Nicholas Everett Jackson

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Professional Appointments

University of Illinois at Urbana-Champaign
- *Assistant Professor of Chemistry* — *2021-Present*
- *AI for Materials Group Leader, Beckman Institute* — *2021-Present*
- *Affiliate (0%) Assistant Professor of Chemical & Biomolecular Engineering* — *2021-Present*
- *Affiliate (0%) Assistant Professor of Materials Science & Engineering* — *2021-Present*

Argonne National Laboratory
- *Assistant Scientist in the Materials Science Division* — *2019-2021*

Education and Training

Argonne National Laboratory and University of Chicago
- *Maria Goeppert Mayer Fellow in the Center for Molecular Engineering* — *2016-2019*
  Supervisor: Juan de Pablo

Northwestern University
- *Ph.D. in Chemistry* — *2011-2016*
  Advisors: Mark Ratner and Lin Chen

Wesleyan University
- *B.A. in Physics w/High Honors* — *2007-2011*
  Advisor: Fred Ellis

Honors and Recognition

Camille Dreyfus Teacher-Scholar Award	*2025*
Cottrell Scholar Award	*2025*
Kavli Foundation Emerging Leader in Chemistry Award	*2025*
Center for Advanced Study Fellow, UIUC	*2024*
School of Chemical Sciences Faculty Teaching Award, UIUC	*2024*
AIChE COMSEF Young Investigator Award	*2024*
ACS COMP OpenEye/Cadence Outstanding Junior Faculty Award	*2024*
Early Career Board, *Journal of Chemical Theory and Computation*	*2023*
RCSA Scialog Fellow: Automating Chemical Laboratories	*2023*
Department of Energy Early Career Program Award	*2023*
Lincoln Excellence for Assistant Professors Scholar, UIUC	*2023*
Selected as a Rising Star, *Applied Physics Letters*	*2023*
Selected as a Rising Star, *Chemistry of Materials "Up-and-Coming" Series*	*2022*
Selected as an Emerging Investigator, *Molecular Systems Design & Engineering*	*2022*
Selected as an Emerging Investigator, *Journal of Chemical Physics*	*2022*
Dreyfus Machine Learning in the Chemical Sciences and Engineering Award	*2021*
ACS Petroleum Research Fund Doctoral New Investigator Award	*2021*
3M Nontenured Faculty Award	*2021*
List of Teachers Ranked as Excellent by their Students x4 (*Sp 21, Fa 22, Sp 23, Fa 23*)	*2021-Present*
ACS PHYS Young Investigator Award	*2019*
Materials Research Society Postdoctoral Award	*2019*
Maria Lastra Excellence in Mentoring Award, University of Chicago	*2019*
Maria Goeppert Mayer Named Fellowship, Argonne National Laboratory	*2016*
Presidential Fellowship, Northwestern University	*2015*
Materials Research Society Graduate Student Silver Award	*2015*

Telluride Science Research Center Paul Barbara Scholarship *2014*
Lambert Award for Excellence in Graduate Research, Northwestern University *2013*
National Science Foundation Graduate Research Fellowship Program *2012*
Phi Beta Kappa, Wesleyan University *2011*
Karl Van Dyke Prize in Physics, Wesleyan University *2010*

Pre-Prints

*indicates corresponding author(s), ^ indicates equal contributions, indicates undergraduate authors

[**] Zhu, S.; Jackson, N.E. "Reconstructing Electronic Property Distributions from the Coarse-Grained Resolution with Conditional Flow Matching" Under Review at *J. Chem. Theory Comput.*

[**] Raghuraman, V.; Jackson, N.E.* "Reactive Atomistic Simulations of Doping-Driven Co-Aggregation in P3HT:F4TCNQ" *Under Review at J. Phys. Chem.* DOI: 10.26434/chemrxiv.15005840/v1

[**] Zhang, H.; Jackson, N.E.* "Machine Learned NMR Predictions for Condensed Phase Polymer Films" *Under Review at Nat. Commun.* DOI: 10.26434/chemrxiv.15001687/v1

Publications since UIUC

*indicates corresponding author(s), ^ indicates equal contributions, indicates undergraduate authors

[**49**] Too, M.; Jackson, N.E.* "A Model Hamiltonian Map for Organic Semiconductor Doping Regimes" *J. Chem. Phys.* **2026**.

[48] Iyer, S.; Yu, Z.; Jackson, N.E.* "Computational Exploration of the Structure and Mechanical Behaviour of Hybrid Epoxy-Acrylate Dual-Cure Systems" *Soft Matter* **2026** https://doi.org/10.1039/D6SM00122J.

[**47**] Jang, S.; Wu, J.L.; Jackson, N.E.; Schroeder, C.M.; Evans, C.M. "Enhanced Crystallinity and Electrical Conductivity in Conjugated Polymers via Dynamic Covalent Bond Exchange" *Macromolecules*, **2026.**

[**46**] Jackson, N.E.* ``A Theory of Electronic Structure for Coarse-Grained Resolutions" *J. Chem. Phys.* 165, 034116, **2026***. Editor's Pick*. https://doi.org/10.1063/5.0329731

[**45**] Kim, S.; Schroeder, C.M.; Jackson, N.E.* "Generative Multi-Property Refinement of Polymer Chemistries" *Macromolecules*, **2026**. https://doi.org/10.1021/acs.macromol.6c00564.

[**44**] Kidder, K.; Kim, S.; Jackson, N.E.* "On the Prospect of Chemically Transferable Coarse-Grained Electronic Structure Models for Soft Materials" *J. Phys. Chem. B*, **2026**. https://doi.org/10.1021/acs.jpcb.6c00843.

[**43**] Qiu, H.; Jackson, N.E.* "Computational Insights into the Salt-Induced Modulation of Electron Transporting Conjugated Polyelectrolytes" *Macromolecules*, **2026,** 59, 6, 3872-3884. https://doi.org/10.1021/acs.macromol.5c02692

[42] DeBernardo, A.; Jackson, N.E.* "Machine Learning Graph Convolutional Electronic Propagators" *J. Chem. Phys.* 164, 044104, **2026**. https://doi.org/10.1063/5.0305033.

[41] Wu, J.; Friday, D.M.; Hwang, C.; Yi, S.; Torres-Flores, T.C.; Burke, M.D.; Diao, Y.; Schroeder, C.M.; Jackson, N.E.* "Democratizing Chemical Machine Learning with Community-Engaged Test Sets" *Digit. Discov.* **2026**, 5, 304-309. https://doi.org/10.1039/D5DD00424A.

[40] Palacio-Betancur, V.; Jackson, N.E.* "Molecular Charge Topology Governs Polar Nematic Order *J. Am. Chem. Soc.* **2025**, 147, 51, 46841-46846. https://doi.org/10.1021/jacs.5c18760.

[39] Verma, A.; Wang, C.-I.; Espera, R.; Raghuraman, V.; Jackson, N.E.* "Conformation Mediated Doping in P3HT:F4TCNQ Dimers from Density Functional Theory" *J. Phys. Chem. A*. **2025**, 129, 44, 10108-10116. https://doi.org/10.1021/acs.jpca.5c05040.

