Andrew S. **Rosen**

Assistant Professor, Princeton University
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Academic Appointments

Princeton University — *Princeton, NJ*
Assistant Professor of Chemical and Biological Engineering — 2024 – Present

Education and Training

University of California, Berkeley — *Berkeley, CA*
Miller Research Fellow — 2021 – 2024
Department of Materials Science and Engineering
Faculty Host: 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

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 – 2024
Presidential Fellowship, Northwestern University – The Graduate School — 2021 – 2022
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 – 2021
George Thodos Teaching Assistant Award (×2), Northwestern University CBE — 2017 & 2018
National Defense Science and Engineering Graduate Fellowship, U.S. Dept. of Defense — 2017 – 2021
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

Under Review

31. Deep Learning of Ab Initio Hessians 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* (under review).

30. 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*, arXiv:2401.00096 (2024).

29. 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*, arXiv:2311.01491 (2023).

Published

28. MOFDiff: Coarse-Grained Diffusion for Metal–Organic Framework Design
X. Fu, T. Xie, **A.S. Rosen**, T.S. Jaakkola, J.A. Smith*, *ICLR* (in press).

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. Vinyl 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. Formation of an Unprecedented Uranium Paddlewheel 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).

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"

Editorials

1. Reflections in Search of Faculty Positions

   H. Mao, **A.S. Rosen**, D. Sanchez, V. Sanchez, S. Cranford*, *Matter*, 6, 300–307 (2023).

Teaching

Northwestern University

Teaching Assistant for CHEM ENG 451: Applied Molecular Modeling — Jan. 2020 – Mar. 2020

- "Always helpful, always cheerful. One of the best TAs I've had. Always willing to help but makes sure you put in the work."
- "Andrew really knows what he is talking about. He is able to explain things very well in terms that help you understand."

Northwestern University

Teaching Assistant for CHEM ENG 211: Thermodynamics — Sep. 2018 – Dec. 2018

- "Andrew is the best TA I have ever had. He cared about our success and was able to clearly convey even the most challenging concepts."
- "Andrew was always very helpful and responded to emails with very well thought out responses that always

beyond answered my questions. He's also just a very nice person and one of the best TAs I've ever worked with."

Northwestern University

Teaching Assistant for CHEM ENG 404: Advanced Thermodynamics Jan. 2018 – Mar. 2018

- "Andrew Rosen is a gift to this university. I've never stumped him on a question, I always leave conversations about questions fully-satisfied and then some."
- "Phenomenal at responding to questions while encouraging students' abilities to reason through problems. Found the right balance between guidance and provoking students' thoughts in class."

Northwestern University

Teaching Assistant for CHEM ENG 212: Phase Equilibrium and Staged Separations Mar. 2017 – Jun. 2017

- "Whoever is reading this, I want you to know that this TA was (and most likely will ever be) the best TA I have ever met. It's crazy how committed he is to the students learning the class and how much he wishes to see them understand the material."
- "Best TA I have ever had the privilege of knowing. He is always happy to help not only do homework problems but get us to LEARN how to do them front and back."

Service

Academic Peer-Review

ResearcherID: G-2407-2014

- Journals (45+ total reviews): *Nature Machine Intelligence, Matter, Journal of the American Chemical Society, JACS Au, Nature Communications, ACS Materials Letters, ACS Applied Materials and Interfaces, 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*
- Grants (3+ total reviews): DOE BES, ACS PRF, Swiss National Supercomputing Centre

Open-Source Software Development

- Active creator and maintainer of multiple large-scale material property databases, such as the QMOF Database and the MOF Explorer interface on the Materials Project
- Maintainer and lead developer of the following codes: `quacc`, Atomic Simulation Environment (`ASE`)
- Contributor to over 100 packages in computational chemistry, materials science, and workflow orchestration

Thesis Committees

- Quinn Galacher, CBE (Ph.D. student): advisor Michael Webb

Conference Chair

- "Data Science for Catalysis" session, ACS Fall Meeting, 2023

Materials Project

Materials Project Foundation Member 2023 – Present

- Guide the future directions of the Materials Project software ecosystem

Letters to a Pre-Scientist

Scientist PenPal 2019 – Present

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

Rosen Review

Chemical Engineering Review Website 2011 – Present

- Created and continue to update an educational website to explain STEM concepts to students around the world
- Over its lifetime, the site has been viewed 1,000,000+ times with visitors from 191 countries

AIChE CRE

Social Media Team 2019 – 2023

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

Presentations

32. "Discovering Heterogeneous Catalysts with Unique Electronic Structure Properties." *Flatiron Institute Initiative for Computational Catalysis Inaugural Workshop*, 2024. (Oral, Invited)

31. "Free-Atom-Like *d*-States Beyond the Dilute Limit of Single-Atom Alloys." *ACS Fall 2023 Meeting*, 2023. (Oral, Invited)

30. "The Present and Future of Materials Databases: Metal–Organic Framework Edition." *Materials Research Data Alliance Annual Meeting*, 2023. (Oral, Invited)

29. "Discovering Tunable Materials with Unprecedented Properties via High-Throughput Quantum Chemistry." *Massachusetts Institute of Technology, Department of Materials Science and Engineering*, 2023. (Oral, Invited)

28. "Discovering Tunable Materials with Unprecedented Properties via High-Throughput Quantum Chemistry." *University of California, San Diego, Department of NanoEngineering*, 2023. (Oral, Invited)

