

Andrew S. Rosen

Assistant Professor, Princeton University

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Academic Appointments

Princeton University

Assistant Professor, Department of Chemical and Biological Engineering
Associated Faculty, Princeton Materials Institute
Associated Faculty, Princeton Institute for Computational Science and Engineering
Participating Faculty, Center for Statistics and Machine Learning

Princeton, NJ

2024 - Present

Education and Training

University of California, Berkeley

Miller Research Fellow
Department of Materials Science and Engineering
Mentor: Prof. Kristin A. Persson

Berkeley, CA

2021 - 2024

Northwestern University

Ph.D. in Chemical Engineering
Advisors: Prof. Randall Q. Snurr, Prof. Justin M. Notestein

Evanston, IL

2016 - 2021

Tufts University

B.S. in Chemical Engineering, *summa cum laude*

Medford, MA

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
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 , 55 th APS Plasma Physics Conference	2013
Tau Beta Pi , Tufts University	2013

Publications

* = corresponding author | † = equal contribution | [Google Scholar](#) | ORCID: 0000-0002-0141-7006
> 2100 citations via Google Scholar, *h*-index \geq 19

Under Review

37. Atomate2: Modular Workflows for Materials Science

A.M. Ganose*, H. Sahasrabudde, 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. 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*, arXiv:2401.00096 (2024).

33. 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

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)*, 38 (2024). 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. Sahasrabudde, 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 CO₂ 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. Yildirim*, 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. Zr₆O₈ 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 O₂ Binding: Design Rules and Ambient Temperature O₂ 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/SiO₂ 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 MoS₂ 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

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 Dieng (Princeton University, Computer Science).

Teaching

Princeton University

CBE 504: Chemical Reactor Engineering

Fall 2024

Overall Course Quality: 4.77/5.0, Instructor Lecture Quality: 4.90/5.0

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 6.02×10^{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 of California, Berkeley

Graduate Students

- Pratham Kamath, MSE (2023 – 2024)

Northwestern University

Undergraduate Researchers

- Shaelyn Iyer, ChBE (2020 – 2021)

University Service

Department of Chemical and Biological Engineering, Princeton University

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

Thesis and General Exams Committees, Princeton University

- Russel Kwon, CBE (advisor: David Graves)
- Winnie Huang, CBE (advisors: Michele Sarazen, Marcella Lusardi)
- Samuel Moore, CBE (advisor: Michele Sarazen)
- Quinn Gallagher, CBE (advisor: Michael Webb)
- Nicholas Kalamaris, CBE (first proposition; advisor: Christos Maravelias)
- Jiaen Wu, CBE (first proposition; advisor: Emily Davidson)

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

External Service

Manuscript Peer-Review

ResearcherID: G-2407-2014

- 55+ reviews: *Nature Machine Intelligence*, *Nature Reviews Chemistry*, *Matter*, *Journal of the American Chemical Society*, *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

- 4+ reviews: 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*

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*

Conference Chair

- “Data Science for Catalysis” session, ACS Fall Meeting, 2023

Invited Presentations

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.