[38] Ferguson, A.;…;Jackson, N.E.;…*et al.* "The Future of Artificial Intelligence and the Mathematical and Physical Sciences (AI+MPS)" *arXiv*. **2025**. DOI: 10.48550/arXiv.2509.02661.

[37] Wang, C.-I.*; Lindsay, A.C.; Jackson, N.E.* "Machine learning for electronic couplings: opportunities and challenges" *APL Comp. Phys.* **2025**, 1, 021501. *Invited for Inaugural Issue. Selected as a Feature Article by the Editors.* https://doi.org/10.1063/5.0297213

[36] Raghuraman, V.; Verma, A.; Jackson, N.E.* "All-Atom Reactive Monte Carlo Molecular Dynamics for Molecular Doping in Organic Semiconductors" *J. Chem. Theory Comput.* **2025**, 21, 20, 10527-10536. https://doi.org/10.1021/acs.jctc.5c01206.

[35] Samajdar, R.; Yang, H.; Yi, S.; Wang, C-.I.; Putnam, S.T.; Pence, M.A.; Lindsay, G.S.; Meigooni, M.; Liu, X.; Ren, J.; Moore, J.S.; Tajkhorshid, E.; Gewirth, A.A.; Rodriguez-Lopez, J.; Jackson, N.E.; Schroeder, C.M. "Electrochemically Mediated Au-C(sp^2) Anchors for Molecular Electronics" *J. Phys. Chem. C* **2025**, 129, 39, 17458-17471. https://doi.org/10.1021/acs.jpcc.5c06124.

[34] Chen, J.; Jackson, N.E.* "A Machine Learning Model for Copolymer Radical Reactivity Ratio Predictions with Frontier-Orbital Insights" *Chem. Mater.* **2025**, 37, 19, 7894-7907. https://doi.org/10.1021/acs.chemmater.5c01608. *Invited for "Machine Learning for Materials Chemistry" Issue.*

[33] Xu, Z.; Wang, Z.; Zhang, R.; Verma, A.; Neu, J.S.; Bairagya, P.; Jeon, S.; Damron, A.M.; Rinehart, J.M.; Wagner, J.S.; Sabury, S.; Luo, X.; Österholm, A.M.; Mei, J.; Moore, J.S.; You, W.; Reynolds, J.R.; Jackson, N.E.; Diao, Y. "Ubiquitous Chiral Symmetry Breaking of Conjugated Polymers via Liquid-Liquid Phase Separation" *J. Am. Chem. Soc.*, **2025**, 2025, 147, 37, 33530–33544. https://doi.org/10.1021/jacs.5c07995.

[32] Shah, A.K.; Dey, A.; Luo, L.; Amador, B.; Philippy, P.; Zhong, M.; Ouyang, S. Friday, D.M.; Bianchi, D.; Jackson, N.; Zanibbi, R.; Han, J. "Multimodal Search in Chemical Documents and Reactions" https://arxiv.org/abs/2502.16865, *48th International ACM SIGIR Conference on Research and Development in Information Retrieval*, **2025**.

[31] Iyer, S.; Jackson, N.E.* "In-silico exploration of metabolite-derived soft materials using a chemical reaction network" *Chem. Mater.* **2025**, 37, 8, 2877-2888. https://doi.org/10.1021/acs.chemmater.5c00163

[30] Sivilotti, S.L.; Friday, D.M.; Jackson, N.E.* "Active Learning High Coverage Sets of Complementary Reaction Conditions" *Digit. Discov.* **2025**, 4, 846-852. https://doi.org/10.1039/D4DD00365A

[29] Kim, S.; Schroeder, C.M.; Jackson, N.E.* "Functional Monomer Design for Synthetically Accessible Polymers" *Chem. Sci.* ***2025.*** 16, 4755-4767. https://doi.org/10.1039/D4SC08617A.

[28] Jackson, N.E.*; Savoie, B.M. "Ten Problems for Polymer Reactivity Prediction" *Macromolecules* **2025**, 58, 4, 1737-1754. https://doi.org/10.1021/acs.macromol.4c02582.

[27] Yu, Z.; Jackson, N.E.* "Shortest paths govern bond rupture in thermoset networks" *Macromolecules* **2025**, 58, 3, 1728-1736. https://doi.org/10.1021/acs.macromol.4c02438.

[26] Yu, Z.; Jackson, N.E.* "Chemically transferable electronic coarse-graining for polythiophenes," *J. Chem. Theory Comput.* **2024**, 20, 20, 9116-9127. https://doi.org/10.1021/acs.jctc.4c00804

[25] Samajdar, R.; Meigooni, M.; Yang, H.; Li, J.; Jackson, N.E.; Mosquera, M.; Tajkhorshid, E.; Schroeder, C.M. "Understanding the role of secondary structure on electron transport in peptides using single-molecule techniques," *Proc. Natl. Acad. Sci.* **2024**, 121 (32) e2403324121, https://doi.org/10.1073/pnas.2403324121.

[24] Angello, N.^; Friday, D.M.^; Hyung, C.^; Yi, S.^; Cheng, A.; Flores, T; Jira, E.; Wang, W.; Aspuru-Guzik, A.*; Burke, M.*; Schroeder, C.M.*; Diao, Y.*; Jackson, N.E.* "Closed-Loop Transfer Enables AI to Yield Chemical Knowledge," *Nature,* 633, 351-358, **2024**, https://www.nature.com/articles/s41586-024-07892-1.

- https://phys.org/news/2024-08-ai-black-team-key-chemistry.html

[23] Wang, C.-I.; Maier, J.C.; Jackson, N.E.* "Accessing the Electronic Structure of Liquid Crystalline Semiconductors with Bottom-Up Electronic Coarse-Graining," *Chem. Sci.* **2024**, 15, 8390-8403, https://doi.org/10.1039/D3SC06749A.

[22] Verma, A.; Jackson, N.E.* "Assessing Molecular Doping Efficiency in Organic Semiconductors with Reactive Monte Carlo," *J. Chem. Phys.* 160, 104106 (**2024**). https://doi.org/10.1063/5.0197816.

[21] Yu, Z.; Jackson, N.E.* "Exploring Thermoset Fracture with A Quantum Chemically Accurate Model of Bond Scission," *Macromolecules*, **2024**, 57, 4, 1414-1425. https://doi.org/10.1021/acs.macromol.3c02549.

[20] Maier, J.C.; Wang, C.-I.; Jackson, N.E.* "Distilling Coarse-Grained Representations of Molecular Electronic Structure Using Continuously Gated Message Passing," *J. Chem. Phys.* 160, 024109 (**2024**). https://doi.org/10.1063/5.0179253.

[19] Charette, B.J.; King, S.R.; Chen, J.; Holm, A.R.; Malme, J.T.; Cook, R.D. Schaller, R.D.; Jackson, N.E.; Olshansky, L. "Excited State Dynamics in a Conformationally Fluxional Copper Coordination Complex," *J. Phys. Chem. A.* **2023**, 127, 37, 7747-7755. https://doi.org/10.1021/acs.jpca.3c04269.

