Andrew S. **Rosen**

Assistant Professor, Princeton University
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Academic Appointments

Princeton University — *Princeton, NJ*
Assistant Professor, Department of Chemical and Biological Engineering — 2024 – Present
Associated Faculty, Princeton Materials Institute
Associated Faculty, Princeton Institute for Computational Science and Engineering
Associated Faculty, Center for Statistics and Machine Learning
Associated Faculty, Andlinger Center for Energy and the Environment
Associated Faculty, Computational Sciences Department, Princeton Plasma Physics Laboratory

Education and Training

University of California, Berkeley — *Berkeley, CA*
Miller Research Fellow, Department of Materials Science and Engineering — 2021 – 2024
Mentor: Prof. Kristin A. Persson

Northwestern University — *Evanston, IL*
Ph.D. in Chemical Engineering — 2016 – 2021
Advisors: Prof. Randall Q. Snurr, Prof. Justin M. Notestein

Tufts University — *Medford, MA*
B.S. in Chemical Engineering, *summa cum laude* — 2011 – 2015

Honors & Awards

Outstanding Teaching Award, Princeton University – SEAS — 2025
Royal Society of Chemistry Outstanding Reviewer, Digital Discovery — 2023
Distinguished Young Scholar, University of Washington – Chemical Engineering — 2022
Miller Research Fellowship, University of California, Berkeley — 2021
Presidential Fellowship, Northwestern University – The Graduate School — 2021
Distinguished Graduate Researcher Award, Northwestern University CBE — 2020
Outstanding Research Mentor Award, International Institute for Nanotechnology — 2020
CAS Future Leader, American Chemical Society — 2020
CoMSEF Graduate Student Award – Honorable Mention, AIChE CoMSEF — 2020
ACS Division of Inorganic Chemistry Travel Award, ACS Division of Inorganic Chemistry — 2020
ACS Catalysis Division Travel Award, ACS Catalysis Division — 2019
Ryan Fellowship, International Institute for Nanotechnology — 2018
George Thodos Teaching Assistant Award (×2), Northwestern University CBE — 2017 & 2018
National Defense Science and Engineering Graduate Fellowship, U.S. Dept. of Defense — 2017
Class of 1947 Victor Prather Prize, Tufts University — 2015
Goldwater Scholarship, Barry Goldwater Scholarship Foundation — 2014
Summer Research Scholarship, Tufts University — 2014
National Undergraduate Fellowship, Princeton Plasma Physics Laboratory — 2013

Outstanding Poster Presentation Award, 55th APS Plasma Physics Conference 2013
Tau Beta Pi, Tufts University 2013

Publications

* corresponding author | = equal contribution | Google Scholar | ORCID: 0000-0002-0141-7006
> 4200 citations via Google Scholar, *h*-index $\geq$ 27

Pre-Prints and Articles Under Review

44. Predicting the Thermodynamic Limits of Metal–Organic Framework Metastability
B. Dallmann, A. Saha, **A.S. Rosen***. *Under review.*

43. The Open Molecules 2025 (OMol25) Dataset, Evaluations, and Models
D.S. Levine, M. Shuaibi, M. Hasyim, K. Michel, E.W.C. Spotte-Smith, M.G. Taylor, M.R. Hasyim, K. Michel, I. Batatia, G. Csányi, M. Dzamba, P. Eastman, N.C. Frey, X. Fu, V. Gharakhanyan, A.S. Krishnapriyan, J.A. Rackers, S. Raja, A. Rizvi, **A.S. Rosen**, Z. Ulissi, S. Vargas, C.L. Zitnick, S.M. Blau*, B.M. Wood*. arXiv:2505.08762 (2025).

Published and In Press

42. Beyond Big Data in Quantum Chemistry
A.S. Rosen*, *Nature Chemical Engineering*, 3, 79 (2026).

41. Capturing the Complexities of Catalyst–Support Interactions with the Help of Machine Learning
A.S. Rosen*, *Angewandte Chemie International Edition*, 64, e202521310 (2025).

40. Multi-Gas Adsorption with Single-Site Cooperativity in a Metal–Organic Framework
K.M. Carsch, H.Z.H. Jiang, R.A. Klein, **A.S. Rosen**, P. Summerhill, J.L. Peltier, A.J. Huang, R.A. Murphy, M.N. Dods, Hope A. Silva, Z. Hasanbasri, H. Kwon, S.L. Karstens, Y. Yabuuchi, J. Böergel, J.W. Taylor, K.R. Meihaus, K.C. Bustillo, A.M. Minor, K.A. Persson, C.M. Brown, R.D. Britt, N.P. Stadie, J.R. Long*, *Science*, 390, 808–812 (2025).

