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Cambridge, MA

Lucas Attia

LinkedIn
Google Scholar
Personal Website

PhD Candidate · MIT Chemical Engineering | DOE Computational Science Graduate Fellow

Chemical engineering PhD researcher with expertise in pharmaceutical nanotechnology, molecular simulation, and machine learning. Accomplished communicator, with 8 peer-reviewed publications, 41+ presentations at conferences and symposia, and 12 award-winning presentations. Experienced fundraiser, securing $330k in scholarships, $380k in fellowships, and $100k in grant funding.

Education

Massachusetts Institute of Technology (MIT) — **Cambridge, MA**
PhD Chemical Engineering — *2021 – 2026 (expected)*
- Minor: Machine Learning
- Thesis (working title): *Nanoemulsion-Templated Drug Nanoparticles for Advanced Oral Delivery*

University of Delaware — **Newark, DE**
Honors B.S. Chemical Engineering with Distinction, GPA: 3.92 — *2017 – 2021*
- Minors: Chemistry, Computer Science
- Thesis: *Computational Modeling of Fluid Flow through Open Cellular Foams and Lattice Structures*

Technical Experience

Eli Lilly and Company — **Boston, MA**
Cheminformatics Intern — *Summer 2024*
- Developing cheminformatics workflows to computationally design lipid nanoparticles (LNPs) for the delivery of genetic medicine.

MIT Department of Chemical Engineering — **Cambridge, MA**
PhD Research Fellow, Doyle Group — *2021 – Present*
- Programmed deep learning models to predict organic solubility, with leading performance on unseen solutes (open source code), leading to a manuscript accepted in Nature Communications, an invitation to present at the Computational Pharmaceutics Symposium (2024), and the MDPI Pharmaceuticals Award (2024). Model distributed through a Python package, website, Wolfram Alpha package, and Rowan Scientific's platform. Presented work at MIT Molecular ML Conference (2024) and the MIT Health and Life Science Collaborative Symposium (2024).
- Simulated the effects of excipients on nanoparticle crystallinity using atomistic molecular dynamics (open source code), leading to a published manuscript and an invited presentation at MIT Math Department seminar. Recognized with Merck Poster Award, CRS Annual Meeting (2024); Langmuir Graduate Award, ACS CSSS (2024); Dow Travel Award, MIT ChemE (2024)
- Invented hydrogel encapsulation systems to control release kinetics of nanoparticle-based drugs, published in Advanced Healthcare Materials and featured in MIT News. Recognized with Best Seminar Award, MIT ChemE (2023); Best Poster, Preclinical Form and Formulation GRC (2023); Best Poster, APS Virtual Polymer Physics Symposium (2023).
- Managed 2 undergraduate researchers and 1 research technician on daily research tasks and long-term project deliverables.
- Raised $100k through Koch Institute Frontier Research Program to computationally design PROTAC nanoparticle formulations.

Lawrence Berkeley National Laboratory — **Berkeley, CA**
Machine Learning Intern, Blau Group — *Summer 2023*
- Developed graph-based deep learning models to predict optical nanoparticle properties. Incorporated capability for data augmentation, which improved model accuracy by 27 % (open source code), resulting in a manuscript under review. Presented results at ACS CSSS, MRS Fall Meeting, and MIT Soft Materials Seminar.

University of Delaware — **Newark, DE**
Undergraduate Researcher, Fromen Group — *2017 – 2021*
- Modeled fluid flow through 3-D printed lattice structures using computational fluid dynamics (CFD) to optimize lattice design, leading to a published manuscript and my undergraduate thesis.
- Determined efficacy of metal organic frameworks (MOFs) nanoparticles as aerosolizable pulmonary drug delivery vehicles, contributing to two published manuscripts. Earned Goldwater Scholarship.

Merck & Co. — **Boston MA**
Discovery Pharmaceutical Sciences Intern — *Summer 2020*
- Created research plan for statistical modeling and multi-scale simulation of a lipid nanoparticle (LNP) production process.
- Evaluated and implemented software alternative for data storage of proprietary drug candidate risk assessment (RA) documents.
- Digitized drug candidate risk assessments to standardize and structure data collection for future analysis.

