Aditya **Nandy**

Assistant Professor of Chemical and Biomolecular Engineering at UCLA

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Education

Massachusetts Institute of Technology — *Cambridge, MA*

Ph.D. in Theoretical Chemistry — *Aug. 2017 - Apr. 2023*

- NSF Graduate Research Fellow (NSF-GRFP), Robert T. Haslam Presidential Fellow (maximum of 5 per year, per department), Department of Chemistry Award for Outstanding Teaching, Schmidt Science Fellowship Nominee (1 of 8), ACS COMP CCG Award (1 of 5), AIChE CoMSEF Award Winner (1 of 2).
- Thesis: Using Data-Driven Models to Understand Transition Metal Catalyst Energy Landscapes and Metal-Organic Framework Stability; Ph.D. advised by Prof. Heather J. Kulik

University of California, Berkeley — *Berkeley, CA*

B.S. in Chemical Engineering (Minor: Chemistry) — *Aug. 2013 - May 2017*

- High Honors, Regents' and Chancellor's Scholar, Leadership Award Scholar, Dean's List, Genentech USBTD Scholar, Tau Beta Pi

Experience

University of California, Los Angeles (UCLA) — *Westwood, CA*

Assistant Professor of Chemical and Biomolecular Engineering (CBE) — *July 2025*

- Running my own research group in the CBE department. Starting on July 1, 2025.

Independent Postdoctoral Fellowship at the University of Chicago — *Chicago, IL*

Postdoctoral Fellow — *September 2023 - PRESENT*

- Collaborative research with Professors Suriyanarayanan Vaikuntanathan, Eduardo Perozo, Benoit Roux, and Yuehaw Khoo.
- Collaboration with Professor Yamuna Krishnan.

Professor Heather J. Kulik's Group at the Massachusetts Institute of Technology — *Cambridge, MA*

Ph.D. Student — *Aug. 2017 - Apr. 2023*

- Research assistant in the group of Professor Heather J. Kulik (http://hjkgrp.mit.edu/).
- Lead developer and maintainer for `text_mining_tools` software package: https://github.com/hjkgrp/text_mining_tools
- Lead contributor and maintainer to `molSimplify` software package: https://github.com/hjkgrp/molSimplify.
- System administrator for our supercomputer (named gibraltar!). Handled both hardware and software. Performed maintenance and updates.
- Teaching assistant for 5.60 (Thermodynamics and Kinetics) (Fall 2017 / Spring 2018). Lab assistant for 10.637 (Fall 2021). Rated 7.0/7.0 for overall teaching ability for all semesters.
- Grader for 10.637 (Computational Chemistry) (Fall 2018 / Fall 2020).
- Primary host for Greater Boston Area Theoretical Chemistry Seminar (Put on by Graduate Students of MIT, Harvard, and BU). Responsible for inviting and hosting Professors Francesco Evangelista (Emory), Berend Smit (EPFL/UC Berkeley), Shaama Sharada (USC), Teresa Head-Gordon (UC Berkeley), Eugene Koonin (NIH), Jason Goodpaster (UMn), Laura Gagliardi (UMn), and William Jorgensen (Yale).
- Presented research to both scientific (conferences) and general (MIT Energy Night, outreach programs) audiences.
- Worked on and published collaborative projects with experimentalists (Mircea Dinca group at MIT.; Connie Lu group at UMn via Inorganometallic Catalyst Design Center; Phillip Milner group at Cornell) and other computational scientists (Getman group at Clemson via Inorganometallic Catalyst Design Center).
- Mentored undergraduate students from diverse backgrounds (Conrad Goffinet, MIT ChemE S.B. 2020, S.M. 2021; Anna Bair, MIT Chemistry S.B. 2023; Freya Edholm, MIT ChemE/Mathematics S.B. 2023; David Gonzalez Narvaez; University of Puerto Rico at Cayey Chemistry B.S. 2023).

Genentech Inc., Late Stage Pharmaceutical Development — *South San Francisco, CA*

Intern — *May 2016 - Aug. 2016*

- Investigated protein-excipient interactions using various analytical techniques, including but not limited to dynamic light scattering (DLS) and relaxation-dispersion nuclear magnetic resonance (NMR) spectroscopy. Elucidated special properties of L-arginine for drug formulations.
- Maintained a major collaboration with protein analytical chemistry.
- Began a collaboration with Genentech's molecular dynamics (MD) core team to verify experimental data.
- Presented findings as a poster, and published paper regarding arginine work in *J. Phys. Chem. B* (4th author).