39. A Foundation Model for Atomistic Materials Chemistry
I. Batatia=, P. Benner=, Y. Chiang=, A.M. Elena=, D.P. Kovács=, J. Riebesell†, X.R. Advincula, M. Asta, M. Avaylon, W.J. Baldwin, F. Berger, N. Bernstein, A. Bhowmik, S.M. Blau, V. Cărare, J.P. Darby, S. De, F. Della Pia, V.L. Deringer, R. Elijošius, Z. El-Machachi, F. Falcioni, E. Fako, A.C. Ferrari, A. Genreith-Schriever, J. George, R.E.A. Goodall, C.P. Grey, S. Han, W. Handley, H.H. Heenen, K. Hermansson, C. Holm, S. Hofmann, J. Jaafar, S. Hofmann, K.S. Jakob, H. Jung, V. Kapil, A.D. Kaplan, N. Karimitari, J.R. Kermode, N. Kroupa, J. Kullgren, M.C. Kuner, D. Kuryla, G. Liepuoniute, J.T. Margraf, I.-B. Magdău, A. Michaelides, J.H. Moore, A.A. Naik, S.P. Niblett, S.W. Norwood, N. O'Neill, C. Ortner, K.A. Persson, K. Reuter, **A.S. Rosen**, L.L. Schaaf, C. Schran, B.X. Shi, E. Sivonxay, T.K. Stenczel, V. Svahn, C. Sutton, T.D. Winburne, J. Tilly, C. van der Oord, S. Vargas, E. Varga-Umbrich, T. Vegge, M. Vondrák, Y. Wang, W.C. Witt, F. Zills, G. Csányi*, *Journal of Chemical Physics*, 163, 184110 (2025).

38. An Accurate and Efficient Framework for Modelling the Surface Chemistry of Ionic Materials
B.X. Shi, **A.S. Rosen**, T. Schäfer, A. Grüneis, V. Kapil, A. Zen, A. Michaelides*, *Nature Chemistry* (2025).

37. Computational Investigation of the Impact of Metal–Organic Framework Topology on Hydrogen Storage Capacity
K. Liu, H. Chen, T. Islamoglu, **A.S. Rosen**, X. Wang, O.K. Farha, R.Q. Snurr*, *Molecular Systems Design & Engineering*, 10, 817–835 (2025).

36. Accelerated Data-Driven Materials Science with the Materials Project
M.K. Horton, P. Huck, R.X. Yang, J.M. Munro, S. Dwaraknath, A.M. Ganose, R.S. Kingsbury, M. Wen, J.-X. Shen, T.S. Mathis, A.D. Kaplan, K. Berket, J. Riebesell, J. George, **A.S. Rosen**, E.W.C. Spotte-Smith, M.J. McDermott, O.A. Cohen, A. Dunn, M. Kuner, G.M. Rignanese, G. Hautier, G. Petretto, D. Waroquiers, S.M. Griffin,

J.B. Neaton, D.C. Chrzan, M. Asta, S. Cholia, G. Ceder, S.P. Ong, A. Jain, K.A. Persson*, *Nature Materials* (2025).

35. Atomate2: Modular Workflows for Materials Science
A.M. Ganose*, H. Sahasrabuddhe, M. Asta, K. Beck, T. Biswas, A. Bonkowski, J. Bustamante, X. Chen, Y. Chiang, J. Clary, D. Chrzan, O. Cohen, C. Ertural, M. Gallant, J. George, S. Gerits, R. Goodall, R. Guha, G. Hautier, M. Horton, A.D. Kaplan, R.S. Kingsbury, M.C. Kuner, B. Li, X. Linn, M.J. McDermott, R.S. Mohanakrishnan, A.N. Naik, J.B. Neaton, K.A. Persson, G. Petretto, T.A.R. Purcell, F. Ricci, B. Rich, J. Riebesell, G.-M. Rignanese, **A.S. Rosen**, M. Scheffler, J. Schmidt, J.-X. Shen, A. Sobolev, R. Sundararaman, C. Tezak, V. Trinquet, J.B. Varley, D. Vigil-Fowler, D. Wang, D. Waroquiers, M. Wen, H. Yang, H. Zheng, J. Zheng, Z. Zhu, A. Jain*, *Digital Discovery*, 4, 1944–1973 (2025).