[18] Jackson, N.E.*; Savoie, B.M.*; Statt, A.*; Webb, M.A.* "Introduction to Machine Learning for Molecular Simulation," *J. Chem. Theory Comput.* **2023**, 19, 14, 4335-4337. https://doi.org/10.1021/acs.jctc.3c00735 *Invited Guest Editor for Special Issue.*

[17] Jackson, N.E.*; Luther, J.M.*; Savoie, B.M.*; Wu, K.* "Photophysics in emerging photovoltaics," *J. Chem. Phys.* 159, 020401 (**2023**). https://doi.org/10.1063/5.0161842. *Invited Guest Editor for Special Issue.*

[16] Guo, J.; Woo, V.; Andersson, D.; Hoyt, N.; Williamson, M.; Foster, I.; Benmore, C.; Jackson, N.E.; Sivaraman, G. "AL4GAP: Active Learning Workflow for Generating DFT-SCAN Accurate Machine-Learning Potentials for Combinatorial Molten Salt Mixtures," *J. Chem. Phys.* **2023**. 159, 024802. https://doi.org/10.1063/5.0153021.

[15] Wang, C.-I.; Maier, J.C.; Jackson, N.E.* "Identifying Coarse-Grained Representations for Electronic Predictions," *J. Chem. Theory Comput.* **2023**, 19, 15, 4982-4990. https://doi.org/10.1021/acs.jctc.3c00466.

[14] Yu, Z.; Jackson, N.E.* "Machine learning quantum-chemical bond scission in thermosets under extreme deformation," *Appl. Phys. Lett.* 122, 211906, **2023**. https://doi.org/10.1063/5.0150085, *Editor's Pick, Selected for Rising Star Collection, Invited for Accelerate Materials Discovery and Phenomena Special Issue.*

[13] Khasbaatar, A.; Cheng, A.; Jones, A.L.; Komar, J.; Kwok, J.J.; Lin, O.; Jackson, N.E.; Chen, Q.; Reynolds, J.R.; Diao, Y. "Solution Aggregate Structures of Donor Polymers Determine the Processing Resiliency of Non-Fullerene Organic Solar Cells," *Chem. Mater.* **2023**, 35, 7, 2713-2729. https://doi.org/10.1021/acs.chemmater.2c02141.

[12] Kim, S.; Schroeder, C.M.; Jackson, N.E.* "Open Macromolecular Genome: Generative Design of Synthetically Accessible Polymers," *ACS Polymers Au.* **2023**, 3, 4, 318-330. https://doi.org/10.1021/acspolymersau.3c00003.

[11] Friday, D.M.; Jackson, N.E.* "Electron and Ion Transport in Semi-Dilute Conjugated Polyelectrolytes: View from a Coarse-Grained Tight-Binding Model," *Mol. Syst. Des. Eng.,* **2023**, 8, 743-755. https://doi.org/10.1039/D2ME00285J, *Invited for Emerging Investigators Series. Finalist for 2023 Outstanding Early Career Paper Award.*

[10] Wang, C.-I.; Jackson, N.E.* "Bringing Quantum Mechanics to Coarse-Grained Soft Materials Modeling," *Chem. Mater.* **2023**, 35, 4, 1470-1486. https://doi.org/10.1021/acs.chemmater.2c03712, *Invited for "Up-and-Coming" Investigator Series.*

[9] Maier, J.C.; Jackson, N.E.* "Bypassing Backmapping: Coarse-grained electronic property distributions using heteroscedastic Gaussian processes," *J. Chem. Phys.* **2022**, 157, 174102. https://doi.org/10.1063/5.0101038, *Featured on cover of issue 17, Selected for Emerging Investigator Series.*

[8] Guo, J.; Ward, L.; Babuji, Y.; Hoyt, N.; Williamson, M.; Foster, I.; Jackson, N.E.; Benmore, C.; Sivaraman, G. "A Composition Transferable Machine Learning Potential for LiCl-KCl Molten Salts Validated by HEXRD," *Phys. Rev. B,* **2022**, 106, 014209. https://doi.org/10.1103/PhysRevB.106.014209.

[7] Friday, D.M.; Jackson, N.E.* "Modeling the Interplay of Conformational and Electronic Structure in Conjugated Polyelectrolytes," *Macromolecules,* **2022**, 55, 5, 1866-1877. https://doi.org/10.1021/acs.macromol.2c00007.

[6] Yu, H.; Li, J.; Li, S.; Jackson, N.E.; Moore, J.S.; Schroeder, C.M. "Efficient Intermolecular Charge Transport in pi-Stacked Pyridinium Dimers using Cucurbit[8]uril Supramolecular Complexes," *J. Am. Chem. Soc.* **2022**, 144, 7, 3162. https://doi.org/10.1021/jacs.1c12741.

[5] Sivaraman, G; Jackson, N.E.* "Coarse-Grained Density Functional Theory Predictions via Deep Kernel Learning," *J. Chem. Theory Comput.* **2022**, 18, 2, 1129-1141. https://doi.org/10.1021/acs.jctc.1c01001.

[4] Li, J.; Pudar, S.; Yu, H.; Li, S.; Moore, J.S.; Rodriguez-Lopez, J.; Jackson, N.E.; Schroeder, C.M. "Reversible Switching of Molecular Conductance in Viologens is Controlled by the Electrochemical Environment," *J. Phys. Chem. C* **2021**, 125, 40, 21862-21872. https://doi.org/10.1021/acs.jpcc.1c06942.

[3] Maier, J.C.; Jackson, N.E.* "Sequence-Controlled Electron Transport in Conjugated Copolymers," *Macromolecules* **2021**, 54, 15, 7060-7069. https://doi.org/10.1021/acs.macromol.1c01194.

[2] Sivaraman, G.; Guo, J.; Ward, L.; Hoyt, N.; Williamson, M.; Foster, I.; Benmore, C.; Jackson, N.E.* "Automated Development of Molten Salt Machine Learning Potentials: Application to LiCl," *J. Phys. Chem. Lett.* **2021**, 12, 17, 4278-4285. https://doi.org/10.1021/acs.jpclett.1c00901.

[1] Jackson, N.E.* "Coarse-Graining Organic Semiconductors: The Path to Multiscale Design," *J. Phys. Chem. B.*, **2021**, 125, 2, 485-496. https://doi.org/10.1021/acs.jpcb.0c09749.

Publications Prior to UIUC

*indicates corresponding author(s), ^ indicates equal contributions

[49] Cohen, A.; Jackson, N.E.*; de Pablo, J.J.* "Anisotropic Coarse-Grained Model for Conjugated Polymers: Investigations into Solution Morphologies," *Macromolecules*, 2021, 54, 8, 3780-3789.