Professor Jeffrey A. Reimer's Group at the University of California, Berkeley — *Berkeley, CA*

Undergraduate Researcher — *Jan. 2015 - Aug. 2017*

- Designed and built a tuneless ssNMR probe as well as a pressure control system, including complicated circuitry and valve-work (required machining, simple circuit building, programming in python, and engineering.
- Modeled NMR experiments using DFT calculations. Validated experimental data using DFT calculations. Performed various characterization experiments, including 1-pulse and CP/MAS on various nuclei.
- Contributed to a project in collaboration with Prof. Jeffrey Long's group that led to publication of a paper in *Chem. Sci.* (6th author).
- Secured funding to work independently twice - 1. Regents' and Chancellor's Research Fellowship, and 2. Chevron Scholarship.
- Independently wrote a senior thesis. Published thesis project in *J. Phys. Chem. C* (1st author).

# Peer-Reviewed Publications (‡ denotes equal contribution, * denotes corresponding author)

54. Chakraborti, P.; Mukherjee, S.; Oettinger, D.; **Nandy, A.***; Krishnan, Y.*; Walter, M.G.* Mechanistic Basis of the Voltage-Sensitivity of Thiazolothiazole Dyes. *submitted*.
53. Saha, R.; Vazquez-Salazar, A.; **Nandy, A.***; and Chen, I.A.* Fitness Landscapes and Evolution of Catalytic RNA. *Annu. Rev. Biophys.*, **2024**, *53*, 109-125.