34. Computational Modeling of a High-Entropy Alloy for Enhanced Ammonia Synthesis
J.H. Baratta, **A.S. Rosen***, *Chem Catalysis*, 5, 101426 (2025).

33. Machine Learned Potential for High-Throughput Phonon Calculations of Metal-Organic Frameworks
A.M. Elena[=], P.D. Kamath[=], T.J. Inizan, **A.S. Rosen**, F. Zanca, K.A. Persson*, *npj Computational Materials*, 11, 125 (2025).

32. A Recipe for Charge Density Prediction
X. Fu*, **A.S. Rosen**, K. Bystrom, R. Wang, A. Musaelian, B. Kozinsky, T. Smidt, T.S. Jaakola, *Advances in Neural Information Processing Systems (NeurIPS)*, 37, 9727–9752 (2025).

31. Analytical *Ab Initio* Hessian from a Deep Learning Potential for Transition State Optimization
E.C.-Y. Yuan, A. Kumar, X. Guan, E.D. Hermes, **A.S. Rosen**, J. Zádor, T. Head-Gordon*, S.M. Blau*, *Nature Communications*, 15, 8865 (2024).

30. Investigating the Behavior of Diffusion Models for Accelerating Electronic Structure Calculations
D. Rothchild, **A.S. Rosen**, E. Taw, C. Robinson, J.E. Gonzalez*, A.S. Krishnapriyan*, *Chemical Science*, 15, 13506–13522 (2024).

29. cclib 2.0: An Updated Architecture for Interoperable Computational Chemistry
E. Berquist[†], A. Dumi[†], S. Upadhyay[†], O.D. Abarbanel, M. Cho, S. Gaur, V. Hugo Cano Gil, G.R. Hutchinson, O.S. Lee, **A.S. Rosen**, S. Schamnad, F.S.S. Schneider, C. Steinmann, M. Stolyarchuk, J.E. Vanderzande, W. Zak, K.M. Langner*, *Journal of Chemical Physics*, 161, 042501 (2024).

28. MOFDiff: Coarse-Grained Diffusion for Metal–Organic Framework Design
X. Fu*, T. Xie, **A.S. Rosen**, T.S. Jaakkola, J.A. Smith*, *International Conference on Learning Representations (ICLR)*, 12, (2024).

27. Structured Information Extraction from Scientific Text with Large Language Models
J. Dagdelen, A. Dunn, S. Lee, N. Walker, **A.S. Rosen**, G. Ceder, K.A. Persson, A. Jain*, *Nature Communications,* 15, 1418 (2024).

26. Jobflow: Computational Workflows Made Simple
A.S. Rosen, M. Gallant, J. George, J. Riebesell, H. Sahasrabuddhe, J.X. Shen, M. Wen, M.L. Evans, G. Petretto, D. Waroquiers, G.-M. Rignanese, K.A. Persson, A. Jain, A.M. Ganose*, *Journal of Open Source Software,* 9, 5995 (2024).

25. Tetrazine-Linked Covalent Organic Frameworks with Acid Sensing and Photocatalytic Activity
A. Zadehnazari, A. Khosropour, A.A. Altaf, **A.S. Rosen**, A. Abbaspourrad*, *Advanced Materials*, 2311042 (2024).

24. Evidence of a Uranium-Paddlewheel Node in a Catecholate-Based Metal–Organic Framework
J.G. Knapp, X. Wang, **A.S. Rosen**, X. Wang, X. Gong, M. Schneider, T. Elkin, K.O. Kirlikovali, M. Fairley, M.D. Krzyaniak, M.R. Wasielewski, N.C. Gianneschi, R.Q. Snurr, O.K. Farha*, *Angewandte Chemie International Edition*, 62, e202305526 (2023).

23. An Ecosystem for Digital Reticular Chemistry
K.M. Jablonka, **A.S. Rosen**, A.S. Krishnapriyan, B. Smit*, *ACS Central Science*, 9, 563–581 (2023).
— Highlighted in *Chemistry World*

22. Free-Atom-Like *d* States Beyond the Dilute Limit of Single-Atom Alloys
A.S. Rosen, S. Vijay, K.A. Persson*, *Chemical Science*, 14, 1503–1511 (2023).