[48] Yu, B.; Rumyantsev, A.M.; Jackson, N.E.; Liang, H.; Ting, J.M.; Meng, S.; Tirrell, M.V.; de Pablo, J.J. "Complex Coacervation of Statistical Polyelectrolytes: Role of Monomer Sequences and Formation of Inhomogeneous Coacervates," *Mol. Syst. Des. Eng.* 2021, 6, 790-804.

[47] Rumyantsev, A.M.; Jackson, N.E.; Johner, A.; de Pablo, J.J. "Scaling Theory of Net-Neutral Sequence-Specific Polyampholytes," *Macromolecules*, 2021, 54, 8, 3780-3789.

[46] Rumyantsev, A.M.; Jackson, N.E.; de Pablo, J.J. "Polyelectrolyte Complex Coacervates: Recent Developments and New Frontiers," *Annu. Rev. Condens. Matter Phys.* 2021, 12:1.

[45] Wu, H.; Yu, B.; Ting, J.M.; Meng, S.; Jackson, N.E.; de Pablo, J.J.; Tirrell, M.V. "Spatiotemporal Formation and Growth Kinetics of Polyelectrolyte Complex Micelles with Millisecond Resolution," *ACS Macro Lett.*, 2020, 9, 11, 1674-1680.

[44] Webb, M.A.; Jackson, N.E.; Gil, P.S.; de Pablo, J.J. "Targeted Sequence Design within the Coarse-Grained Polymer Genome," *Sci. Adv.* 2020, 6 : eabc6216.

[43] Yu, B.; Rauscher, P.M.; Jackson, N.E.; Rumyantsev, A.M.; de Pablo, J.J. "Crossover from Unentangled to Entangled Dynamics in Salt-Free Polyelectrolyte Complex Coacervates," *ACS Macro. Lett.* 2020, 9, 9, 1318-1324.

[42] Bagchi, K.; Deng, C.; Bishop, C.; Li, Y.; Jackson, N.E.; Yu, L.; Toney, M.F.; de Pablo, J.J.; Ediger, M.D. "Over what length scale does an inorganic substrate perturb the structure of a glassy organic semiconductor?" *ACS Appl. Mater. Interfaces*, 2020, 12, 26717-26726.

[41] Sivaraman, G.^; Jackson, N.E.^*; Sanchez-Lengeling, B.; Vasquez-Mayagoitia, A.; Aspuru-Guzik A.; Vishwanath, V.; de Pablo, J.J.* "A machine learning workflow for molecular analysis: application to molecular melting points," *Mach. Learn.: Sci. Technol.*, 2020, 1, 025015.

[40] Jackson, N.E.*; Bowen, A.S.; de Pablo, J.J.* "Efficient Multiscale Optoelectronic Prediction for Conjugated Polymers," *Macromolecules*, 2020, 53, 482-490.

[39] Rumyantsev, A.M.; Jackson, N.E; Yu, B.; Ting, J.M.; Tirrell, M.V.; de Pablo, J.J. "Controlling Complex Coacervation via Random Polyelectrolyte Sequences," *ACS Macro. Lett.*, 2019, 8, 10, 1296-1302.

[38] Jackson, N.E.^; Webb, M.A.^; de Pablo, J.J. "Recent Advances in Machine Learning Towards Multiscale Soft Materials Design," *Curr. Opin. Chem. Eng.*, 2019, 23:1-9.

[37] de Pablo, J.J.; Jackson, N.E.; Webb, M.A.; Chen, L-C.; Moore, J.; Morgan, D.; Pollock, T.; Schlom, D.; Toberer, E.; Analytis, J.; Dabo, I.; DeLongchamp, D.; Fiete, G.; Grason, G.; Hautier, G.; Mo, Y.; Rajan, K.; Reed, E.; Rodriguez, E.; Stevanovic, V.; Suntivich, J.; Thornton, K.; Zhao, J-C.; "New Frontiers for the Materials Genome Initiative, *npj Comput. Mater.*, 2019, 5, 1, pp 41.

[36] Jackson, N.E.; Bowen, A.S.; Antony, L.W.; Webb, M.A.; Vishwanath, V.; de Pablo, J.J. "Electronic Structure at Coarse-Grained Resolutions from Supervised Machine Learning," *Sci. Adv.*, 2019, 5 (3); eaa1190.

[35] Bagchi, K.; Jackson, N.E.; Gujral, A.; Huang, C.; Toney, M.F.; Yu, L.; de Pablo, J.J. Ediger, M.D. "Origin of anisotropic molecular packing in vapor deposited Alq_3 glasses," *J. Phys. Chem. Lett.*, 2019, 10, pp 164-170.

[34] Bowen, A.; Jackson, N.E.; Reid, D.R.; de Pablo, J.J. "Structural Correlations and Percolation in Twisted Perylene Diimides using a Simple Anisotropic Coarse-Grained Model," *J. Chem. Theory Comput.*, 2018, 14, (12), pp 6495-6504.

[33] Reid, D.R.; Jackson, N.E.; Bourque, A.J.; Snyder, C.R.; Jones, R.L.; de Pablo, J.J. "Aggregation and Solubility of a Model Conjugated Donor-Acceptor Polymer," *J. Phys. Chem. Lett.*, 2018, 9 (16), pp 4802-4807.

[32] Kohlstedt, K.L.; Jackson, N.E.; Savoie, B.M.; Ratner, M.A. "Introduction to Organic Semiconductors Using Accessible Undergraduate Chemistry Concepts," *J. Chem. Educ.*, 2018, 95 (9), pp 1500-1511.

[31] Jackson, N.E.; Webb, M.A.; de Pablo, J.J. "Layered Nested Markov Chain Monte Carlo," *J. Chem. Phys.*, 2018, 149, 072326.

[30] Yu, J.^; Jackson, N.E.^; Xu, X.; Morgenstern, Y.; Kaufman, Y.; Ruths, M.; de Pablo, J.J.; Tirrell, M. "Multivalent counterions diminish the lubricity of polyelectrolyte brushes," *Science*, 2018, 360 (6396), pp 1434-1438.

[29] Langenberg, M.; Jackson, N.E.; de Pablo, J.J.; Muller, M. "Role of translational entropy in spatially inhomogeneous, coarse-grained models," *J. Chem. Phys.*, 2018, 148, 094112.

[28] Yu, J.^; Jackson, N.E.^; Xu, X.; Brettmann, B.K.; Ruths, M.; de Pablo, J.J.; Tirrell, M. "Multivalent Ions Induce Lateral Structural Inhomogeneities in Polyelectrolyte Brushes," *Sci. Adv.*, 2017, 3 (12); eaao1497.

[27] Antony, L.W.; Jackson, N.E.; Lyubimov, I.; Vishwanath, V.; Ediger, M.D.; de Pablo, J.J. "Influence of Vapor Deposition on Structural and Charge Transport Properties of Ethyl Benzene Films," *ACS Cent. Sci*, 2017, 3 (5), pp 415-424.

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[20] Storm, F.E.; Olsten, S.T.; Hansen, T.; De Vico, L.; Jackson, N.E.; Ratner, M.A.; Mikkelsen, K.V. “Boron Subphthalocyanine Based Molecular Triad Systems for the Capture of Solar Energy,” *J. Phys. Chem. A*, 2016, 120 (390), pp 7694-7703.

