

# Austin M. Mroz

Eric & Wendy Schmidt AI in Science Postdoctoral Fellow, Imperial College London  
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<b>Education</b>	<u>University of Oregon (UO), Eugene, OR, USA</u> 2017-2021 Doctorate of Philosophy, <b>Physical Chemistry</b> <u>Rose-Hulman Institute of Technology (RHIT), Terre Haute, IN, USA</u> Bachelor of Science, <b>Mechanical Engineering</b> 2012-2016 Masters of Science, <b>Chemistry</b> 2015-2017
<b>Research</b>	<u>Schmidt AI in Science Postdoctoral Fellowship, Imperial College London</u> Nov 2023 - present
<b>Experience</b>	<i>Department of Chemistry, I-X</i> <ul style="list-style-type: none"><li>– developing data-driven optimization algorithms for closed-loop chemical discovery platforms</li><li>– building open-source tools to improve the accessibility of data-driven optimization algorithms for chemical applications</li><li>– working at the department level as a part of the Equipment, Facilities and Data Management Strategy Team to develop a white paper guiding the data strategy for the Department of Chemistry at Imperial College London</li></ul> <u>Postdoctoral Research Associate, Imperial College London</u> Jun 2021 - Nov 2023 <i>Department of Chemistry, Prof. Kim Jelfs Group</i> <ul style="list-style-type: none"><li>– developed large-scale, open-source workflows to accelerate the discovery of novel porous liquids, a new class of materials combining the fast mass transfer of liquids with the permanent porosity of solid sorbents</li><li>– demonstrated a closed-loop, experimental-theoretical workflow for the discovery of novel CO<sub>2</sub> sorbents, as part of an industry collaboration between Imperial College London and BP through BP-ICAM</li></ul>
<b>Honors &amp; Awards</b>	<u>Global Incentive Fund</u> May 2024 <i>Awarded £9000 to develop a 2-day symposium featuring early career researchers working in materials discovery at Technical University of Munich</i> <u>Emerging Leader in Electronic Structure Theory, iOP Publishing</u> Dec 2022 <u>Graduate Student Award for Excellence in the Teaching of Chemistry</u> Sep 2018 - Jun 2019 <u>Dean's First Year Merit Awards, University of Oregon</u> Sep 2017 - Jun 2018
<b>Publications</b>	Judge, E.; Azzouzi, M.†; <b>Mroz, A. M.</b> †; del Rio Chanona, E. A.; and Jelfs, K. E.* “Applying multi-fidelity Bayesian optimization in chemistry: Open challenges and major considerations.” <b>2024</b> , DOI: 10.48550/arXiv.2409.07190; <i>Submitted</i> († <b>equal contribution</b> )  <b>Mroz, A. M.</b> *; Toka, P. N.; del Rio Chanona, E. A.; and Jelfs, K. E.* “Web-BO: Towards increased accessibility of Bayesian optimization for chemistry.” <i>Faraday Discussions</i> , <b>2024</b> , DOI: 10.1039/D4FD00109E; (github.com/austin-mroz/web-bo)  <b>Mroz, A. M.</b> ; Egleston, B. D.; Sherwood, J.; Morel, R. C.; Jelfs, K. E.; and Greenaway, R. L.* “Predicting solubility and size-exclusivity towards the rational design of porous liquid solutions.”, <b>2024</b> , <i>Submitted</i> .