Before Independent Career at UCLA Chemical and Biomolecular Engineering

52. Oh, C.; **Nandy, A.**; Yue, S.; Kulik, H.J.* MOFs with the Stability for Practical Gas Adsorption Applications Require New Design Rules. *submitted.*
51. Pitt, T.; Jia, H.; Azbell, T. J.; Zick, M.E.; **Nandy, A.**; Kulik, H.J.; and Milner, P. J.* Benchmarking N_2O Adsorption and Activation in Coordinatively Unsaturated Metal-Organic Frameworks. *J. Mater. Chem. C*, **2024**, *12*, 3164-3174.
50. Jia, H.; Duan, C.; Kevlishvili, I.; **Nandy, A.**; Liu, M.; and Kulik, H.J.* Computational Discovery of Co-doped Single-Atom Catalysts for Methane-to-Methanol Conversion. *ACS Catal.*, **2024**, *14*, 2992−3005.
49. Adamji, H.; Kevlishvili, I.; **Nandy, A.**; Roman-Leshkov, Y.; Kulik, H.J. Large-scale Comparison of Fe and Ru Polyolefin C–H Activation Catalysts. *J. Catal.*, **2024**, *431*, 115361.
48. Yue, S.; **Nandy, A.**; and Kulik, H.J.* Discovering Molecular Coordination Environments for Selective Ion Binding Using Machine Learning. *J. Phys. Chem. B*, **2023**, *127*, 10592–10600.
47. Edholm, F.; **Nandy, A.**; Reinhardt, C.; Kastner, D.W.; and Kulik, H.J.* Protein3D: Enabling Analysis and Extraction of Metal-Containing Sites from the Protein Data Bank with molSimplify. *J. Comput. Chem.*, **2024**, *45*, 352-361.
46. Vennelakanti, V.; Taylor, M. G.; **Nandy, A.**; Duan, C.; and Kulik, H.J.* Assessing the Performance of Approximate Density Functional Theory on 95 Experimentally Characterized Fe(II) Spin Crossover Complexes. *J. Chem. Phys.*, **2023**, *159*, 024120.
45. Adamji, H.; **Nandy, A.**; Kevlishvili, I.; Roman-Leshkov, Y.; and Kulik, H.J.* Computationally Guided Discovery of Stable Metal-Organic Frameworks that are Promising Methane to Methanol Catalysts. *J. Am. Chem. Soc.*, **2023**, *145*, 14365–14378.
44. **Nandy, A.**; Taylor, M.G.; and Kulik, H.J.* Identifying Underexplored and Untapped Regions in the Chemical Space of Transition Metal Complexes. *J. Phys. Chem. Lett*, **2023**, *14*, 5798–5804.
43. Cytter, Y.; **Nandy, A.**; Duan, C.; and Kulik, H.J.* Insights into the Deviation from Piecewise Linearity in Transition Metal Complexes from Supervised Machine Learning Models. *Phys. Chem. Chem. Phys.*, **2023**, *25*, 8103-8116.
42. **Nandy, A.**; Yue, S.; Oh, C.; Duan, C.; Terrones, G.; Chung, Y.G.; and Kulik, H.J.* A Database of Ultrastable MOFs Reassembled from Stable Fragments with Machine Learning Models. *Matter*, **2023**, *6*, 1-19.
41. Yue, S.; Oh, C.; **Nandy, A.**; Terrones, G.; and Kulik, H.J.* Effects of MOF Linker Rotation and Functionalization on Methane Uptake and Diffusion. *Mol. Sys. Des. Eng.*, **2023**, *8*, 527-537.
40. Terrones, G.; Duan, C.; **Nandy, A.**; and Kulik, H.J.* Low-Cost Machine Learning Prediction of Excited State Properties of Iridium-Centered Phosphors. *Chem. Sci.*, **2023**, *14*, 1419-1433.
39. Kastner, D. W.; **Nandy, A.**; Mehmood, R.; and Kulik, H.J.* Mechanistic Insights Into Substrate Positioning Across Non-heme Fe(II)/alpha-ketoglutarate-dependent Halogenases and Hydroxylases. *ACS Catal.*, **2023**, *13*, 2489-2501.
38. Duan, C.; **Nandy, A.**; Terrones, G.; Kastner, D. W.; and Kulik, H.J.* Rapid Exploration of a 32.5M Compound Chemical Space with Active Learning to Discover Density Functional Approximation Insensitive and Synthetically Accessible Transitional Metal Chromophores. *JACS Au*, **2023**, *3*, 391-401.
