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Personal Website

Lucas Attia

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

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Chemical engineering PhD researcher with expertise in pharmaceutical nanotechnology and cheminformatics. Accomplished communicator, with 10 peer-reviewed publications, 60+ presentations at conferences and symposia, and 12 award-winning presentations. Experienced fundraiser, securing $330k in scholarships, $380k in fellowships, and $350k in grant funding. My long-term research vision is to digitize drug formulation by integrating data-driven and physics-based modeling with experiments.

EDUCATION

Massachusetts Institute of Technology (MIT)   **Cambridge, MA**
PhD Chemical Engineering   *2021 – 2026 (expected)*
- Minor: Machine Learning
- Thesis: *Engineering drug nanoparticle formation, structure, and processing for oral bioavailability enhancement*

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*

RESEARCH EXPERIENCE

MIT Department of Chemical Engineering   **Cambridge, MA**
PhD Research Fellow, Doyle Group   *2021 – Present*

DEEP LEARNING (DL) FOR MOLECULAR PROPERTY PREDICTION
- Programmed DL models to accurately predict organic solubility, published in *Nature Communications* and featured in MIT News. Resulted in 1 award, 6 invited talks, and 7 other presentations.
- Deployed models through a website, Python package, and Rowan Scientific's platform. Maintain open source code.
- Lead active collaboration with Neopoly Ltd to develop a causal DL architecture for molecular property prediction. Resulted in 4 presentations, a conference paper at NeurIPS 2025 and a manuscript in preparation.

MOLECULAR DYNAMICS (MD) SIMULATIONS FOR NANOFORMULATION DESIGN
- Simulated the effects of excipients on nanoparticle crystallinity using MD (open source code), leading to a publication in *ACS AMI*. Recognized with 5 awards, 1 invited talk, and 10 contributed presentations.
- Raised $100k through Koch Institute Frontier Research Program to simulate PROTAC-surfactant interactions using MD and enable efficient PROTAC nanoparticle design.

HYDROGEL-BASED DRUG DELIVERY SYSTEMS
- Invented hydrogel encapsulation systems to control release kinetics of nanoparticle-based drugs, published in *Advanced Healthcare Materials* and featured in MIT News. Resulted in 4 awards and 9 presentations.
- Patented process to formulate ultra high-concentration injectable antibody suspensions, leading to a manuscript published in *Advanced Materials* and featured in MIT News. Also led to an active collaboration with GSK and $250k through the MIT Northpond Seed program.
- Managed 2 undergraduate researchers and 1 technician on daily tasks and project deliverables.

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.

PROFESSIONAL EXPERIENCE

Eli Lilly and Company   **Boston, MA**
Cheminformatics Intern   *Summer 2025*
- Built ML models to predict lipid nanoparticle (LNP) properties and biological activity. Virtually screened candidate lipids, recommended hits for experimental validation, and discovered new design rules for lipid chemical modifications.
- Deployed ML models to production server, enabling user scientists to access real-time inference. Maintained GitHub repository.

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.

Merck & Co.   **Boston MA**
Discovery Pharmaceutical Sciences Intern   *Summer 2020*
- Created research plan for statistical modeling and multi-scale simulation of a LNP production process.
- Digitized drug candidate risk assessments to standardize data collection and storage for future analysis.

SOFTWARE SKILLS

Languages	Python, bash, MATLAB, Git, LaTeX
Machine Learning	Deep learning, Pytorch, sklearn
Cheminformatics	rdkit, mordred, deepchem, chemprop
Molecular Dynamics	GROMACS, CHARMM, PyMOL, xtb
Scientific Computing	High performance computing, slurm, parallelization

EXPERIMENTAL SKILLS

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

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

Awards
- **MIT Open Data Prize**, Massachusetts Institute of Technology   2025
- **AIChE PD2M Student Award**, AIChE   2025
- **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

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

LEADERSHIP

Massachusetts Institute of Technology   **Cambridge, MA**
Graduate Communication Fellow   *2022 – Present*
- Awarded prestigious 4-year Chemical Engineering fellowship to lead scientific communication efforts in the department.
- Deliver 3+ workshops on technical communication to department annually. Coach 60+ peers through 120+ hours of appointments.

Committee on Intellectual Property   *2024 – Present*
- Recommend MIT-level policy guidelines to improve technology transfer and translation.
- Advocated for science-based policy and federal research support with congressional offices with the MIT Science Policy Review. Covered in MIT News feature.