- Kai, A.; **Mroz, A. M.**; Jelfs, K. E.; Cooper, A. I.; Little, M. A.; and Greenaway, R. L.\* “Construction of an organic cage-based porous ionic liquid using an amination strategy.”, **2024**, *Submitted*.
- Zhou, J.; Yang, Y.; **Mroz, A. M.**; and Jelfs, K. E.\* “PolyCL: Contrastive Learning for Polymer Representation Learning via Explicit and Implicit Augmentations.”, **2024**, DOI: 10.48550/arXiv.2408.07556, *Submitted*.
- Zhu, M.; **Mroz, A. M.**; Gui, L.; Jelfs, K. E.; Bemporad, A.; del Rio Chanona, E. A.; Lee, Y. S.\* “Discrete and mixed-variable experimental design with surrogate-based approach.”, **2024**, DOI: 10.26434/chemrxiv-2024-h37x4, *Submitted*.
- Mroz, A. M.\***; Turciani, L.; Jelfs, K. E.\* “SMORES: An electric field-based measure of sterics,” *Electron. Struct.*, **2023**, 5, 4; (github.com/austin-mroz/SMORES)  
Invited, featured article in 2022 Emerging Leaders Issue
- Zhou, J.; **Mroz, A. M.**; Jelfs, K. E.\* “Deep generative design of porous organic cages via a variational autoencoder,” *Digital Discovery*, **2023**, 2, 6, 1925-1936.
- Mroz, A. M.**; Posligua, V.; Tarzia, A.; Wolpert, E. H.; Jelfs, K. E.\* “Into the Unknown: How Computation Can Help Explore Uncharted Material Space,” *J. Am. Chem. Soc.*, **2022**, 144, 41, 18730-18743.
- Mroz, A. M.**; Davenport, A. M.; Sterling, J.; Davis, J.; Hendon, C.H.\* “An electric field-based approach for quantifying effective volumes and radii of chemically affected space,” *Chem. Sci.*, **2022**, 13, 6558-6566. (github.com/austin-mroz/STREUSEL)
- Egleston, B. D.†; **Mroz, A. M.†**; Jelfs, K. E.\*; Greenaway, R. L.\* “Porous liquids – the future is looking emptier,” *Chem. Sci.*, **2022**, 13, 5042-5054. († **equal contribution**)
- Hanna, S. L.; Debela, T. T.; **Mroz, A. M.**; Syed, Z. H.; Kirlikovali, K. O.; Hendon, C. H.\*; Farha, O. K.\* “Identification of a Metastable Uranium Metal-Organic Framework Isomer Through Non-Equilibrium Synthesis.” *Chem. Sci.*, **2022**, 13, 13032-13039.
- Yoon, S.; Talin, A. A.; Stavila, V.; **Mroz, A. M.**; Bennett, T. D.; He, Y.; Keen, D. A.; Hendon, C. H.; Allendorf, M. D.\*; So, M. C.\* “From n- to p-type material: effect of metal ion on charge transport in metal-organic materials,” *ACS. Appl. Mater. Interfaces*, **2021**, 13, 44, 52055-52062.
- Mancuso, J. L.; **Mroz, A. M.**; Le, K. N., Hendon, C.H.\* “Electronic Structure Modeling of Metal-Organic Frameworks,” *Chem. Rev.*, **2020**, 16, 8641.
- LeRoy, M. A.; **Mroz, A. M.**; Mancuso, J. L.; Miller, A.; Van Cleve, A.; Check, C.; Heinz, H.; Hendon, C. H.; Brozek, C. K.\* “Post-synthetic modification of ionic liquids using ligand-exchange and redox coordination chemistry,” *J. Mater. Chem. A*, **2020**, 8, 22674.
- Hamann, D. M.; Bardgett, D.; Bauers, S.R.; Kasel, T. W.; **Mroz, A. M.**; Hendon, C. H.; Medlin, D. L.; Johnson, D. C.\* “Influence of Nanoarchitecture on Charge Donation and Electrical Transport Properties in [(SnSe)<sub>1+δ</sub>][TiSe<sub>2</sub>]<sub>q</sub> Heterostructures,” *Chem. Mater.*, **2020**, 32, 5802.
- Donor, M. T.; **Mroz, A. M.**; Prell, J. S.\* “Experimental and theoretical investigation of overall energy deposition in surface-induced unfolding of protein ions,” *Chem. Sci.*, **2019**, 10, 1497.