21. Effect of Composition and Local Environment on CO_2 Adsorption on Nickel and Magnesium Oxide Solid Solutions
A. Peng, **A.S. Rosen**, R.Q. Snurr*, H. Kung*, *Journal of Physical Chemistry C*, 126, 19705–19714 (2022).

20. A Flexible and Scalable Scheme for Mixing Computed Formation Energies from Different Levels of Theory
R. Kingsbury, **A.S. Rosen**, A. Gupta, J. Munro, S.P. Ong, A. Jain, S. Dwaraknath, M.K. Horton, K.A. Persson*, *npj Computational Materials*, 8, 195 (2022).

19. High-Throughput Predictions of Metal–Organic Framework Electronic Properties: Theoretical Challenges, Graph Neural Networks, and Data Exploration
A.S. Rosen*, V. Fung, P. Huck, C.T. O'Donnell, M.K. Horton, D.T. Truhlar, K.A. Persson, J.M. Notestein, R.Q. Snurr, *npj Computational Materials*, 8, 112 (2022).
— Highlighted in *MRS Bulletin*, 47, 886 (2022).

18. Exploring Mechanistic Routes for Light Alkane Oxidation with an Iron-Triazolate Metal–Organic Framework
A.S. Rosen, J.M. Notestein*, R.Q. Snurr*, *Physical Chemistry Chemical Physics*, 24, 8129–8141 (2022).
— Selected by the editors as a 2022 HOT *PCCP* article.

17. Realizing the Data-Driven, Computational Discovery of Metal–Organic Framework Catalysts
A.S. Rosen, J.M. Notestein*, R.Q. Snurr*. *Current Opinion in Chemical Engineering*, 35, 100760 (2022).

16. Fine-Tuning A Robust Metal–Organic Framework Towards Enhanced Clean Energy Gas Storage
Z. Chen, M.R. Mian, S.-J. Lee, H. Chen, X. Zhang, K.O. Kirlikovali, S. Shulda, P. Melix, **A.S. Rosen**, P.A. Parilla, T. Gennett, R.Q. Snurr, T. Islamoglu*, T. Yildrim*, O.K. Farha*, *Journal of the American Chemical Society*, 143, 18838–18843 (2021).

15. Machine Learning the Quantum-Chemical Properties of Metal–Organic Frameworks for Accelerated Materials Discovery
A.S. Rosen*, S.M. Iyer, D. Ray, Z. Yao, A. Aspuru-Guzik, L. Gagliardi, J.M. Notestein, R.Q. Snurr, *Matter*, 4, 1578–1597 (2021).
— Featured on the cover of *Matter* and previewed in *Patterns*, 2, 100239 (2021).

14. Zr_6O_8 Node-Catalyzed Butene Hydrogenation and Isomerization in the Metal–Organic Framework NU-1000
K.E. Hicks, **A.S. Rosen**, Z.H. Syed, R.Q. Snurr, O.K. Farha*, J.M. Notestein*, *ACS Catalysis*, 10, 14959–14970 (2020).

13. Supramolecular Porous Assemblies of Atomically Precise Catalytically Active Cerium-Based Clusters
M.C. Wasson, X. Zhang, K. Otake, **A.S. Rosen**, S. Alayoglu, M.D. Krzyaniak, Z. Chen, L.R. Redfern, L. Robison, F.A. Son, Y. Chen, T. Islamoglu, J.M. Notestein, R.Q. Snurr, M.R. Wasielewski, O.K. Farha*, *Chemistry of Materials*, 32, 8522– 8529 (2020).

12. Comparing GGA, GGA+*U*, and Meta-GGA Functionals for Redox-Dependent Binding at Open Metal Sites in Metal–Organic Frameworks
A.S. Rosen, J.M. Notestein*, R.Q. Snurr*, *Journal of Chemical Physics*, 152, 24101 (2020).

11. Topological Effects on Separation of Alkane Isomers in Metal–Organic Frameworks

N.S. Bobbitt, **A.S. Rosen**, R.Q. Snurr*, *Fluid Phase Equilibria*, 519, 112642 (2020).

10. High-Valent Metal-Oxo Species at the Nodes of Metal–Triazolate Frameworks: The Effects of Ligand Exchange and Two-State Reactivity for C–H Bond Activation
    A.S. Rosen, J.M. Notestein*, R.Q. Snurr*, *Angewandte Chemie International Edition*, 59, 19494–19502 (2020).