27. "Discovering Tunable Materials with Unprecedented Properties via High-Throughput Quantum Chemistry." *University of Colorado Boulder, Department of Chemical and Biological Engineering*, 2023. (Oral, Invited)

26. "Discovering Tunable Materials with Unprecedented Properties via High-Throughput Quantum Chemistry." *University of Illinois, Urbana-Champaign, Department of Materials Science and Engineering*, 2023. (Oral, Invited)

25. "Discovering Tunable Materials with Unprecedented Properties via High-Throughput Quantum Chemistry." *Yale University, Department of Chemical and Environmental Engineering*, 2023. (Oral, Invited)

24. "Discovering Tunable Materials with Unprecedented Properties via High-Throughput Quantum Chemistry." *University of California, Santa Barbara, Department of Chemical Engineering*, 2023. (Oral, Invited)

23. "Discovering Tunable Materials with Unprecedented Properties via High-Throughput Quantum Chemistry." *University of Washington, Department of Chemical Engineering*, 2023. (Oral, Invited)

22. "Discovering Tunable Materials with Unprecedented Properties via High-Throughput Quantum Chemistry." *Princeton University, Department of Chemical and Biological Engineering*, 2023. (Oral, Invited)

21. "Computationally Accelerated Discovery of Atomically and Electronically Tunable Clean Energy Materials." *Materials Research Society Fall Meeting*, 2022. (Poster)

20. "Accelerated Prediction of Metal–Organic Framework Electronic Properties Via High-Throughput Quantum-Chemical Calculations and Machine Learning." *AIChE National Meeting*, 2022. (Oral)

19. "Computationally Accelerated Discovery of Atomically and Electronically Tunable Clean Energy Materials."*AIChE National Meeting*, 2022. (Poster)

18. "Navigating the Metal–Organic Framework Universe with High-Throughput Quantum Chemistry." *Stati tical Thermodynamics and Molecular Simulations Virtual Seminar Series*, 2022. (Oral, Invited)

17. "Discovering Tunable Materials with Unprecedented Properties Using High-Throughput Quantum Chemistry." *University of Washington Distinguished Young Scholars Seminar Series*, 2022. (Oral, Invited)

16. "Machine Learning the Quantum-Chemical Properties of Metal–Organic Frameworks for Accelerated Materials Discovery with a New Electronic Structure Database." *AIChE National Meeting*, 2021. (Oral)

15. "The QMOF Database: Accelerating the Discovery of Metal–Organic Frameworks with Targeted Electronic Structure Properties." *Open Databases Integration for Materials Design Workshop*, 2021. (Oral, Invited)

14. "Machine Learning the Quantum-Chemical Properties of Metal–Organic Frameworks for Accelerated Materials Discovery with a New Electronic Structure Database." *Materials Research Society Spring Meeting*, 2021. (Oral)

13. "Tuning the Reactivity of Metal–Triazolate Frameworks for the Catalytic Oxidation of Strong C–H Bonds." *AIChE National Meeting*, 2020. (Oral)

12. "Leveraging Quantum-Chemical Screening Methods to Guide the Discovery of Promising Metal–Organic Frameworks." *AIChE National Meeting*, 2020. (Poster)

11. "A Guided Journey Through the Metal–Organic Framework Universe: New Materials for Longstanding Challenges." *Distinguished Graduate Researcher Award Presentation*, 2020. (Oral, Invited)

10. "High-Valent Metal-Oxo Species for C–H Activation and Where to Find Them: A Computationally Guided Expedition." *Catalysis Club of Chicago Symposium*, 2020. (Oral)

9. "Combining Quantum Chemistry and Supercomputing to Accelerate the Discovery of Promising Metal–Organic Frameworks." *Northwestern SPIE-MRSEC Seminar Series*, 2020. (Oral, Invited)

8. "Reactive, High-Valent Metal-Oxo Species Incorporated within Metal–Triazolate Frameworks." *12th AIChE Midwest Regional Conference*, 2020. (Oral)

7. "Combining Supercomputing and Quantum Chemistry to Optimize the Design of Modular Nanoporous Materials for Increased Energy Security." *1st Annual NDSEG Conference*, 2019. (Poster)

6. "Structure–Activity Relationships that Identify Metal–Organic Framework Catalysts for Methane Activation." *26th North American Catalysis Society Meeting*, 2019. (Oral)

5. "One Step Closer to the Holy Grail: Designing MOFs for the Catalytic Oxidation of Methane." *Catalysis Club of Chicago Symposium*, 2019. (Poster)

4. "Structure–Activity Relationships to Identify Promising Metal–Organic Frameworks for the Catalytic Oxidation of Methane." *ACS Spring 2019 National Meeting*, 2019. (Oral)

3. "Thermodynamic Stability and Kinetic Favorability of MoS_2 Edge Sites for Alkane Dehydrogenation." *Catalysis Club of Chicago Symposium*, 2018. (Poster)

2. "DFT Study of Metal Oxide Nanoclusters for C–H Bond Activation." *SUNCAT Summer Institute: Fundamentals and Applications of Heterogeneous Catalysis*, 2017. (Poster)

1. "Validation of X-ray Line Ratios for Electron Temperature Profiles in Tokamak Plasmas." *55th American Physical Society – Division of Plasma Physics Conference*, 2013. (Poster)

Memberships

Materials Research Society	2021 – Present
American Chemical Society (CATL, COMP)	2011 – Present
American Institute of Chemical Engineers (CRE, CoMSEF)	2011 – Present
Catalysis Club of Chicago	2018 – 2021