Software Skills

Languages	Python, MATLAB, Julia, Unix, R, C+, Git, LaTeX,
Molecular Dynamics	GROMACS, CHARMM, polymer simulation, molecular visualization
Scientific Computing	High performance computing, slurm, parallelization
Machine Learning	Unsupervised learning, deep neural networks, Pytorch, keras, sklearn
Cheminformatics	rdkit, mordred, deepchem, chemprop

Experimental Skills

Nanomaterials	Nanoemulsion design, dynamic light scattering (DLS), scanning electron microscopy (SEM), fluorescent spectroscopy, transmission electron microscopy (TEM)
Soft Materials	Hydrogel synthesis, rheological characterization, droplet microfluidics
Crystallography	X-ray diffraction (XRD), Raman spectroscopy, differential scanning calorimetry (DSC)

Select Honors and Awards

Fellowships

- **Chemical Engineering Communication Lab Fellowship**, Massachusetts Institute of Technology 2022 – 2026
- **Rosemary Wojtowicz Fellowship Fund**, Massachusetts Institute of Technology 2021 – 2022
- **Simon (1968) Fellowship Fund**, Massachusetts Institute of Technology 2021 – 2022
- **Computational Science Graduate Fellowship**, U.S. Department of Energy 2021 – 2025
- **Graduate Research Fellowship Program**, National Science Foundation (declined) 2021 – 2024
- **Harward Munson Fellowship**, University of Delaware 2021
- **Summer Scholars Science and Engineering Scholarship**, University of Delaware 2019
- **Summer Research Internship**, NASA Delaware Space Grant Consortium 2018

Scholarships

- **American Association of University Professors Undergraduate Award**, University of Delaware 2021
- **Robert L. Pigford Undergraduate Award for Chemical Engineering**, University of Delaware 2020
- **NASA Undergraduate Tuition Scholarship**, NASA Delaware Space Grant 2020
- **Engineering Alumni Association Scholarship**, University of Delaware 2020
- **Barry M. Goldwater Scholarship**, The Barry Goldwater Scholarship and Excellence in Education Foundation 2020
- **Trustee Scholarship**, University of Delaware 2017 – 2021
- **Diamond State Scholarship**, Delaware Department of Education 2017 – 2021

Awards

- **Pharmaceuticals Travel Award**, MDPI 2024
- **Graduate Student Council Travel Grant**, MIT Graduate Student Council 2024
- **Dow Travel Award**, MIT Department of Chemical Engineering 2024
- **Merck Best Poster Award**, Controlled Release Society Annual Program and Exposition 2024
- **Langmuir Graduate Student Award**, American Chemical Society Colloid and Surface Science Symposium 2024
- **Best Student Seminar Award**, MIT Department of Chemical Engineering 2024
- **National Finalist**, Dissolution Research Presentation International, Society for Pharmaceutical Dissolution Science 2023
- **3rd Place Poster Award**, Virtual Polymer Physics Symposium, American Physical Society 2023
- **Best Poster Award**, Preclinical Form and Formulation for Drug Discovery Gordon Research Conference 2023
- **Future Leaders in Chemical Engineering Symposium Award**, North Carolina State University 2020
- **1st Place, Intern Elevator Pitch Competition**, Merck & Co. 2020
- **2nd Place Poster in Materials Science and Engineering**, AIChE Annual Student Conference 2019
- **General Honors Award**, University of Delaware 2019
- **3rd Place Poster, Biotechnology and Biomedical Career Fair Poster Reception**, University of Delaware 2019
- **National Merit Scholarship Finalist**, National Merit Scholarship Corporation 2017
- **Future Scientist Award**, U.S. Department of Agriculture 2016

Leadership

Gordon Research Seminar **Cambridge, MA**

Conference Planning Chair (peer-elected), Preclinical Form and Formulation for Drug Discovery *2023 – 2025*

- Develop conference program focused on applications of computational tools in drug formulation, delivery, and development.
- Communicate with industrial and academic stakeholders to fund-raise and promote conference.

MIT Chemical Engineering Communication Lab **Cambridge, MA**

Graduate Communication Fellow *2022 – Present*

- Awarded prestigious departmental fellowship to engage with scientific and technical communication efforts in the department.
- Deliver 3+ workshops on technical communication to department annually.
- Coached 50+ peers in various oral, written, and visual communication over the course of 110+ hours of coaching appointments.