President, Graduate Christian Fellowship   *2022 – 2024*
- Guide student group efforts in service, ministry, fund-raising, and community building as peer-nominated leader.

Graduate Teaching Fellow   *Spring 2024*
- Taught 14 students in Chem. Eng. course 10.494B: Therapeutic Nanoparticle Manufacturing, and 16 students in 10.493: Electrochemical Energy.

Gordon Research Seminar   **(remote)**
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.

Polygence   **(remote)**
Mentor   *2022 – Present*
- Supervise 50+ high school student research projects from initial design through completion and publication.

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.

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.

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. Natajaya, C., **Attia, L.**, Burns, J., Doyle, P.S. "Causal molecular machine learning for property prediction and molecular optimization". *ACS Central Science* (in preparation).

2. **Attia, L.**, Evbarunegbe, N., Spjuth, O., Seal, S. "Interpreting and Visualizing VSA Descriptors Through VSA Explainer". *ACS Journal of Chemical Information and Modeling* (in preparation).

3. **Attia, L.**, Nguyen, D., Lui, K., Qin, Q., Doyle, P.S. (2026) "Size-controlled templating of drug nanoparticles from nanoemulsion precursors for versatile nanoformulation". *ACS Chemistry of Materials*, 38, 1, 473–485.
   10.1021/acs.chemmater.5c02892.

4. Sivonxay, E., **Attia, L.**, ..., Blau. S.M.(2025) "Gradient-based optimization of complex nanoparticle heterostructures enabled by deep learning on heterogeneous graphs". *Nature Computational Science*, 1-13.
   doi.org/10.1038/s43588-025-00917-3

5. Zheng, T., **Attia, L.**, Teng, J.. Doyle, P.S. (2025) "High-concentration antibody formulation via solvent-based dehydration ". *Advanced Materials*, e16429.
   10.1002/adma.202516429

6. **Attia, L.**, Burns, J., Doyle, P.S., Green, W.H. (2025) "Data-driven Organic Solubility Prediction at the Limit of Aleatoric Uncertainty". *Nature Communications*, 16(1), 7497.
   doi:10.1038/s41467-025-62717-7

7. **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

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

9. **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

10. 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

11. 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

12. 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., Doyle, P.S., Green, W.H. "Data-Driven Organic Solubility Prediction at the Limit of Aleatoric Uncertainty". *Open Data Prize Award Reception*. Massachusetts Institute of Technology, Cambridge, MA, October 2025.

2. **Attia, L.**, D., Doyle, P.S. "Engineering drug nanoparticle structure, function, and processing for oral bioavailability enhancement". *Bioproduct Research & Development*. Eli Lilly & Co., Boston, MA, August 2025.

3. **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.

4. **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.

5. **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.

6. **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.

7. **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.

8. **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**]

Oral Presentations

1. Natajaya, C., Burns, J., **Attia, L.**., Doyle, P.S. "Causal Molecular Machine Learning for Property Prediction and Optimization". *Cambridge Cheminformatics Network Meetings*, Cambridge, UK, November 2025.

2. Natajaya, C., Burns, J., **Attia, L.**., Doyle, P.S. "Causal Molecular Machine Learning for Property Prediction and Optimization". *AIChE National Conference*. Boston, MA, November 2025.

3. **Attia, L.**, Nguyen, D., Liu, K., Qi, Q.M., and Doyle, P.S. "Size-Controlled Templating of Lipophilic Drug Nanoparticles from Nanoemulsion Precursors for Versatile Nanoformulation". *AIChE National Conference*. Boston, MA, November 2025.

4. Zheng, T., **Attia, L.**, Teng, J., Doyle, P.S. "A Novel Solvent-Based Dehydration Process for High-Concentration Aqueous Antibody Suspensions". *AIChE National Conference*. Boston, MA, November 2025.

5. Burns, J.W., **Attia, L.**, Doyle, P.S., Green, W.H. "Organic Solubility Prediction at the Aleatoric Limit with Neural Networks". *AIChE National Conference*. Boston, MA, November 2025.

6. Zheng, T., **Attia, L.**, Teng, J., Doyle, P.S. "A Novel Solvent-Based Dehydration Process for High-Concentration Aqueous Antibody Suspensions". *Preclinical Form and Formulation for Drug Discovery Gordon Research Seminar*. Portland, ME, June 2025.