37. Cho, Y.; **Nandy, A.**; Duan, C.; and Kulik, H.J.* DFT-Based Multireference Diagnostics in the Solid State: Application to Metal–Organic Frameworks. *J. Chem. Theory Comput.*, **2023**, *19*, 1, 190–197.
36. Duan, C.; **Nandy, A.**; Meyer, R.; Arunachalam, N.; and Kulik, H.J.* A Transferable Recommender Approach for Selecting the Best Density Functional Approximations in Chemical Discovery. *Nat. Comput. Sci.*, **2023**, *3*, 38–47.
35. Arunachalam, N.; Gugler, S.; Taylor, M. G.; Duan, C.; **Nandy, A.**; Janet, J. P.; Meyer, R.; Oldenstaedt, J.; Chu, D. B. K.; and Kulik, H.J.* Ligand Additivity Relationships Enable Efficient Exploration of Transition Metal Chemical Space *J. Chem. Phys.*, **2022**, *157*, 184112.
34. **Nandy, A.**; Adamji, H.; Kastner, D.W.; Vennelakanti, V.; Nazemi, A.; Liu, M.; and Kulik, H.J.* Using Computational Chemistry to Reveal Nature's Blueprints in Single-Site Catalyst C–H Activation. *ACS. Catal.*, **2022**, *12* (15), 9281-9306.
33. Duan, C.; **Nandy, A.**; Adamji, H.; and Kulik, H. J.* Machine Learning Models Predict Calculation Outcomes with the Transferability Necessary for Computational Catalysis. *J. Chem. Theory Comput.*, **2022**, *18* (7), 4282-4292.
32. **Nandy, A.**; Duan, C.; Goffinet, C.; and Kulik, H. J.* New Strategies for Direct Methane-to-Methanol Conversion from Active Learning Exploration of 16 Million Catalysts. *JACS Au*, **2022**, *2* (5), 1200-1213.
31. Cytter, Y.; **Nandy, A.**; Bajaj, A.; and Kulik, H. J.* Divergent Ligand Additivity Effects in Two Types of Delocalization Errors From Approximate Density Functional Theory. *J. Phys. Chem. Lett.*, **2022**, *13* (20), 4549-4555.
30. Duan, C.; Chu, D. B. K.; **Nandy, A.**; and Kulik, H. J.* Detection of Multi-Reference Character Imbalances Enables a Transfer Learning Approach for Virtual High Throughput Screening with Coupled Cluster Accuracy at DFT Cost *Chem. Sci.*, **2022**, *13*, 4962-4971.
29. Bajaj, A.; Duan, C.; **Nandy, A.**; Taylor, M. G.; and Kulik, H. J.* Molecular Orbital Projectors in Non-empirical jmDFT Recover Exact Conditions in Transition Metal Chemistry. *J. Chem. Phys.*, **2022**, *156*, 184112.
28. **Nandy, A.**‡; Terrones, G.‡; Arunachalam, N.; Duan, C.; Kastner, D. W.; Kulik, H. J.* MOFSimplify, machine learning models with extracted stability data of three thousand metal–organic frameworks *Sci. Data.*, **2022**, *9*, 74.
27. Duan, C.‡; **Nandy, A.**‡; and Kulik, H. J.* Machine Learning for the Discovery and Design of Materials. *Ann. Rev. Chem. Eng.*, **2022**, *13*, 405-429.
26. Harper, D.‡; **Nandy, A.**‡; Arunachalam, N.; Duan, C.; Janet, J.P.; and Kulik, H. J.* Representations and Strategies for Transferable Machine Learning Models in Chemical Discovery *J. Chem. Phys.*, **2022**, *156*, 074101.
25. Jia, H.; **Nandy, A.**; Liu, M.; and Kulik, H. J.* Modeling the Roles of Rigidity and Dopants in Single-Atom Methane-to-Methanol Catalysts. *J. Mater. Chem. A.*, **2022**, *10*, 6193-6203.
24. Liu, M.; Nazemi, A.; Taylor, M. G.; **Nandy, A.**; Duan, C. and Kulik, H. J.* Large-Scale Analysis of the Electronic and Geometric Properties of Bio-Inspired Mo/W complexes. *ACS Catal.*, **2022**, *12* (2), 383-396.
23. **Nandy, A.**‡; Duan, C.‡; and Kulik, H. J.* Audacity of huge: overcoming challenges of data scarcity and data quality for machine learning in computational materials discovery. *Curr. Opin. in Chem. Eng.*, **2022**, 36, 100778.