MIT Department of Chemical Engineering **Cambridge, MA**

Graduate Teaching Fellow *Spring 2024*

- Taught 14 students in 10.494B: Therapeutic Nanoparticle Manufacturing, and 16 students in 10.493: Electrochemical Energy.

University of Delaware **Newark, DE**
President's Strategic Planning Committee, Office of the President *2021*

- Served as the dean-nominated student representative on a cross-functional committee to conduct post-COVID planning.
- Strategized institutional-level changes to incorporate experiental learning and field work into undergraduate curricula.

University of Delaware **Newark, DE**
Public Relations Chair (peer-elected), Engineers Without Borders *2017 – 2021*

- Partnered with international communities to design engineering solutions, including a water distribution system in the Philippines and a well water system in Malawi.
- Developed a corporate sponsorship package to recruit corporate sponsors, managed publication of biannual newsletter, and coordinated press releases with the University Communications Office.
- Mentored underclassmen in academic and career development through formal mentorship program.

University of Delaware **Newark, DE**
Planning Committee (faculty-selected), AIChE Chapter *2019 – 2020*

- Reformed organizational structure of the chapter to streamline workflows and dedicate executive board positions to K-12 STEM Outreach and Diversity & Inclusion.

Publications

1. **Attia, L.***, Nguyen, D.*, Lui, K., Qin, Q., Doyle, P.S., "Size-controlled templating of drug nanoparticles from nanoemulsion precursors for versatile nanoformulation". *Chemistry of Materials* (in preparation).

2. **Attia, L.**, Burns, J., Doyle, P.S., Green, W.H. "Data-driven Organic Solubility Prediction at the Limit of Aleatoric Uncertainty". *Nature Communications* (accepted).
doi:10.26434/chemrxiv-2024-93qp3

3. Sivonxay, E., **Attia, L.**, Spotte-Smith, E.W.C., Sanchez-Lengeling, B., Xia, X., Barter, D., Chan, E.M., Blau. S.M., "Inverse Design of Complex Nanoparticle Heterostructures via Deep Learning on Heterogeneous Graphs". *Nature Computational Science* (in review).
10.26434/chemrxiv-2024-1dw4q

4. **Attia, L.**, Nguyen, D., Gokhale, D., Zheng, T., Doyle, P.S. (2024) "Surfactant-polymer complexation and competition on drug nanocrystal surfaces controls crystallization". *ACS Applied Materials & Interfaces*, 16, 26, 34409–34418.
doi:10.1021/acsami.4c06815

5. Raines, K., Agarwal, P., Augustijns, P., Alayoubi, A., **Attia, L.**, Bauer-Brandl, A., ..., Polli, J. E. (2023) "Drug Dissolution in Oral Drug Absorption: Workshop Report." *The AAPS Journal*, 25(6)
doi:10.1208/s12248-023-00865-8

6. **Attia, L.**, Chen, L.H., Doyle, P.S., (2023) "Orthogonal gelations to synthesize core-Shell hydrogels Loaded with nanoemulsion-templated drug nanoparticles for versatile oral drug delivery". *Advanced Healthcare Materials*, 12(31), 2301667
doi:10.1002/adhm.202301667

7. Woodward, I., **Attia, L.**, Patel, P., Fromen, C.A. (2021). "Scalable 3D-printed lattices for pressure control in fluid applications". *AIChE Journal*, 67(12).
doi:10.1002/aic.17452

8. Jarai, B.M., Stillman, Z.S., **Attia, L.**, Decker, G.E., Bloch, E.D., Fromen, C.A. (2020). "Evaluating UiO-66 Metal-Organic Framework (MOF) Nanoparticles as Acid-Sensitive Carriers for Pulmonary Drug Delivery Applications". *ACS Applied Materials & Interfaces*, 12:35 38989–39004.
doi: 10.1021/acsami.0c10900

9. Decker, G.E., Stillman, Z.S., **Attia, L.**, Fromen, C.A., Bloch, E.D. (2019). "Controlling size, defectiveness, and fluorescence in nanoparticle uio-66 through water and ligand modulation". *Chemistry of Materials*, 31(13), 4831-4839.
doi: 10.1021/acs.chemmater.9b01383

Select Presentations

Invited Talks

1. **Attia, L.**, Burns, J., Nguyen, D., Doyle, P.S., Green, W.H. "Organic Solubility Prediction at the Limit of Aleatoric Uncertainty". *Seminar in Fluid Mechanics and Transport Phenomena*. Massachusetts Institute of Technology, Cambridge, MA, May 2025.