7. Burns, J.W., **Attia, L.**, Doyle, P.S., Green, W.H. "Organic Solubility Prediction at the Limit of Aleatoric Uncertainty". *Rowan Scientific Seminar Series*, Boston, MA, April 2025.

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

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

10. Burns, J.W., **Attia, L.**, Doyle, P.S., Green, W.H. "Organic Solubility Prediction at the Limit of Aleatoric Uncertainty". *Computational Research in Boston and Beyond*, MIT Department of Mathematics, Cambridge, MA, January 2025.

11. Burns, J.W., **Attia, L.**, Doyle, P.S., Green, W.H. "Organic Solubility Prediction at the Limit of Aleatoric Uncertainty". *Computational Research in Boston and Beyond*, MIT Department of Mathematics, Cambridge, MA, January 2025.

12. Sivoxnay, E., **Attia, L.**, Xia, X., Helms, B.A., Chan, E., Blau, S.M. "Enabling Inverse Design of Nanoparticle Photophysics via Deep Learning on Heterogeneous Graphs". *Materials Research Society Fall Meeting*. Hynes Convention Center, Boston, MA, December 2024.

13. Burns, J.W., **Attia, L.**, Doyle, P.S., Green, W.H. "Organic Solubility Prediction at the Limit of Aleatoric Uncertainty". *MIT Department of Chemical Engineering Seminar*. Cambridge, MA, November 2024.

14. Burns, J.W., **Attia, L.**, Doyle, P.S., Green, W.H. "Organic Solubility Prediction at the Limit of Aleatoric Uncertainty". *MIT Computational Science and Engineering Community Seminar*, Cambridge, MA, November 2024.

15. 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.

16. **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.

17. **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.

18. **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**]

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

20. **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.

21. **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. [**3rd place Presentation Award**]

22. **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. [**National Finalist Award**]

23. **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.

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

25. **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.

26. **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.

27. **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.

28. 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)

29. 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.**, Doyle, P.S. "Developing a bottom-up pharmaceutical nanoformulation approach using soft materials, molecular simulation, and deep learning". *AIChE National Conference*, Boston, MA, November 2025.

2. **Attia, L.**, Burns, J., Lau, J., Attia, P.M. "Multi-fidelity deep learning for liquid battery electrolyte solvent stability prediction ". *8th Artificial Intelligence in Chemistry Symposium*, Cambridge, UK, September 2025.

3. Sivoxnay, E., **Attia, L.**, Xia, X., Helms, B.A., Chan, E., Blau, S.M. "Enabling Inverse Design of Nanoparticle Photophysics via Deep Learning on Heterogeneous Graphs". *Molecular Foundry Annual User Meeting*. Lawrence Berkeley National Lab, Berkeley, CA, August 2025.

4. **Attia, L.**, Burns, J., Doyle, P.S., Green, W.H. "Organic Solubility Prediction at the Limit of Aleatoric Uncertainty". *8th Artificial Intelligence in Chemistry Symposium*, Cambridge, UK, September 2025.

5. Natajaya, C., Burns, J., **Attia, L.**. "Causal Chemprop: Causal Machine Learning for Molecular Property Prediction and Optimization". *8th Artificial Intelligence in Chemistry Symposium*, Cambridge, UK, September 2025.

6. Natajaya, C., Burns, J., **Attia, L.**. "Causal Chemprop: Causal Machine Learning for Molecular Property Prediction and Optimization". *High Throughput Chemistry, Gordon Research Conference*, New London, NH, July 2025.

7. **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.

8. **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.

9. **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**]

10. **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.

11. **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.

12. 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.

13. 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.

14. 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.

15. 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**]

16. **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.

17. **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**]

18. **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.

19. **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.

20. **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.

21. **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.**].

22. **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**].

23. **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

Forum Planner, MIT Veritas Forum	2022 – 2023
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

REFERENCES

- Patrick S. Doyle, Massachusetts Institute of Technology
- Caitlin Steir, Massachusetts Institute of Technology
- Scott Brown, Eli Lilly (former)
- Sean Kyle Bedingfield, Eli Lilly
- Samuel M. Blau, Lawrence Berkeley National Laboratory
- Catherine A. Fromen, University of Delaware
- Suzanne D'Addio, Merck
- Pierre Daublain, Merck