Sutton, E.C.; McDevitt, C. E.; Prochnau, J.Y.; Yglesias, M. V.; **Mroz, A. M.**; Yang, M. C.; Cunningham, R.M.; Hendon, C.H.; DeRose, V.J.\* “Nucleolar Stress Induction by Oxaliplatin and Derivatives,” *J. Am. Chem. Soc.*, **2019**, 141, 18411

McDevitt, C. E.; Yglesias, M. V.; **Mroz, A. M.**; Sutton, E.C.; Yang, M. C.; Hendon, C.H.; DeRose, V.J.\* “Monofunctional platinum(II) compounds and nucleolar stress; is phenanthriplatin unique?,” *J. Biol. Inorg. Chem.*, **2019**, 24, 899

Kasel, T. W.†; Deng, Z.†; **Mroz, A. M.**†; Hendon, C. H.; Butler, K. T.; Canepa, P., “Metal-free perovskites for non linear optical materials,” *Chem. Sci.*, **2019**, 10, 8187-8194. († **equal contributions**)

**Mroz, A. M.**, “Pro- and Antioxidant Activity of Selenomethionine: Preventative Measures against Metal-Mediated DNA Oxidation,” M. Sc., Rose-Hulman Institute of Technology, Terre Haute, IN, **2017**.

**Teaching** Bayesian optimization workshop, Imperial College London Sep 2024

**Experience** *AIchemy, UK’s AI-hub for chemistry*

- Independently developed and delivered a **3 hour workshop** on Bayesian optimization basics for chemical applications
- Tailored teaching materials to **35 participants**, including post-graduate students, postdoctoral scholars, and senior academics in the Department of Chemistry at Imperial College London
- Material focused on Bayesian optimization basics and tailored to beginner-level
- Deployed a teaching tool that I developed and built as part of the learning framework

Bayesian optimization for guided chemical design, Imperial College London Sep 2024

*Sargent Centre for Process Systems Engineering, Bayesian optimization Summer School*

- Independently developed and delivered a **3 hour workshop** on Bayesian optimization for guided chemical design
- Tailored teaching materials to **90 participants** comprised of diverse backgrounds (chemical engineering, software engineering, chemistry, physics) and from a variety of posts (industry professionals, post-graduate students, postdoctoral scholars, and senior academics)
- Material focused on chemistry-specific considerations required for implementing Bayesian optimization for chemical and materials design
- Deployed a teaching tool that I developed and built as part of the learning framework

AI for Materials, Imperial College London Jan 2021 - present

*Lab instructor; MSc Digital Chemistry program*

- Developed and led a practical course (“AI for Materials”) as a part of the Digital Chemistry MSc program at Imperial College London
- Designed and implemented teaching materials for introducing students to AI for materials property prediction problems
- Led a team of 4 teaching assistants

General Chemistry I-III, University of Oregon Sep 2017 - Sep 2020

*Lab instructor*

- Taught and led 2 sections of the wet lab course for the first year of General Chemistry