2. **Attia, L.**, Nguyen, D., and Doyle, P.S. "Templating lipophilic drug nanoparticles from nanoemulsion precursors for bioavailability enhancement". *UM-AAPS PharmAdvance Conference*. University of Mississippi, Oxford, MS, April 2025.

3. **Attia, L.**, Burns, J., Nguyen, D., Doyle, P.S., Green, W.H. "Organic Solubility Prediction at the Limit of Aleatoric Uncertainty". *Symposium on Computational Pharmaceutics - AI and Modeling in Pharma 4.0*. University of Macau Department of Pharmaceutical Sciences, Macua, China, December 2024.

4. **Attia, L.**, Sivoxnay, E., Xia, X., Helms, B.A., Chan, E., Blau, S.M.. "Inverse Design of Upconverting Nanoparticles via Deep Learning on Physics-Infused Heterogeneous Graphs". *Seminar in Fluid Mechanics and Transport Phenomena*. Massachusetts Institute of Technology, Cambridge, MA, October 2024.

5. **Attia, L.**, Nguyen, D., Gokhale, D., Zheng, T., Doyle, P.S. "Revealing the molecular origins of surface condition-dependent nanoparticle structure using classical molecular simulations". *Computational Research in Boston and Beyond*. MIT Department of Mathematics, Cambridge, MA, June 2024.

Oral Presentations

1. **Attia, L.**, Weiss, T. "Communicating through Visual Design". *Department of Chemical Engineering Workshop*. Cambridge, MA, February 2025.

2. **Attia, L.**, Ripley, K. "Delivering an effective poster". *Department of Chemical Engineering Individual Laboratory Experience, MIT*. Cambridge, MA, February 2025.

3. Burns, J.W., **Attia, L.**, Doyle, P.S., Green, W.H. "Organic Solubility Prediction at the Limit of Aleatoric Uncertainty". *Pfizer Chemistry Connect*, Cambridge, MA, November 2024.

4. **Attia, L.**, Doyle, P.S. "Bottom-up templating of drug nanoparticles in core-shell hydrogel particles for versatile oral drug delivery". *Controlled Release Society Annual Meeting and Exposition*. Bologna, Italy, July 2024.

5. **Attia, L.**, Sivoxnay, E., Xia, X., Helms, B.A., Chan, E., Blau, S.M. "Inverse Design of Upconverting Nanoparticles via Deep Learning on Physics-Infused Heterogeneous Graphs". *American Chemical Society Colloids and Surface Science Symposium*. University of Washington, Seattle, WA, June 2024.

6. **Attia, L.**, Nguyen, D., Gokhale, D., Zheng, T., Doyle, P.S. "Understanding and predicting drug nanoparticle crystallinity using molecular simulation". *American Chemical Society Colloids and Surface Science Symposium*. University of Washington, Seattle, WA, June 2024. [**Langmuir Graduate Award Session**]

7. **Attia, L.**, Ripley, K. "Delivering an effective poster". *Department of Chemical Engineering Individual Laboratory Experience, MIT*. Cambridge, MA, February 2024.

8. **Attia, L.**, Sivoxnay, E., Xia, X., Helms, B.A., Chan, E., Blau, S.M.. "Inverse Design of Upconverting Nanoparticles via Deep Learning on Physics-Infused Heterogeneous Graphs". *Materials Research Society Fall Meeting*. Boston, MA, December 2023.

9. **Attia, L.**, Doyle, P.S. "Templating drug nanoparticles inside hydrogels for next generation pharmaceutical formulation". *MIT Department of Chemical Engineering Seminar*. Cambridge, MA, October 2023. [**Best Seminar Award**]

10. **Attia, L.**, Chen, L.-H., Doyle, P.S. "Orthogonal gelations to synthesize core-shell hydrogels for versatile oral drug delivery". *American Physical Society Virtual Polymer Physics Symposium 2023*. Virtual, August 2023.