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Invited Presentations

1.	(Upcoming) ACS Spring, Degradation of Polymers and Composite Materials, New Orleans, LA	2027
2.	(Upcoming) MRS Spring, Unraveling the Fundamentals of Doping in pi-Conjugated Semiconductors	2027
3.	(Upcoming) Department Seminar – Penn State University, Chemistry	2027
4.	(Upcoming) Department Seminar, Harvey Mudd College, Chemistry	2026
5.	(Upcoming) MRS Fall, Fundamentals of Organic and Hybrid Mixed Conductors, Boston, MA	2026
6.	(Upcoming) ACS Fall, Data Analytics and AI: Polymers, Chemistry, and Manufacturing, Chicago, IL	2026
7.	(Upcoming) ACS Fall, Machine Learning Meets Electronic Structure Theory, Chicago, IL	2026
8.	NOBCChE Midwest Regional Symposium, Columbus, OH	2026
9.	Machine Learning for Materials and Molecular Discoveries (ML2MD), Uppsala, Sweden	2026
10.	CECAM "Physics-Aware Machine Learning for Molecules and Materials", Cornell Tech, NY	2026
11.	Theory Seminar – UC Berkeley, Chemistry & Chemical Engineering	2026
12.	Department Seminar – Stanford University, Chemistry	2026
13.	Department Seminar – Purdue University, Chemistry	2026
14.	Department Seminar – University of Wisconsin – Madison, Chemistry	2026
15.	Schmidt AI + Science Seminar Series – University of Chicago	2026
16.	Department Seminar – University of Notre Dame, Chemistry	2026
17.	Department Seminar – Northwestern University, Chemistry	2026
18.	Theoretical Chemistry Seminar – Northwestern University	2026
19.	Department Seminar – University of Chicago, Molecular Engineering	2026
20.	Department Seminar – Princeton University, Materials Institute	2025
21.	Department Seminar – Columbia University, Chemistry	2025
22.	Department Seminar – Case Western Reserve University, Chemistry	2025
23.	Department Seminar – Case Western Reserve University, Macromolecular Eng.	2025
24.	3rd International Symposium on Machine Learning in Quantum Chemistry, UT-Knoxville	2025
25.	Data Chemistry Bootcamp Speaker – University of Notre Dame	2025
26.	Department Seminar – University of Colorado – Boulder, Chemistry	2025
27.	Department Seminar – North Carolina State University, Chemical Engineering	2025
28.	Telluride Science Research Center Conference on Polymer Physics	2025
29.	University of Missouri Advancing Materials Frontiers with Creativity and Data Science NRT Program (Student-Invited)	2025
30.	Kavli Foundation Emerging Leader in Chemistry Award Lecture	2025
31.	ACS Spring, Data Analytics and AI for Manufacturing and Healthcare session, San Diego, CA.	2025
32.	APS March, Generative models and machine learning in chemical physics session, Anaheim, CA.	2025
33.	University of Delaware NRT MIDAS Training Program Seminar	2024
34.	AIChE COMSEF Plenary Session	2024

35. ACS Fall COMP Awards Session 2024
36. Institute for Mathematical and Statistical Innovation, Learning Collective Variables and Coarse-Grained Models Workshop, Chicago, IL 2024
37. (Virtual) UNC Chapel Hill – ONR MURI for Molecular Doping of Organic Electronic Materials Seminar Series 2024
38. (Virtual) Materials Research Data Alliance (MaRDA) Annual Meeting 2024
39. AIChE COMSEF Plenary Session 2023
40. (Virtual) Seminar for British Petroleum on AI in Materials Engineering 2023
41. (Virtual) Rice University, NSF Center for Adopting Flaws as Features 2023
42. ACS Northwest Meeting Computational and Theoretical Chemistry Symposium 2023
43. 2023 TechConnect World "AI for Advanced Materials Design" Symposium 2023
44. ACS Spring, Advances in Coarse-Graining and Multiscale Modeling Symposium 2023
45. ACS Spring, New Directions in the Physical Chemistry of Organic Semiconductors Symposium 2023
46. Department Seminar – Ohio University, Chemical and Biomolecular Engineering 2023
47. (Virtual) Helmholtz Institute-Muenster, Machine Learning in Physical Chemistry Seminar Series 2022
48. ARO-MDP Data-Driven Design of Heterogeneous Materials Workshop, UChicago 2022
49. (Virtual) Sandia National Laboratory, New Mexico Machine Learning Symposium 2021
50. (Virtual) 3M Materials Informatics and Machine Learning Seminar 2021
51. (Virtual) Department Seminar – Fordham University, Chemistry. 2021
52. (Virtual) Argonne National Laboratory, AI and HPC Seminar Series. 2021
53. (Virtual) CECAM, Multiscale simulations of soft matter: new method developments and mathematical foundations 2020

Professional Service

Conference or Workshop Organization and Chairing

- Frontiers in AI and Molecular Modeling Session, ACS Spring 2027, New Orleans. Co-Organizers: Yamil Colón, Mike Webb.
- Organic Electronics & Photonics Session, APS Spring 2027, Atlanta.
- Co-Organizers: Xiaodan Gu, Enrique Gomez.
- International Workshop on Polymer Data (2026), Washington DC. Co-Organizers: Tengfei Luo, Brett Savoie, Junichiro Shiomi, Ryo Yoshida. https://polymerdataworkshop.nd.edu/. Raised $7500 from Beckman Institute to support workshop.
- AIChE Area 1a programming committee (2024-2027)
- Obtained $12,000 Euro from Centre Européen de Calcul Atomique et Moléculaire (CECAM) to co-organize the first US-based CECAM workshop: "Frontiers of Computational Reaction Prediction" at the University of Chicago in July 2024. https://chemistry.illinois.edu/news/2024-02-21t164021/nick-jackson-leading-first-ever-us-based-cecam-workshop.
- ACS COMP "Advances in Coarse-Grained and Multiscale Modeling", Indianapolis, IN (Spring '23) – Co-organizer and session chair.
- AIChE Annual Meeting COMSEF "Machine Learning for Soft Materials" ('22,'23) – Co-organizer and session chair.

Guest Editorships and Editorial Board Service

- *Chemical Reviews*, Topic Editor in AI (2025-2027)
- *Lin X. Chen Festschrift, Journal of Chemical Physics,* Guest Editor (2026).
- *Journal of Chemical Theory and Computation,* Early Career Board (2023-2025)
- *Journal of Chemical Theory and Computation*, Guest Editor for 2023 Special Issue on "Machine Learning for Molecular Simulation."
- *Journal of Chemical Physics*, Guest Editor for 2023, Vol. 159, Issue 2. Focus Issue on "Photophysics in Emerging Photovoltaics."