9. Tuning the Redox Activity of Metal–Organic Frameworks for Enhanced, Selective O_2 Binding: Design Rules and Ambient Temperature O_2 Chemisorption in a Cobalt–Triazolate Framework
    A.S. Rosen, M.R. Mian, T. Islamoglu, O.K. Farha, J.M. Notestein, R.Q. Snurr*, *Journal of the American Chemical Society*, 142, 4317–4328 (2020).

8. Identification Schemes for Metal–Organic Frameworks to Enable Rapid Search and Cheminformatics Analysis
    B.J. Bucior, **A.S. Rosen**, M. Haranczyk, Z. Yao, M.E. Ziebel, O.K. Farha, J.T. Hupp, J.I. Siepmann, A. Aspuru-Guzik, R.Q. Snurr*, *Crystal Growth and Design*, 19, 6682–6697 (2019).

7. Structure–Activity Relationships that Identify Metal–Organic Framework Catalysts for Methane Activation
    A.S. Rosen, J.M. Notestein*, R.Q. Snurr*, *ACS Catalysis*, 9, 3576–3587 (2019).
    — Featured in C&EN

6. Identifying Promising Metal–Organic Frameworks for Heterogeneous Catalysis via High-Throughput Periodic Density Functional Theory
    A.S. Rosen, J.M. Notestein*, R.Q. Snurr*, *Journal of Computational Chemistry*, 40, 1305–1318 (2019).

5. Evidence for Copper Dimers in Low-Loaded CuO_x/SiO_2 Catalysts for Cyclohexane Oxidative Dehydrogenation
    S.L. Nauert, **A.S. Rosen**, H. Kim, R.Q. Snurr, P.C. Stair, J.M. Notestein*, *ACS Catalysis*, 8, 9775–9789 (2018).

4. Comprehensive Phase Diagrams of MoS_2 Edge Sites Using Dispersion-Corrected DFT Free Energy Calculations
    A.S. Rosen, J.M. Notestein*, R.Q. Snurr*, *Journal of Physical Chemistry C*, 122, 15318–15329 (2018).

3. Correlations, Trends and Potential Biases among Publicly Accessible Web-Based Student Evaluations of Teaching
    A.S. Rosen*, *Assessment and Evaluation in Higher Education*, 43, 31–44 (2018).
    — Featured in *Inside Higher Ed* and VOA News

2. A Detailed Combined Experimental and Theoretical Study on Dimethyl Ether/Propane Blended Oxidation
    E.E. Dames, **A.S. Rosen**, B.W. Weber, C.W. Gao, C-J. Sung, W.H. Green*, *Combustion and Flame*, 168, 310–330 (2016).

1. Validation of X-ray Line Ratios for Electron Temperature Determination in Tokamak Plasmas
    A.S. Rosen, M.L. Reinke*, J.E. Rice, A.E. Hubbard, J.W. Hughes, *Journal of Physics B*, 47, 105701 (2014).
    — Selected as an article representing "the best work published in the *Journal of Physics B* in 2014"

Research Grants

Total: $1,630,000 | Rosen's share: $1,445,000

7. **Undisclosed Foundation**: "AI-Guided Discovery of Heterogeneous Catalysts with Unbound Potential." Single PI. Award: $200,000 (11/2025–10/2026).

6. **NSF Office of Advanced Cyberinfrastructure** (Cyberinfrastructure for Sustained Scientific Innovation):

"Collaborative Research: Frameworks: SINAPSE: Scalable Infrastructure for AI-coupled Predictive Simulation Enhancement." Co-PI. Award to Rosen: $725,000 (10/2025–09/2028).

5. **New Industrial Collaborations Grant** (Meta Platforms, Princeton Office of the Dean for Research): "Development of an AI-Ready Dataset for Next-Generation Battery Materials." Single PI. Award: $275,000 (07/2025–06/2027).
4. **SEAS Innovation Grant** (Princeton SEAS): "A Combined Experimental and Computational Approach for Accelerated Zeolite Discovery via Pre-Nucleation Building Units." Lead PI. Award: $230,000. Award to Rosen: $100,000. (01/2026–12/2027).
3. **SEAS Innovation Seed Grant** (Princeton SEAS): "Democratizing the Computational Discovery of Clean Energy Materials." Single PI. Award: $50,000 (06/2025–08/2025).
2. **Materials Research Science and Engineering Center Seed Grant** (Princeton Center for Complex Materials): "Developing Thermodynamic and Kinetic Stability Relationships for Porous Framework Materials." Single PI. Award: $60,000 (02/2025–01/2026).
1. **AI Seed Grant** (Princeton Laboratory for Artificial Intelligence): "AI-Accelerated Discovery of Porous Materials with Confined Electrons for Challenging Chemical Transformations." Lead PI. Award: $90,000. Award to Rosen: $45,000 (01/2025–06/2026).