22. **Nandy, A.**; Duan, C.; and Kulik, H. J.* Using Machine Learning and Data Mining to Leverage Community Knowledge for the Engineering of Stable Metal-Organic Frameworks. *J. Am. Chem. Soc.*, **2021**, *143* (42), 17535-17547.
21. Taylor, M. G.; **Nandy, A.**; Lu, C. C.; and Kulik, H. J.* Deciphering Cryptic Behavior in Bimetallic Transition Metal Complexes with Machine Learning. *J. Phys. Chem. Lett.*, **2021**, *12* (40), 9812-9820.
20. Vennelakanti, V.; **Nandy, A.**; Kulik, H. J.* The Effect of Hartree-Fock Exchange on Scaling Relations and Reaction Energetics for C–H Activation Catalysts. *Top. Catal.*, **2022**, *65*, 296-311.
19. **Nandy, A.**‡; Duan, C.‡; Taylor, M. G.; Liu, F.; Steeves, A. H. and Kulik, H. J.* Computational Discovery of Transition-metal Complexes: From High-throughput Screening to Machine Learning. *Chem. Rev.*, **2021**, *121* (16), 9927-10000.
18. Duan, C.; Liu, F.; **Nandy, A.**; Kulik, H. J.* Putting Density Functional Theory to the Test in Machine-Learning-Accelerated Materials Discovery. *J. Phys. Chem. Lett.*, **2021**, *12* (19), 4628-4637.
17. Janet, J.P.; Duan, C.;**Nandy, A.**; Liu, F.; and Kulik, H. J.* Navigating Transition-Metal Chemical Space: Artificial Intelligence for First-Principles Design. *Acc. Chem. Res.*, **2021**, *54* (3), 532-545.
16. **Nandy, A.**; Kulik, H. J.* Why Conventional Design Rules for C-H Activation Fail for Open Shell Transition Metal Catalysts *ACS Catal.*, **2020**, *10* (24), 15033-15047.
15. Moosavi, S. M.; **Nandy, A.**; Jablonka, K. M.; Ongari, D.; Janet, J. P.; Boyd, P. G.; Lee, Y.; Smit, B.*; Kulik, H. J.* Understanding Diversity in the Metal-Organic Framework Ecosystem. *Nat. Commun.* **2020**, *11*, 4068.
14. **Nandy, A.**‡; Chu, D. B. K‡; Harper, D. R.; Duan, C.; Arunachalam, N.; Cytter, Y.; Kulik, H. J.* Large-Scale Comparison of 3*d* and 4*d* Transition Metal Complexes Illuminates the Reduced Effect of Exchange on Second-Row Spin-State Energetics. *Phys. Chem. Chem. Phys.* **2020**, *22*, 19326-19341.
13. Duan, C.; Liu, F.; **Nandy, A.**; Kulik, H. J.* Semi-supervised Machine Learning Enables the Robust Detection of Multireference Character at Low Cost. *J. Phys. Chem. Lett.* **2020**, *11* (16), 6640-6648.
12. Duan, C.; Liu, F.; **Nandy, A.**; Kulik, H. J.* Data-Driven Approaches Can Overcome the Cost–Accuracy Trade-Off in Multireference Diagnostics. *J. Chem. Theory Comput.* **2020**, *16* (7), 4373-4387.
11. Taylor, M. G.‡; Yang, T.‡; Lin, S.‡; **Nandy, A.**; Janet, J.P.; Duan, C.; Kulik, H. J.* Seeing is Believing: Experimental Spin States from Machine Learning Model Structure Predictions. *J. Phys. Chem. A*, **2020**, *124* (16), 3286-3299.
10. **Nandy, A.**; Zhu, J.; Janet, J. P.; Duan, C.; Getman, R. B.; Kulik, H. J.* Machine Learning Accelerates the Discovery of Design Rules and Exceptions in Stable Metal-Oxo Intermediate Formation. *ACS Catal.* **2019**, *9* (9), 8243-8255.
9. Janet, J. P.; Duan, C.; Yang, T.; **Nandy, A.**; Kulik, H. J.* A Quantitative Uncertainty Metric Controls Error in Neural Network-Driven Chemical Discovery. *Chem. Sci.*, **2019**, *10*, 7913-7922.
8. Duan, C.; Janet, J. P.; Liu, F.; **Nandy, A.**; Kulik, H. J.* Learning from Failure: Predicting Electronic Structure Calculation Outcomes with Machine Learning Models. *J. Chem. Theory Comput.*, **2019**, *15* (4), 2331-2345.
7. Janet, J. P.; Liu, F.; **Nandy, A.**; Duan, C.; Yang, T.; Lin, S.; Kulik, H. J.* Designing in the Face of Uncertainty: Exploiting Electronic Structure and Machine Learning Models for Discovery in Inorganic Chemistry. *Inorg. Chem.*, **2019**, *58* (16), 10592-10606.
6. **Nandy, A.**‡; Duan, C.‡; Janet, J. P.; Gugler, S. O.; Kulik, H. J.* Strategies and Software for Machine Learning Accelerated Discovery in Transition Metal Chemistry. *Ind. Eng. Chem. Res.*, **2018**, *57* (42), 13973-13986.
5. **Nandy, A.**; Forse, A. C.; Witherspoon, V. J.*; Reimer, J. A.* NMR Spectroscopy Reveals Adsorbate Binding Sites in the Metal-Organic Framework UiO-66(Zr). *J. Phys. Chem. C*, **2018**, *122* (15), 8295-8305.
4. Khirich, G.*; Holliday, M. J.; Lin, J. C.; **Nandy, A.** Measurement and Characterization of Hydrogen-Deuterium Exchange Chemistry Using Relaxation Dispersion NMR Spectroscopy. *J. Phys. Chem. B*, **2018**, *122* (8), 2368-2378.
3. Ford, A. C.; Chui, W. F.; Zeng, A. Y.; **Nandy, A.**; Liebenberg, E.; Carraro, C.; Kazakia, G.; Alliston, T.; O'Connell, G. D.* A Modular Approach to Creating Large Engineered Cartilage Surfaces. *J. Biomech.*, **2018**, *67*, 177-183.
2. Barin, G.; Peterson, G. W.; Crocellà, V.; Xu, J.; Colwell, K. A.; **Nandy, A.**; Reimer, J. A.; Bordiga, S.; Long, J. R.* Highly Effective Ammonia Removal in a Series of Brønsted Acidic Porous Polymers: Investigation of Chemical and Structural Variations. *Chem. Sci.*, **2017**, *8*, 4399-4409.
1. Bezci, S. E.; **Nandy, A.**; O'Connell, G. D.* Effect of Hydration on Healthy Intervertebral Disk Mechanical Stiffness. *J. Biomech. Eng.*, **2015**, *137* (10), 101007.