11. **Attia, L.**, Chen, L.-H., Doyle, P.S. "Programmable pulsatile dissolution of drug nanocrystals from core-shell hydrogel particles". *Dissolution Research Presentation International: United States*. Virtual, August 2023.

12. **Attia, L.**, Chen, L.H., Doyle, P.S. "Core shell hydrogel particles as a platform for versatile drug product manufacturing". *Preclinical Form and Formulation for Drug Discovery, Gordon Research Seminar*. West Dover, VT, June 2023.

13. **Attia, L.**, Ripley, K. "Delivering an effective poster". *Department of Chemical Engineering Individual Laboratory Experience, MIT*. Cambridge, MA, April 2023.

14. **Attia, L.**, Chen, L.H., Doyle, P.S. "Dual gelation for the synthesis of core-shell hydrogel particles". *New England Complex Fluids Workshop at Brandies University*. Waltham, MA, August 2022.

15. **Attia, L.**, Woodward, I., Malholtra, A., Vlachos, D., Lu, X.L., Fromen, C.A. "Computational Modeling of Fluid Flow through Open Cellular Foams and Lattice Structures". *University of Delaware Undergraduate Thesis Defense*. Virtual, May 2021.

16. **Attia, L.**, Daublain, P., Dorsey, P., D'Addio, S. "First Principles Simulations and Statistical Models for Lipid Nanoparticle Production and Risk Assessment Software Platform Transition". *Merck Boston Summer Intern Poster Symposium*. Virtual, August 2020.

17. Stillman, Z.S.*, Decker, G.E., **Attia, L.**, Bloch, E.D., Fromen, C.A., "Understanding particle size measurements of UiO-66 via defectiveness". *ACS Annual Spring Meeting, INORG: Chemistry of Materials*. Philadelphia, PA, March, 2020. (*conference canceled due to COVID-19)

18. Jarai, B.M.*, Stillman, Z.S., Decker, G.E., **Attia, L.**, Abbas, S., Bloch, E.D., Fromen, C.A.. "Utilizing UiO-66 Metal-Organic Frameworks (MOFs) As Pulmonary Drug Delivery Vehicles". AIChE Annual Conference, Bionanotechnology for Drug Delivery. Orlando, FL, United States, November 2019.

Poster Presentations

1. **Attia, L.**, Burns, J., Nguyen, D., Green, W.H., Doyle, P.S., "Deep-learning guided design of nanoformulations with improved bioavailability". *MIT Life Sciences & Health Symposium*, Cambridge, MA, December 2024.

2. **Attia, L.**, Burns, J., Doyle, P.S., Green, W.H. "Organic Solubility Prediction at the Limit of Aleatoric Uncertainty". *Molecular Machine Learning Conference @ MIT* Cambridge, MA, November 2024.

3. **Attia, L.**, Nguyen, D., Gokhale, D., Zheng, T., Doyle, P.S. "Surfactant-polymer complexation and competition on drug nanocrystal surfaces controls crystallinity". *Controlled Release Society Annual Meeting and Exposition*. Bologna, Italy, July 2024. [**Best Poster Award**]

4. **Attia, L.**, Nguyen, D., Gokhale, D., Zheng, T., Doyle, P.S. "Surfactant-polymer complexation and competition on drug nanocrystal surfaces controls crystallinity". *Modeling and Simulation Applications in Pharmaceutical Development and Manufacturing, AIChE P2DM*. Cambridge M.A., May 2024.

5. **Attia, L.**, Nguyen, D., Gokhale, D., Zheng, T., Doyle, P.S. "Surfactant-polymer complexation and competition on drug nanocrystal surfaces controls crystallinity". *Polymer Day, Massachusetts Institute of Technology*. Cambridge M.A., May 2024.

6. Nguyen, D., **Attia, L.**, Gokhale, D., Zheng, T., Doyle, P.S. "Interfacial Competition between Surfactant and Polymer Excipients on a Drug Nanocrystal Surface". *Chemical Engineering Undergraduate Poster Competition*, MIT, Cambridge, MA, April 2024.

7. Nguyen, D., **Attia, L.**, Gokhale, D., Zheng, T., Doyle, P.S. "Interfacial Competition between Surfactant and Polymer Excipients on a Drug Nanocrystal Surface". *National Collegiate Research Conference*, Harvard University, Cambridge, MA, January 2024.