Computing Grants

6. **ALCF Director's Discretionary Award**: "Scalable Foundation Models for Charge Density Prediction." Single PI. Award: 5,000 GPU node hours (11/2025–05/2026).
5. **ALCF Director's Discretionary Award**: "An Off-Equilibrium Metal-Organic Framework Dataset for Training Machine-Learned Potentials." Single PI. Award: 1000 TB valued at $50,000 (09/2025–10/2027).
4. **NERSC High-Impact Science at Scale Award**: "Assessing the Thermodynamic Stability Limits of Nanoporous Materials." Single PI. Award: 25,000 GPU node hours, 5000 CPU node hours (06/2025–12/2025).
3. **NERSC AI for Science Award**: "Development of an Interpretable Machine-Learned Interatomic Potential for Chemical Bonding in Energy Materials." Single PI. Award: 8,000 GPU node hours (06/2025–01/2026).
2. **NSF National Artificial Intelligence Research Resource Pilot**: "Building a Foundational Metal–Organic Framework Dataset for Machine Learning Potentials." Single PI. Award: 100,000 GPU hours valued at approximately $164,000 (04/2025–03/2026).
1. **NSF ACCESS**: "Developing Thermodynamic and Kinetic Stability Relationships for Porous Materials." Single PI. Award: 200,000 ACCESS Credits (01/2025–01/2026).

Teaching

Princeton University

CBE 423/MSE 423: Computational Materials Design and Discovery — Spring 2026
Enrollment: 30

CBE 504: Chemical Kinetics and Reaction Engineering — Fall 2025
Overall Course Quality: **4.82/5.0**, Instructor Lecture Quality: **4.88/5.0**, Enrollment: 24

- Selected quotes: “Andrew Rosen is a gifted instructor. His lectures are well thought out, easy to follow, and engaging”, “Andrew was probably the best professor I had this semester, and never failed to correlate the material in lecture to things that we might actually be interested in.”

CBE 504: Chemical Reactor Engineering Fall 2024

Overall Course Quality: **4.77/5.0**, Instructor Lecture Quality: **4.90/5.0**, Enrollment: 33

- Selected quotes: “Lectures were stunning”, “Dr. Andrew Rosen is hands–down one of the best instructors”, “Prof. Rosen basically wrote a textbook for us… it's 6.02x10^23 better than every kinetics textbook I used in undergrad”

Mentoring

Princeton University

Postdoctoral Researchers

- Dr. Yuliang Shi, Postdoctoral Research Associate (2026 – present)
- Dr. Sihoon Choi, DataX Postdoctoral Research Associate (2025 – present)
- Dr. Hananeh Oliaei, Postdoctoral Research Associate (2025 – present)

Graduate Students

- Isabella Furrick, CBE (2026 – present)
- Julia Baratta, CBE (2025 – present)
- Blake Dallmann, CBE (2025 – present)
- Naisargi Goyal, CBE (2025 – present)

Undergraduate Researchers

- Aryan Saha, ECE (2024 – present)

University Service

University Committees, Princeton University

- Committee on Examinations and Standing (2025 – present)

Department of Chemical and Biological Engineering, Princeton University

- Undergraduate Committee (2024 – present)
- Undergraduate Advising (2025 – present), 11× CBE undergraduates
- Graduate Committee (2024 – 2025)

AI Lab, Princeton University

- Started and am a faculty advisor for an AI for Materials working group and journal club through the AI for Accelerating Invention initiative (2024 – present)
- Reviewed AI Lab Seed Grants (2025)
- Formal career mentor for an AI^2 postdoctoral fellow

Graduate Student Thesis and First Proposition Committees, Princeton University

- 18× CBE graduate students, 1× CEE graduate student

Undergraduate Senior Thesis Committees, Princeton University

- 2× CBE undergraduate students

Center for Statistics and Machine Learning, Princeton University

- Statistics and Machine Learning Minor program evaluator (2025)

Nassau Hall Society, Princeton University

- Panelist for “AI Solving the Unsolvable” (2025)