Peer-Reviewed Book Chapters, Conference Proceedings, and Editorials

2. **Nandy, A.** and Kulik, H.J.* "Learning Design Rules for Catalysts through Computational Chemistry and Machine Learning", in Exploring Chemical Concepts through Theory and Computation, ed. Shubin Liu (in press) **Book chapter.**
1. Duan, C.; **Nandy, A.**; and Kulik, H.J.* "A Density Functional Recommendation Approach for Accurate Predictions of Vertical Spin Splitting of Transition Metal Complexes." ICML 2022 AI for Science Workshop. **Conference proceeding.**

Consulting

Flagship Pioneering, Inc. (FL96) *Cambridge, MA*

Independent Consultant/Key Opinion Leader for FL96 *April 2023-present*

Select Honors & Awards

University of Chicago

2024	**2024 CAS Future Leader**, American Chemical Society	*Columbus, OH*
2024	**Outstanding Reviewer Award**, EES Catalysis (Royal Society of Chemistry)	*London, UK*
2023	**Schmidt AI+Science Fellow**, Schmidt Futures	*Chicago, IL*

Massachusetts Institute of Technology

2022	**AIChE CoMSEF Outstanding Graduate Student Award**, AIChE CoMSEF Division	*Phoenix, AZ*
2022	**Chemical Computing Group Excellence Award for Graduate Students**, American Chemical Society	*Chicago, IL*
2019	**NSF-GRFP Fellow (1 of 13 Chemical Theory Awards)**, National Science Foundation Graduate Research Fellowship Program (NSF-GRFP)	*Alexandria, VA*
2018	**Department of Chemistry Award for Outstanding Teaching**, Massachusetts Institute of Technology	*Cambridge, MA*
2017	**Robert T. Haslam Presidential Fellow**, Massachusetts Institute of Technology	*Cambridge, MA*

University of California, Berkeley

2017	**Most Likely to Succeed as a Chemical Engineer**, American Institute of Chemical Engineers - NorCal	*Berkeley, CA*
2017	**High Honors**, University of California, Berkeley - College of Chemistry	*Berkeley, CA*
2017	**Dean's List**, University of California, Berkeley - College of Chemistry	*Berkeley, CA*
2016	**Chevron Scholarship (8 granted per year)**, Chevron Corporation	*Richmond, CA*
2015	**Genentech Outstanding Student Award (1 granted per year)**, Genentech Inc.	*San Francisco, CA*
2014	**Elected to Tau Beta Pi** , Tau Beta Pi - California Alpha	*Berkeley, CA*
2014	**Berkeley Stem Cell Center Undergraduate Summer Fellowship**, University of California, Berkeley	*Berkeley, CA*
2013, 2016	**The Leadership Award (∼100 granted per year)**, Alumni Association - University of California, Berkeley	*Berkeley, CA*
2013-2017	**The Regents' and Chancellor's Scholarship (Top 1% of applicants)**, University of California, Berkeley	*Berkeley, CA*
2013	**Mills Peninsula Division Scholar**, Palo Alto Medical Foundation	*Palo Alto, CA*

Select Invited Talks

Machine Learning for Chemistry and Materials 2024 — *Santa Fe, NM*

Invited Speaker (Invited by Nikita Fedik and Vidushi Sharma) — *May 2024*

- "Leveraging Community Knowledge to Forge a Path Forward for Transition Metal Complex and Metal-Organic Framework Design"

Molecular Materials Group at Argonne National Laboratory — *Lemont, IL*

Invited Speaker (Invited by Rajeev Assary and Alvaro Vazquez Mayagoitia) — *March 2024*

- "Combining Cheminformatics and Machine Learning to Accelerate Open-Shell Catalyst Discovery"