Panel Reviewer – NSF (CTMC), DOE - EFRC, ONR - MURI
External Ph.D Examiner – Colme Burke, University of Liverpool (2026).
***Ad Hoc* Proposal Reviewer –** DOE (BES/NE-CINR, CTC, SciDac, SCGSR), NSF (CBET, CTMC, DMR, CDS&E), ACS PRF, DFG (Germany), ARO, RCSA, FNR (Luxemborg)
Award Committees – ACS OpenEye Junior Faculty Award
Funding Agency Workshops

- Co-Organizer: NSF "Advancing and Accelerating Materials Innovation Through the Synergistic Interaction among Computation, Experiment, and Theory: Opening New Frontiers" (*npj Comp. Mater*. 2019, 5, 1, 1-23). (7/17)
- Participant: ARO-MDP Data-Driven Design of Heterogeneous Materials (5/22)
- Participant: NSF Sustainable Materials and Manufacturing Square Table (4/21).

Poster Session Judge

- 2025 3rd International Symposium on Machine Learning in Quantum Chemistry
- 2022 Midwest Thermodynamics and Statistical Mechanics
- Fall 2019 ACS PHYS.

Journal Reviewer – *Journal of Physical Chemistry*, *Macromolecules, Science Advances, Journal of Chemical Physics, ACS Macromolecular Letters, Journal of Materials Chemistry C, Angewandte Chemie, ACS Central Science, Nature Review Materials, Nature Synthesis, JACS, PNAS, ACS Nano, Chemical Science, Chemical Physics Letters, ACS Applied Energy Materials, npj Computational Materials, Physical Chemistry Chemical Physics, Chemistry of Materials, Soft Matter, ACS Polymers Au, Nature Machine Intelligence, ChemPhysChem, RSC Digital Discovery, Molecular Simulation, Molecular Informatics, Journal of Chemical Informatics and Modeling, RSC Advances, Fluid Phase Equilibria, Materials Horizons, Materials Today Advances, Communications Physics, Journal of Chemical and Engineering Data, Nanoscale.*
Textbook Reviewer – *Introduction to Computational Physical Chemistry* – Joshua Schrier, ISBN-10: 1938787900.

Grants

Total to Jackson since 2021: $5.2M

National Science Foundation Division of Chemistry: Disciplinary Research Programs – Chemical Theory, Models and Computation Program
Principal Investigator: Nick Jackson
"Electronic Model Development Using Coarse-Grained Molecular Representations"
8/1/26 – 7/31/29 To Jackson: $450,000

Air Force Office of Scientific Research – Organic Materials Chemistry Program
Principal Investigator: Julia Kalow (Northwestern)
Co-Principal Investigators: Nick Jackson, Milan Mrksich (Northwestern)
"*Sequence design in pi-conjugated polymers through encoding-selection decoding"*
8/1/25-7/31/28 Total: $550,000 To Jackson: $160,000

Office of Naval Research – Functional Polymeric and Organic Materials Program
Principal Investigator: Nick Jackson
"Deciphering Molecular Doping in Organic Materials Using Multiscale Simulations"
4/1/26 – 03/31/28 Total: $293,705

NSF Division of Materials Research DMREF
Principal Investigator: Chris Evans

Co-Principal Investigators: Nick Jackson, Rachel Letteri (UVa), Charles Schroeder
"*Collaborative Research: DMREF: AI-guided Discovery of Sustainable Ion-Conducting Peptide Electrolytes"*
9/30/2025 – 8/31/2029 Total: $2,000,000 To Jackson: $421,228

IBM Corporation – IBM-Illinois Discovery Accelerator Institute
Principal Investigator: Heng Ji
Co-Principal Investigators: Ying Diao, Nick Jackson
"Foundational AI Agents for Materials Discovery"
8/1/25-7/31/26 Total: $450,000 To Jackson: $150,000

NSF AI Institute for Molecular Discovery, Synthetic Strategy, and Manufacturing: Molecule Maker Lab Institute (MMLI)
Principal Investigators: Huimin Zhao
Co-Principal Investigators: Scott Denmark, Martin Burke, Heng Ji, Ying Diao
9/1/25 – 8/31/30 Total: $15,000,000 To Jackson: $387,100

Camille Dreyfus Teacher-Scholar Award
Principal Investigator: Nick Jackson
"*A Chemically Transferable Coarse-Grained Electronic Structure Model for Polymers*"
07/01/25-06/31/30 Total: $100,000

Cottrell Scholar Award
Principal Investigator: Nick Jackson
"*Electronic Dynamics Using Coarse-Grained Molecular Representations*"
04/01/25-03/31/28 Total: $120,000

PPG Industries, Inc.
Principal Investigator: Charles Schroeder
Co-Principal Investigator: Nick Jackson
"*Closed-Loop (ML-Based) Discovery and Optimization of Electrochromic Dyes*"
5/1/24-4/31/25 Total: $120,000 To Jackson: $30,000

IBM Corporation – IBM-Illinois Discovery Accelerator Institute
Principal Investigator: Nick Jackson
Co-Principal Investigator: Charles Schroeder
"*A Multi-Task Foundation Model for Polymeric Materials Design via the Open Macromolecular Genome"*
8/1/23 – 7/31/24 Total: $110,000

Department of Energy Early Career Award – Computational and Theoretical Chemistry Program
Principal Investigator: Nick Jackson
"Generalized Electronic Coarse-Graining for the Hierarchical Design of Organic Neuromorphics"
7/1/23 – 6/30/28 Total: $875,000

Office of Naval Research – Functional Polymeric and Organic Materials Program
Principal Investigator: Nick Jackson
"Deciphering Molecular Doping in Organic Materials Using Multiscale Simulations"
9/1/23 – 08/31/26 Total: $488,316

National Science Foundation Future Manufacturing Research Grants: Cyber: Manufacturing USA
Principal Investigator: Michael Cullinan (Texas)
Co-Principal Investigators: Zachariah Page (Texas), Michael Baldea (Texas), Rajesh Menon (Utah)
"Cyber-Enabled, High-Throughput Manufacturing of Multi-Material, 3D Nanostructures"
10/1/22 – 9/30/26 Total: $2,999,732 To Jackson: $421,615

National Science Foundation Division of Chemistry: Disciplinary Research Programs – Chemical Theory, Models and Computation Program
Principal Investigator: Nick Jackson

"Electronic Structure Models Using Coarse-Grained Representations"
4/1/22 – 3/31/25 To Jackson: $450,000

IBM Corporation – IBM-Illinois Discovery Accelerator Institute
Principal Investigator: Huimin Zhao
Co-Principal Investigators: Marty Burke, Ying Diao, Charles Schroeder, Nick Jackson
"*Automation and AI for Organic and Polymeric Materials Discovery"*
12/1/22 – 11/30/23 Total: $500,000 To Jackson: $110,000

Dreyfus Machine Learning in the Chemical Sciences and Engineering Award
Principal Investigator: Nick Jackson
"*Machine Learning Quantum Chemistry Over Coarse-Grained Fields*"
9/1/21 – 8/31/23 Total: $110,261

American Chemical Society Petroleum Research Fund Doctoral New Investigator Award
Principal Investigator: Nick Jackson
"Is There a Tradeoff Between Electronic and Ionic Conduction in Petroleum-Derived Polyelectrolytes?"
9/1/21 – 8/31/23 Total: $110,000