External Service

Manuscript Peer-Review

ResearcherID: G-2407-2014

- 75+ reviews across *Nature Machine Intelligence, Nature Reviews Chemistry, Matter, Journal of the American Chemical Society, Angewandte Chemie*, *JACS Au, Nature Communications, Science Advances*, *ACS Materials Letters, ACS Applied Materials and Interfaces, Advanced Functional Materials, npj Computational Materials, Digital Discovery, Journal of Physical Chemistry C, Journal of Chemical Information and Modeling, Cell Reports Physical Science, PLoS One, Scientific Data, Journal of Open Source Software, F1000Research, STAM Methods, Assessment and Evaluation of Higher Education*

Grant Proposal Peer-Review

- Air Force Office of Scientific Research, Department of Defense (2026)
- Department of Energy, Basic Energy Sciences (2026)
- NSF Division of Chemical, Bioengineering, Environmental and Transport Systems (2025)
- American Chemical Society, Petroleum Research Fund (2025)
- Swiss National Supercomputing Centre (2025)
- Department of Energy, Basic Energy Sciences (2024)
- American Chemical Society, Petroleum Research Fund (2023)
- Swiss National Supercomputing Centre (2023)

Atomic Simulation Environment

Steering Committee (2025 – present)

- Guide the future directions of the Atomic Simulation Environment, which receives >500k downloads per month

Materials Project Software Foundation

Board member and co-founder (2023 – present)

- Guide the future directions of the Materials Project software ecosystem, which has >600k registered users

Open-Source Software Development

- Active creator and maintainer of multiple large-scale material property databases (e.g. QMOF Database, MOF Explorer)
- Maintainer and lead developer of several materials modeling codes (e.g. QuAcc, Atomic Simulation Environment)
- Contributed to over 100 packages in computational chemistry, materials science, and workflow orchestration

Conference Activity

- Co-organizer for the CECAM on "Physics-Aware Machine Learning for Molecules and Materials" (2026)
- Co-chair for "Special Session in Honor of Prof. Randall Snurr's 60th Birthday", CoMSEF, AIChE Annual Meeting (2026)
- Co-chair for "Accelerated Discovery of Inorganic Materials: High-Throughput Experiments, Modeling, and Data Science", MESD, AIChE Annual Meeting (2025)
- Poster judge for AIChE MESD division (2023, 2025)
- Poster judge for AIChE CRE division (2023)
- Co-chair for "Data Science for Catalysis", ACS Fall Meeting (2023)

AIChE Area 1A

Programming Committee (2026 – present)

- Contribute to the overall programming of Area 1A, Thermodynamics and Transport Properties

AIChE CRE

Bin Co-Leader (2026)

- Help organize AIChE session for New Developments in Computational Catalysis

Social Media Team (2019 – 2024)

- Organize and run social media campaigns dedicated to highlighting underrepresented chemical engineers

Letters to a Pre-Scientist

Scientist PenPal (2019 – 2024)

- Outreach to establish relationships between scientists and middle school students in low-income classrooms

Rosen Review

Chemical Engineering Review Website (2011 – 2024)

- Created an educational website viewed 1,000,000+ times with visitors from 191 countries

Strategic Engagements and Science Policy

2. “AI × Material Innovation: Breakthroughs for a Clean Energy Future Workshop.” **Bezos Earth Fund**, 2025.
1. “Semiconductor Materials Accelerator Open Roundtable.” **White House Office of Science and Technology Policy**, 2024.