<b>Student</b>	PhD student assistant supervisor	Sep 2021-present
<b>Supervision</b>	<i>Imperial College London</i>	
	<ul style="list-style-type: none"> <li>– Assistant supervisor of <b>3 PhD students</b> in the Jelfs Group</li> <li>– Participate in project planning, development, direction and troubleshooting</li> </ul>	
	Masters student thesis projects co-supervisor, <i>Imperial College London</i>	Sep 2021-present
	<ul style="list-style-type: none"> <li>– Developed projects for and supervised <b>4 Masters student thesis projects</b></li> <li>– Worked with one student to modify their dissertation for a journal publication</li> </ul>	
	Summer Undergraduate Research Opportunity students, <i>Imperial College London</i>	May 2024-Sep 2024
	<ul style="list-style-type: none"> <li>– Developed projects for and supervised <b>3 undergraduate summer research opportunity students</b> – 2 Chemistry students, and 1 Maths student</li> <li>– Worked with one student to integrate their work into a manuscript I am preparing for another publication</li> </ul>	
<b>Invited Talks</b>	Imperial College London, Chemical Engineering Dept. ECR	Sep 2024
	“The role of simulation and theory in the design of porous liquid solutions”	
	MRS Bulletin (Seattle), Data, Autonomy and Algorithms Session	Apr 2024
	“Toward accelerated, experimental-theoretical closed-loop discovery”	
	Imperial College London, Simulation-Based Inference Symposium	Apr 2023
	“The role of computation in the discovery of synthesisable molecular materials”	
	Argonne National Laboratory, invited seminar	Mar 2023
	“Towards high-throughput autonomous discovery of novel porous liquids”	
	Imperial College London International Women’s Day Symposium	Mar 2022
	“Breaking the Bias”	
	University of Oregon Machine Learning Symposium	Sep 2018
	“Implementing Machine Learning Methods in Pore Characterization of Metal-Organic Frameworks”	
	Rose-Hulman Department of Chemistry Board of Directors Meeting	May 2017
	“Elucidating Oxidative Effects of Selenomethionine”	
<b>Conference Talks</b>	16 <sup>th</sup> International Conference on Materials Chemistry (MC16)	Jul 2023
	“Towards accelerated, experimental-theoretical closed-loop discovery of novel porous liquids”	
	bp-ICAM (International Center for Advanced Materials) Annual Conference	Nov 2022
	“Accelerated discovery of CO <sub>2</sub> capture absorbents via a closed-loop experimental-theoretical workflow”	
	AI in Chemistry, RSC	Sep 2022
	“Identification of improved CO <sub>2</sub> capture absorbents via a closed-loop, experimental-theoretical workflow”	
	ACS National Meeting	Mar 2021
	“Engineering conductive pathways in metal-organic frameworks via p-type bridging interstitials”	
	ACS National Meeting and Expo	Aug 2019
	<i>Machine Learning &amp; Artificial Intelligence in Computational Chemistry Symposium</i>	
	“Pore volumes and surface areas of metal-organic frameworks as descriptors for materials discovery”	

<b>Work Experience</b>	<p><u>Allison Transmission</u>, Indianapolis, IN <span style="float: right;">Jun 2014 - Aug 2014</span></p> <p><i>Product Engineering Intern, Advanced Engineering Department (R&amp;D)</i></p> <ul style="list-style-type: none"> <li>– Recognized an inefficiency in the parts library system and took the initiative to develop and implement a software-based solution that automated the process</li> <li>– Performed a cost study for a product redesign to provide additional design support</li> <li>– Inspected, documented, analyzed and presented observations of a traction failure</li> <li>– Coordinated and facilitated a tensile test and specimen design between two major companies</li> <li>– Managed and organized the competitive assessment of a part from a competitor</li> </ul> <p><u>Rose Hulman Ventures</u>, Terre Haute, IN <span style="float: right;">Mar 2013 - Aug 2013</span></p> <p><i>Design Intern, DowAgro Project Team</i></p> <ul style="list-style-type: none"> <li>– Designed, prototyped and tested a mechanical device for injecting fluid into corn</li> <li>– Developed and implemented ideas for improved maneuverability of the FreedomOne all-terrain wheelchair</li> </ul>
<b>Outreach Activities</b>	<p>The Duck Store, Board of Directors Member <span style="float: right;">Jun 2019 - May 2021</span></p> <p>MadDuck Science Fridays Community Outreach Program, Co-Director <span style="float: right;">Sep 2018 - Sep 2019</span></p> <p>Graduate Assistant, General Chemistry Lab Instructor <span style="float: right;">Nov 2016 - Sep 2019</span></p> <p>Homework Hotline Tutor <span style="float: right;">Sep 2016 - May 2017</span></p> <p>Learning Center Supervisor <span style="float: right;">Mar 2013 - May 2016</span></p>