National Science Foundation Division of Chemistry: Molecule Maker Laboratory Institute (MMLI): An AI Institute for Molecular Discovery Synthetic Strategy and Manufacturing:
Principal Investigators: Huimin Zhao
Co-Principal Investigators: Martin Burke, Jian Peng, Saurabh Sinha, Ying Diao, Scott Denmark
"*Autonomous Materials Discovery for Organic Solar Cells"*
Emerging Opportunities Award – "AI-Guided Molecular Design of Dynamic Mixed Ion/Electron Conductors"
9/1/21 – 8/31/26 Total: $20,000,000 To Jackson: $400,000

3M Nontenured Faculty Award
Principal Investigator: Nick Jackson
"Mapping the Physicochemical Properties of the Charge Transporting Polymer Genome"
5/1/21 – 4/31/24 To Jackson: $45,000

Argonne National Laboratory LDRD Expedition Award
Principal Investigator: Nick Jackson
"An Active Learning Workflow for Machine Learning Forcefield Automation"
9/1/20 – 4/1/21 To Jackson: $70,000

Argonne National Laboratory LDRD Named Fellow Award
Principal Investigator: Nick Jackson
"Microstructural Simulations of Stable Conjugated Polymer Glasses"
10/1/16 – 10/1/19 To Jackson: $450,000

Departmental Service

Vice-Chair of Graduate Admissions Committee	*2026-Present*
Faculty Supervisor for Student-Invited Physical Chemistry Seminar Series	*2026-Present*
Leader of the Department of Chemistry AI Task Force	*2026-Present*
Chemistry Department Klemperer Award Evaluation Committee	*2023*
Chemistry Department Geerdes Travel Award Selection Committee	*2022*
Chemistry Graduate Admissions Committee – Physical & Materials	*2021-2026*
Created the course CHEM452/CHBE413 – Data Science for Chemistry and Engineering, which was approved at the campus level. https://chemistry.illinois.edu/news/2022-10-06/alums-tom-remec-and-susan-morisato-support-new-data-science-initiative	*2021*
Creation and Management of the *Thomas Remec and Susan Morisato Scholarship in Chemical Data Science* (Undergraduate Research Program)	*2021-Present*
Multiple research presentations to UIUC ACS Student Chapter Seminar	*2021-Present*

Creation and maintenance of Center for Advanced Theory and Molecular Simulations (CATMS) website	*2021-Present*
Chemistry Ph.D. Committees (---indicates completed duty): David Durden (Backlund), ~~Zhuang Xu (Diao)~~, ~~Romans Grant (Sweedler)~~, ~~Kevin Adams (Peters)~~, ~~Annika Holm (Mirica)~~, ~~Lawrence Salvati (Dlott)~~, ~~Blake Ocampo (Denmark)~~, Ellie Vandel (Makri), ~~Daniel McIntosh (Hirata)~~, Elisia Meyle (Burke), Nathan Gehrke (Burke), Dongchen Ouyang (Denmark), ~~Autumn Cook (Kuenstler)~~, Arnav Paul (Shukla), ~~Michael Pence (Rodriguez-Lopez)~~, ~~Jagriti Chatterjee (Landes)~~, Omkar Chaudhari (Hirata), Yichen Li (Rodriguez-Lopez), Gaven Hazen (Rodriguez-Lopez), Chetan Prasad (Diao), Faith Kern (Moore), Elizabeth Vrana (Guironnet), Miko Miwa (Shukla), Blake Gross (Jun), Sophie Mazure (Strauss), Gawon Lee (Burke), Anushna Bhattacharyya (Sing), Filippos Drakopoulos (Shukla).	*2021-Present*

University Service

Member of the AI in Education Committee of the LAS AI Task Force	*2026-Present*
Monthly Speaker for AI in Chemistry Event run by the UIUC YCC	*2026*
Beckman Institute Strategic Planning Committee	*2025-2026*
AI for Materials Working Group Leader – Beckman Institute	*2024-Present*
Beckman Institute Program Advisory Committee (Yearly Postdoctoral Fellow selection committee, Yearly Graduate Student Fellow selection committee, Yearly Seed Grant selection committee)	*2023-2026*
IBM-Illinois Discovery Accelerator Institute Seminar Committee	*2023-2025*
Beckman Institute Thomas and Margaret Huang Award for Graduate Research Award Selection Committee	*2023*
ChBE Academic Chat Panelist (10/25)	*2022*
ChBE Ph.D. Committees (--- indicates completed duty): ~~Caroline Li (Schroeder)~~, ~~Azzaya Khasbaatar (Diao)~~, ~~Hsin-Lan Chiang (Shukla)~~, ~~Reeju Samajdar (Schroeder)~~, Siri Phuangthong (Sing), Song Yin (Shukla), Ziqiu Chen (Peters), Adrija Dutta (Shukla), Alyssa Spencer (Makri), Xuenan Mi (Shukla), Banhee Brishti (Mironenko), ~~Lanie Leung (Mironenko~~), Jiqing Zhuang (Mironenko).	*2021-Present*
Materials Science & Engineering Ph.D Committees: ~~Seungjoo Yi (Schroeder),~~ Siddharth Krishnan (Aksimentiev)	*2024 - Present*
Biophysics Tutorials: Tanner Dean (Shukla), Diego Kleiman (Shukla)	*2023 - Present*
Biophysics Ph.D Committees: ~~Diego Kleiman (Shukla)~~	*2024-Present*

Teaching and Pedagogical Training

NSF Molecule Maker Laboratory Institute Organizer and Lecturer for "AI-Empowered Chemistry: A Playbook" - https://online.illinois.edu/catalog/non-credit/offerings/156201. Lecturer.	*2024*
Instructor, CHEM452 Data Science for Chemistry & Engineering, UIUC	*Fall 22,23,25*
Instructor, CHEM442 Structure and Dynamics of Molecules, UIUC	*Spring 21,23,24,25*
ACS New Faculty Workshop	*Summer 2021*
Co-Instructor, MENG24100 Molecular/Materials Modeling I, UChicago	*Fall 2017*
Teaching Intern, CHEM445 Contemporary Spectroscopy, Northwestern	*Spring 2015*
Northwestern University Teaching Certificate Program	*2014-2015*
Teaching Assistant, CHEM101 General Chemistry Laboratory, Northwestern	*2012*
Teaching Assistant, CHEM342 Statistical Thermodynamics, Northwestern	*2012*
Teaching Assistant, CHEM350 Advanced Physical Chem Lab, Northwestern	*2012*
Teaching Assistant, CHEM171 Accelerated Gen Chem Lab, Northwestern	*2011*
Teaching Assistant, PHYS116 General Physics II, Wesleyan	*2010*
Teaching Assistant, PHYS113 General Physics I, Wesleyan	*2009*
Teaching Assistant, PHYS105 The Physics of Sustainability, Wesleyan	*2009*

