Andrew S. **Rosen**

Assistant Professor, Princeton University
A301 Engineering Quadrangle, Princeton University, Princeton, NJ 08544
asrosen@princeton.edu | 609-258-6154 | https://rosen.cbe.princeton.edu

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

Education and Training

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

Publications

* corresponding author | ⁼ equal contribution | Google Scholar | ORCID: 0000-0002-0141-7006

> 2500 citations via Google Scholar, *h*-index ≥ 22

Under Review

39. 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, Z. Hasanbasri, H. Kwon, S.H. Karstens, Y. Yabuuchi, J. Böergel, J.W. Taylor, K.R. Meihaus, K.C. Bustillo, A.M. Minor, K.A. Persson, C.M. Brow, R.D. Britt, N.P. Stadie, J.R. Long*.

38. 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*.

37. 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*, *ChemRxiv* 10.26434/chemrxiv-2025-tcr5h (2025).

36. An Accurate and Efficient Framework for Predictive Insights into Ionic Surface Chemistry
B.X. Shi, **A.S. Rosen**, T. Schäfer, A. Grüneis, V. Kapil, A. Zen, A. Michaelides*, arXiv:2412.17204 (2024).

35. The Materials Project: A Decade of Materials Discovery
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, and K.A. Persson*.

34. 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).

Published

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* (in press).

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). arXiv:2405.19276.

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). arXiv:2310.10732.

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).
— 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"

Editorials

1. Reflections in Search of Faculty Positions
   H. Mao, **A.S. Rosen**, D. Sanchez, V. Sanchez, S. Cranford*, *Matter*, 6, 300–307 (2023).

Grants

5. PI: "Building a Foundational Metal–Organic Framework Dataset for Machine Learning Potentials", National Artificial Intelligence Research Resource Pilot, National Science Foundation. Total: 100,000 GPU hours (04/2025–03/2026).

4. PI: "A Combined Experimental and Computational Approach for Accelerated Zeolite Discovery via Pre-Nucleation Building Units", SEAS Innovation Research Grant, Princeton University. Total: $230,000 (01/2026–12/2027). Co-PIs: Marcella Lusardi, Claire White.

3. PI: "Democratizing the Computational Discovery of Clean Energy Materials", SEAS Innovation Seed Grant, Princeton University. Total: $50,000 (06/2025–08/2025).

2. PI: "Developing Thermodynamic and Kinetic Stability Relationships for Porous Framework Materials", Princeton Center for Complex Materials Seed Grant, Princeton University. Total: $60,000 (02/2025–01/2026).

1. PI: "AI-Accelerated Discovery of Porous Materials with Confined Electrons for Challenging Chemical Transformations", AI Lab Seed Grant, Princeton University. Total: $90,000 (01/2025–06/2026). Co-PI: Adji Buosso Dieng.

Teaching

Princeton University

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

Graduate Students

- 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

- Committee on Examinations and Standing (2025 – present)

Department of Chemical and Biological Engineering, Princeton University

- Undergraduate Committee (2024 – present)
- Graduate Committee (2024 – present)

AI for Materials Engineering Working Group, Princeton University

- Started and lead an AI for Materials Engineering working group through the AI for Accelerating Invention initiative (2024 – present)

Graduate Student Thesis and First Proposition Committees, Princeton University

- Ilya Lyadov (CBE), Matthew Pekarcik (CBE), Andreas Kounis-Melas (CBE), Louis Hoffenberg (CBE), Russell Kwon (CBE), Quinn Gallagher (CBE), Samuel Moore (CBE), Nicholas Kalamaris (CBE), Jiaen Weu (CBE)

Undergraduate Senior Thesis Committees, Princeton University

- Francesca Noviello (CBE), Yvette Olivas Biddle (CBE)

External Service

Manuscript Peer-Review

ResearcherID: G-2407-2014

- 60+ reviews: *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, 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

- 6+ reviews: NSF CBET, DOE BES, ACS PRF, Swiss National Supercomputing Centre

Open-Source Software Development

- Active creator and maintainer of multiple large-scale material property databases (e.g. QMOF Database, MOF Explorer) *accessed 20,000+ times*
- Maintainer and lead developer of several materials modeling codes (e.g. QuAcc, Atomic Simulation Environment) *downloaded 160,000+ times per month*
- Contributed to *over 100 packages* in computational chemistry, materials science, and workflow orchestration

Materials Project Software Foundation

Board member and co-founder (2023 – present)

- Guide the future directions of the Materials Project software ecosystem *used by thousands of people*

Conference Chair

- "Accelerated Discovery of Inorganic Materials: High-Throughput Experiments, Modeling, and Data Science" session, AIChE Annual Meeting, 2025

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

White House Office of Science and Technology Policy

Semiconductor Materials Accelerator Open Roundtable (2024)

- Panelist at the White House for a discussion on accelerated materials R&D for semiconductor manufacturing

AIChE CRE

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*

Invited Presentations

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.