Invited Presentations

30. “Combining Machine Learning and Quantum Chemistry to Guide Materials Design.” **Princeton University**, AI for Accelerating Invention and the Center for Statistics and Machine Learning, 2025.
29. “The Quantum Accelerator: Accessible and Scalable Materials Science Workflows.” **CECAM,** The Atomic Simulation Environment Ecosystem: Present and Perspectives, 2025.
28. “Quantum-Chemical Engineering and Computational Materials Design.” **Princeton University,** Princeton Catalysis Initiative Symposium, 2025.
27. “Discovering Unique Electronic Structure Properties in Solid-State Materials via High-Throughput Simulations.” **Princeton University,** Princeton Materials Institute Symposium, 2025.
26. “Discovering Unique Electronic Structure Properties in Solid-State Materials via High-Throughput Simulations.” **Princeton Plasma Physics Laboratory,** Computational Sciences Department, 2025.
25. “Designing Heterogeneous Catalysts with Free-Atom-Like Electronic States.” **New York Catalysis Society of Metropolitan New York,** Lehigh University, 2025.
24. “Discovering Unique Electronic Structure Properties in Solid-State Materials via High-Throughput Simulations.” **New Jersey Institute of Technology,** Department of Chemistry and Environmental Science, 2025.
23. “Guiding the Design of New Materials with Electronic Structure Calculations in the Big Data Regimes.” **Princeton University,** Chemistry in Solutions and at Interfaces – Computational Chemical Science Center, 2024.
22. “A Data-Driven Approach to Tailor the Electronic Structure Properties of Materials.” **Drexel University,** Department of Chemistry, 2024.
21. “Discovering Unique Electronic Structure Properties in Solid-State Materials via High-Throughput Simulations.” **Rutgers University–Newark,** Department of Physics, 2024.
20. “Accessible and Interoperable Computational Workflows to Satisfy the Data-Hungry Machines.” **AI for Multidisciplinary Exploration and Discovery Workshop on Heterogeneous Catalysis**, Chicago, IL 2024.
19. “Combining High-Throughput Workflows, Quantum Chemistry, and AI for the Discovery of Tunable Materials with Unprecedented Properties.” **University of Pennsylvania,** Penn Institute for Computational Science, 2024.
18. “The Quantum Accelerator: Accessible and Scalable Materials Science Workflows.” **ParslFest**, 2024.
17. “Discovering Heterogeneous Catalysts with Unique Electronic Structure Properties.” **Flatiron Institute,** Initiative for Computational Catalysis Inaugural Workshop, 2024.
16. “Free-Atom-Like *d*-States Beyond the Dilute Limit of Single-Atom Alloys.” **ACS Fall Meeting**, 2023.
15. “The Present and Future of Materials Databases: Metal–Organic Framework Edition.” **Materials Research Data**

Alliance Annual Meeting, 2023.

14. “Discovering Tunable Materials with Unprecedented Properties via High-Throughput Quantum Chemistry.” **Massachusetts Institute of Technology,** Department of Materials Science and Engineering, 2023.

13. “Discovering Tunable Materials with Unprecedented Properties via High-Throughput Quantum Chemistry.” **University of California, San Diego,** Department of NanoEngineering, 2023.

12. “Discovering Tunable Materials with Unprecedented Properties via High-Throughput Quantum Chemistry.” **University of Colorado Boulder,** Department of Chemical and Biological Engineering, 2023.

11. “Discovering Tunable Materials with Unprecedented Properties via High-Throughput Quantum Chemistry.” **University of Illinois, Urbana-Champaign,** Department of Materials Science and Engineering, 2023.

10. “Discovering Tunable Materials with Unprecedented Properties via High-Throughput Quantum Chemistry.” **Yale University,** Department of Chemical and Environmental Engineering, 2023.

9. “Discovering Tunable Materials with Unprecedented Properties via High-Throughput Quantum Chemistry.” **University of California, Santa Barbara,** Department of Chemical Engineering, 2023.

8. “Discovering Tunable Materials with Unprecedented Properties via High-Throughput Quantum Chemistry.” **University of Washington,** Department of Chemical Engineering, 2023.

7. “Discovering Tunable Materials with Unprecedented Properties via High-Throughput Quantum Chemistry.” **Princeton University,** Department of Chemical and Biological Engineering, 2023.

6. “Navigating the Metal–Organic Framework Universe with High-Throughput Quantum Chemistry.” **Statistical Thermodynamics and Molecular Simulations Virtual Seminar Series**, 2022.

5. “Discovering Tunable Materials with Unprecedented Properties Using High-Throughput Quantum Chemistry.” **Distinguished Young Scholars Seminar Series**, University of Washington, 2022.

4. “The QMOF Database: Accelerating the Discovery of Metal–Organic Frameworks with Targeted Electronic Structure Properties.” **Open Databases Integration for Materials Design Workshop**, 2021.

3. “A Guided Journey Through the Metal–Organic Framework Universe: New Materials for Longstanding Challenges.” **Northwestern University**, Distinguished Graduate Researcher Award Presentation, 2020.

2. “High-Valent Metal-Oxo Species for C–H Activation and Where to Find Them: A Computationally Guided Expedition.” **Catalysis Club of Chicago Symposium**, 2020.

1. “Combining Quantum Chemistry and Supercomputing to Accelerate the Discovery of Promising Metal–Organic Frameworks.” **Northwestern SPIE-MRSEC Seminar Series**, 2020.