Outreach

The Jackson Group runs two St. Elmo Brady Outreach Activities at the Booker T. Washington STEM Academy *2025*

Created a Kaggle competition for learning based on the data generated in our 2024 *Nature* paper on closed-loop discovery of photostable compounds https://www.kaggle.com/datasets/dfriday/oligomer-photostability-and-computed-properties *2024*

Recorded two publicly available ML for Chemistry tutorials for the Molecule Maker Lab Institute Youtube Channel: "Turning Molecules into Data" and "How Good is Your Machine Learning Model?" https://www.youtube.com/@MoleculeMaker *2024*

Speaker and panel member for 2030STEM virtual salon #10: Futurecasting – Ensuring New Pathways for Underrepresented Groups in Technically Advanced and Emerging STEM fields, knowledge and skills – Sponsored by the National Academies for Science, Engineering, and Medicine. https://2030stem.org/salon10 *2024*

St. Elmo Brady Academy Outreach Event with Booker T Washington STEM Academy *2024*

Molecule Maker Laboratory Institute (MMLI) Fruit Juice Solar Cells and Machine Learning (Collaboration with The Well Experience) - https://chemistry.illinois.edu/news/2023-05-30/students-researchers-chemical-sciences-lead-middle-school-students-stem-activities *2023*

Beckman Institute Open House "Extracting Strawberry DNA" Interactive Demonstration *2023*

Illinois Academic Leadership and Management Institute (ALMI) Program, https://las.illinois.edu/about/ie/programs/almi *2023*

Mentorship

Postdoctoral Researchers (6)

Dr. Hang Zhang (Ph.D Princeton University w/Mike Webb) *2025-Present*

Dr. Viviana Palacio Betancur (Ph.D University of Chicago w/Juan de Pablo) *2025-Present*

Dr. Katherine Kidder (Ph.D Penn State University w/Will Noid) *2024-Present*

Dr. Vishnu Raghuraman (Ph.D Carnegie Mellon University w/ Michael Widom) *2024-Present*

Dr. Zheng Yu (Ph.D University of Wisconsin – Madison w/Bu Wang) *2022-2024*

Next Position: Postdoctoral Fellow at Princeton University w/Roberto Car

Dr. Chun-I Wang (Ph.D National Chung Cheng University w/Chi Hua) *2021-2024*

Next Position: Asst. Prof. CUNY Lehman College

Graduate Student Researchers (15)

Jinwon Lee, Chemistry Ph.D Student *2025-Present*

Sijing (Paul) Zhu, Chemistry Ph.D Student *2025-Present*

Abigail Miller, Chemistry Ph.D Student (Co-Advised w/Joaquín Rodríguez-López) *2025-Present*

Jingdan Chen, Chemistry Ph.D Student *2024-Present*

Eliza Asani, Chemistry Ph.D Student *2024-Present*

Matthew Too, Chemistry Ph.D Student *2024-Present*

Anna DeBernardo, Chemistry Ph.D. Student *2023-Present*

Huihang Qiu, Chemistry Ph.D. Student *2023-Present*

Jason Wu, Chemistry Ph.D. Student (Co-Advised w/Charles Schroeder) *2023-Present*

Shruti Iyer, Chemistry Ph.D. Student *2022-Present*

Seonghwan Kim, MSE Ph.D. Student (Co-Advised w/Charles Schroeder) *2021-Present*

- *Thesis: "Computational Design of Polymer Chemistry"*
- *Next Position: Postdoctoral Researcher with Juan de Pablo at NYU*

Archana Verma, Ph.D Chemical and Biomolecular Engineering *2021-Present*

- Thesis: "*Thermodynamic Origins of Molecular Doping Efficiency for Advancing Predictive Design of Organic Semiconductors"*

- *Next Position:*

David Friday, Ph.D Chemistry *2020-2025*
- Thesis: *"Computational and Machine Learning Tools for Insights into Conjugated Materials"*
- *Next Position: Scientific Research Advisor at Lilly*

Charlie Maier, Ph.D Physics *2020-2025*
- Thesis: *"Machine Learning-Driven Electronic Models for the Coarse-Grained Resolution of Soft Materials"*
- *Next Position: SAI Postdoctoral Fellow with Brett Savoie at Notre Dame*

Phillip Sin, MSE Ph.D. Student *2021-2023*

Undergraduate Researchers (9)

Aldahir Flores, 2028 ChBE + Data Science *2026-Present*
Shi Chen, 2028 CS + Chemistry *2026-Present*
Isaac Christensen, 2026 CS + Chemistry *2024-2026*
Zylle Constantino, 2025 ChBE *2024-2025*
Next Position: Undergraduate Researcher in Xiao Su group
Ram Ganesan, 2026 CS + Chemistry *2024*
Reesa Espera, 2026 ChBE *2023-2026*
Next Position: Samsung
Sofia Sivilotti, 2025 CS + Chemistry *2023-2025*
Next Position: Data Engineer at Uncountable
Aidan Lindsay, 2025 Chemistry *2023-2025*
Next Position: Ph.D student at University of Chicago Chemistry
Andriy Bilobokyy, 2023 CS + Chemistry *2023*
Next Position: Software Engineer at Northrop Grumman
Andrew Qin, 2023 ChBE *2022-2023*
Next Position: Ph.D. student at NYU Applied Mathematics
Rohini Ramabadran, 2022 CS + Chemistry *2021*
Next Position: Software Engineer at SeatGeek

Group Member Recognition

Beckman Institute Postdoctoral Fellow
Viviana Palacio Betancur (2025)

National Science Foundation Graduate Research Fellowships
Archana Verma (2021), Jason Wu (2024), Anna DeBernardo (2025), Abigail Miller (2026), Aidan Lindsay (2026 – former UG).

Department of Energy Computational Science Graduate Fellowship
Eliza Asani (2025)

Illinois Distinguished Fellowships
Archana Verma (2021), Matthew Too (2024)

Springborn Fellowships
Matthew Too (2024), Abigail Miller (2026)

NCSA Ashby Prize in Computational Science
1st Place - Zheng Yu, Seonghwan Kim, Shruti Iyer, Jason Wu (2024)
https://ai.ncsa.illinois.edu/news-events/2024/05/2024-hackathon-winners-announced/, https://chemistry.illinois.edu/news/2024-05-23/illinois-chemistry-team-wins-computational-science-hackathon

Poster Prizes
Chun-I Wang (MTSM 2022)

ACS Undergraduate Award in Physical Chemistry
Aidan Lindsay (2023), Sofia Sivilotti (2025)

Goldwater Scholar
Aidan Lindsay (2023)

Astronaut Scholarship
Aidan Lindsay (2024)

Remec & Morisato Scholars
Aidan Lindsay (2024), Sofia Sivilotti (2023), Isaac Christensen (2025)

GEICS Inclusive Excellence Leadership Award
Archana Verma (2024)

Oral Presentation Prizes
Archana Verma (1st Prize – ChBE Graduate Research Symposium 2024)

SCS Teaching Excellence Awards
David Friday (2021), Anna DeBernardo (2024), Eliza Asani (2025)