh	Pittsburgh, PA
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Graduate Student Researcher – Wilmer Lab

May 2018 – May 2022

Researcher in a computational materials lab with a focus on metal-organic frameworks (MOFs). My projects focus on the development of a gas sensing array known as an electronic nose. To develop this array, we run high-throughput grand canonical Monte-Carlo (GCMC) simulations of gas adsorption, and with subsequent data analysis and algorithmic design of arrays based in Python. Other projects have included using density functional theory (DFT) to probe the electrical conductivity of MOFs, molecular dynamics (MD) simulations of gas diffusion, and toy models of ligand exchange in MOFs.

University of Pittsburgh	Pittsburgh, PA
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Graduate Student Researcher – Kumta Lab

January 2017 – May 2018

Researched anodes for lithium-metal batteries with a focus on the development of nanostructured electrodes and surface coatings for controlled deposition of lithium and formation of the solid electrolyte interphase. Other projects included developing separators for lithium-sulfur batteries to minimize poly-sulfide dissolution and modification of coin-cells for improved testing.

Lehigh University	Bethlehem, PA
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Nanoporous Film Development

January 2015 – May 2016

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

Lehigh University	Bethlehem, PA
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Solar Power and Storage System

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 was used to determine economically efficient operating conditions.

WORK EXPERIENCE

Applied Separations Inc.	Allentown, PA
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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 CO₂ through a fine-

tipped nozzle. By varying process conditions, nozzle types, and collection methods, we developed an effective and highly reproducible procedure.

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

- “Health-E-Nose: Understanding 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)

Miscellaneous

- Private Tutor for Pre-algebra, Algebra I, Algebra II, Geometry, Physics, and Chemistry (Spring 2020-Present)
- Men’s High School Volleyball Assistant Coach (North Hills High School, Spring 2018)

PUBLICATIONS

Published:

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, 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, *Journal of the American Chemical Society*, 143, 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 CO₂-in-Air Sensing, *Sensors*, 20, 924, (2020). [<https://doi.org/10.3390/s20030924>]

Submitted:

1. 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* (2022). [Submitted]

In Preparation:

3. **B. A. Day** and C. E. Wilmer, Finite Volume Grand Canonical Monte Carlo Simulations: Numerical Approaches for Reproducing the Gibbs-NPT Ensemble for Low Concentration Gases

2. **B. A. Day**, N. I. Ahualli, and C. E. Wilmer, Multiplexed E-Noses: Improving Sensitivity through Multiple Pressure Sampling
1. **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)

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 Ω XE 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 Ω XE Departmental Research Day, University of Pittsburgh, Pittsburgh, PA, USA, February 14, 2020.

Non-presenting Author (Oral & Poster):

(* indicates presenting author)

3. P. Thanapisitikul*, B. Gattu, P. M. Shanthi, **B. A. Day**, M. K. Datta, and P. N. Kumta, "Surface Patterning of Lithium Metal: Novel Approach to Stable Li Metal Anodes", 233rd ECS National Conference, Seattle, WA, USA, May 14, 2018. (Oral Presentation)
2. B. Gattu*, P. M. Shanthi, P. Thanapisitikul, **B. A. Day**, M. K. Datta, O. I. Velikokhatnyi, and P. N. Kumta, "Suppression of Dendrite in Lithium Sulfur Batteries Using a Composite Polymer Electrolyte", 233rd ECS National Conference, Seattle, WA, USA, May 13, 2018. (Oral Presentation)
1. **B. A. Day**, B. Gattu*, P. M. Shanthi, M. K. Datta, and P. N. Kumta, "Surface Modification of Porous Foam Electrodes: Stabilization of Solid Electrolyte Interphase Formation in Li-Metal Batteries", 233rd ECS National Conference, Seattle, WA, USA, May 14, 2018. (Oral Presentation)

AWARDS & HONORS

Conferences:

- University of Pittsburgh's Ω XE Departmental Research Day – 2nd Place Oral Presentation Award, (Pittsburgh, PA, August 26, 2021)

Last Updated: March 4, 2022

- Pittsburgh Quantum Institute Poster Session Travel Award Winner (Pittsburgh, PA [Web-based], April 17, 2020)

Business Competitions:

B. A. Day “Health-E-Nose”

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:

- Product Development and Management Association (PDMA) Pitch Competition (Carnegie Mellon University, November 11, 2021)
- Big Idea Center’s Forge Student Accelerator (University of Pittsburgh’s Innovation Institute, August 30, 2021 – May 2, 2022)
- Blast Furnace Student Accelerator (University of Pittsburgh’s 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)

UNIVERSITY INVOLVEMENT & LEADERSHIP

- Co-founder and Lead Organizer of STEM & Society Lecture Series (University of Pittsburgh, July 2020 – January 2021)
- Pittsburgh Quantum Institute Lab Liaison (University of Pittsburgh, May 2020-May 2021)
- Graduate Student Organizing Committee (University of Pittsburgh, May 2018 – Current)
- Chemical Engineering Safety Review Board (University of Pittsburgh, May 2018 – May 2020)
- Volunteer at Chem Fest, National Chemistry Week Celebration (Carnegie Science Center, Oct 16-22, 2016)

SKILLS

Language	English (Native), Latin (10+ Years), French (Beginner)
Software	
GitHub	https://github.com/birdday
Development	Python, Bash, Java, C#
Scientific	RASPA, CP2K, LAMMPS, Aspen Plus, Aspen Dynamics, MATLAB
Graphics / Video	Blender, Inkscape
Laboratory	Scanning Electron Microscopy with EDX Analysis, Atomic Force Microscopy, RAMAN Microscopy, Impedance Spectroscopy, X-Ray Diffraction, Small-Angle X-Ray Scattering, Arbin Battery Cycling, Sputter Coater, Glove Box, Ball Milling, Tube and Box Furnace, High-Pressure Gases

REFERENCES

References available upon request.