8. Nguyen, D., **Attia, L.**, Gokhale, D., Zheng, T., Doyle, P.S. "Interfacial Competition between Surfactant and Polymer Excipients on a Drug Nanocrystal Surface". *Microsystems Annual Research Conference*, MIT Microsystems Technologies Laboratory, Brenton Woods, NH, January 2024.

9. Nguyen, D., **Attia, L.**, Gokhale, D., Zheng, T., Doyle, P.S. "Interfacial Competition between Surfactant and Polymer Excipients on a Drug Nanocrystal Surface". *AIChE National Student Conference*, Orlando, FL, October 2023. [**2nd Place Poster Award**]

10. Nguyen, D., **Attia, L.**, Gokhale, D., Zheng, T., Doyle, P.S. "Interfacial Competition between Surfactant and Polymer Excipients on a Drug Nanocrystal Surface". *AIChE National Student Conference*, Orlando, FL, October 2023. [**1st Place Poster Award**]

11. **Attia, L.**, Nguyen, D., Gokhale, D., Doyle, P.S. "Interfacial competition on a drug nanocrystal surface". *Department of Energy Computational Science Graduate Fellowship Annual Program Review*. Washington D.C., July 2023.

12. **Attia, L.**, Chen, L.H., Doyle, P.S. "Core shell hydrogel particles as a platform for versatile drug product manufacturing". *Preclinical Form and Formulation for Drug Discovery, Gordon Research Seminar*. West Dover, VT, June 2023. [**Best Poster Award**]

13. **Attia, L.**, Chen, L.H., Doyle, P.S. "Core shell hydrogel particles as a platform for versatile drug product manufacturing". *Preclinical Form and Formulation for Drug Discovery, Gordon Research Conference*. West Dover, VT, June 2023.

14. **Attia, L.**, Chen, L.H., Doyle, P.S. "Core-Shell Hydrogel Particles for the Formulation of Hydrophobic Small-Molecule APIs". *Department of Energy Computational Science Graduate Fellowship Annual Program Review*. Arlington, VA, July 2022.

15. **Attia, L.**, Stillman, Z.S., Decker G.E., Bloch, E.D., Fromen, C.A. "Evaluation of UiO-66 Nanoparticles as Pulmonary Drug Delivery Vehicles". *NCSU Future Leaders in Chemical Engineering Symposium*. Virtual, October 2020.

16. **Attia, L.**, Stillman, Z.S., Decker G.E., Bloch, E.D., Fromen, C.A. "Evaluating the Fluid and Aerodynamic Properties of Uio-66 Nanoparticles". *AIChE Annual Student Conference*. Orlando, FL, November 2019. [**2nd Place Poster Award - Materials Science and Eng.**].

17. **Attia, L.**, Stillman, Z.S., Decker, G.E., Jarai, B.M., Bloch, E.D., Fromen, C.A. "Fluid and Aerodynamic Properties of UiO-66 Nanoparticles with Varying Defectiveness and Cargo-Loading". *Biotechnology and Biomedical Career Fair Poster Reception*. Newark, DE, October 2019. [**3rd Place Poster Award**].

18. **Attia, L.***, Stillman, Z.S, Abbas, S., Decker, G.E., Bloch, E., Fromen, C.A. "Evaluating Metal-Organic Frameworks as Pulmonary Drug Delivery Vehicles". *AIChE Annual Student Conference*, Pittsburgh, PA, November 2018.

Activities and Service

President, MIT Graduate Christian Fellowship	2022 – 2024
Content Contributor, MIT Graduate Admissions Blog	2021 – Present
Graduate Dorm Officer, Massachusetts Institute of Technology	2021 – 2022
Academic Tutor, University of Delaware Office of Academic Enrichment	2019-2021
Planning Committee, University of Delaware Veritas Forum	2019-2021
Thermodynamics Grader, University of Delaware	2021
International Education Experience, University of Delaware Institute for Global Studies	
• Tokyo, Japan: Studied psychology of language with Prof. Tamara Medina.	2020
• Padova, Italy: Studied materials science and Italian history at University of Padova with Prof. Ismat Shah.	2019
• Rosseau, Dominica: Studied economics and geography of Caribbean islands with Prof. Anthony Seraphin.	2018