Marcos Sotomayor Group Meeting at UChicago — *Chicago, IL*

Invited Speaker — *February 2024*

- "Modeling Emergent Phenomena in Outer Hair Cells"

Shuwen Yue Group Meeting at Cornell — *Ithaca, NY*

Invited Speaker — *February 2024*

- "Combining Cheminformatics and Machine Learning to Accelerate Open-Shell Catalyst Discovery"

Telluride Science Workshop: Activation of Small Molecules — *Telluride, CO*

Invited Speaker (Invited by Jenny Y. Yang, Nadia Leonard, and David C. Lacy) — *June 2024*

- "Combining Cheminformatics and Machine Learning to Accelerate Open-Shell Catalyst Discovery"

NIST Workshop: Integrating Crystallographic and Computational Approaches to Carbon-Capture Materials for the Mitigation of Climate Change — *Rockville, MD*

Invited Speaker (Invited by Eric Cockayne); Co-chair for Discussion on Machine Learning for Gas Adsorption — *November 2023*

- "Leveraging Community Knowledge to Quantify and Engineer Stability in MOFs for Gas Adsorption"

Randall Q. Snurr and Linda Broadbelt Group Meetings at Northwestern — *Evanston, IL*

Invited Speaker — *October 2023*

- "Combining Cheminformatics and Machine Learning to Accelerate Open-Shell Catalyst Discovery"

American Chemical Society Fall 2023 Meeting — *San Francisco, CA*

Invited Speaker (Invited to CATL Session on Data Science by Hongliang Xin, Nong Artrith, and John Kitchin — *August 2023*

- "Using Text-Mining and Community Knowledge to Quantify and Engineer Stability in MOFs"

Telluride Science Workshop: Machine Learning and Informatics for Chemistry and Materials — *Telluride, CO*

Invited Speaker — *June 2023*

- "Data-driven Exploration of Transition Metal Complexes and Metal-Organic Frameworks by Leveraging Computational and Experimental Data"

Statistical Thermodynamics and Molecular Simulations Seminar *Virtual (New Haven, CT)*

Virtual Seminar Speaker Invited by Prof. Amir Haji-Akbari and Prof. Sapna Sarupria *January 2023*

- "Sifting Through 16M Catalysts for Methane-to-Methanol Catalyst Design Under Weak Thermodynamic Scaling"

Select Contributed Talks

American Chemical Society Meeting, CATL Division *San Francisco, CA*

Graduate Student Representing Kulik Group *March 2021*

- Presented an oral presentation on broken linear free energy relationships in single site catalysis.

American Institute of Chemical Engineers Virtual Meeting (2020) *San Francisco, CA*

Graduate Student Representing Kulik Group *November 2020*

- Presented an oral presentation on broken linear free energy relationships in single site catalysis.

Department of Energy, Energy Frontiers Research Center (EFRC) Review *Gaithersburg, MD*

Graduate Student Representing Kulik Group within Inorganometallic Catalyst Design Center (ICDC) *February 2020*

- Co-presented an oral presentation with Prof. Matthew Neurock regarding collaborative work from within ICDC. Presented work from Kulik, Getman, Gagliardi, Neurock, and Truhlar groups.

American Institute of Chemical Engineers Annual Meeting (2019) *Orlando, FL*

Graduate Student Representing Kulik Group *November 2019*

- Presented an oral presentation regarding surrogate model development for investigation of light alkane oxidation catalysts.

Inorganometallic Catalyst Design Center All-Hands Meeting *Minneapolis, MN*

Graduate Student Representing Kulik Group *October 2019*

- Presented an oral presentation regarding surrogate model development for investigation of light alkane oxidation catalysts. Specifically focused on applications to experimental work, and how active learning can result in robust model development.

26th North American Catalysis Society Meeting (2019) *Chicago, IL*

Graduate Student Representing Kulik Group *June 2019*

- Presented an oral presentation regarding surrogate model development for investigation of light alkane oxidation catalysts.

New England Catalysis Society (NECS) Meeting (2018) *Boston, MA*

Graduate Student Representing Kulik Group *December 2018*

- Presented an oral presentation regarding surrogate model development for novel transition metal catalyst discovery.

Inorganometallic Catalyst Design Center Subgroup Meeting (2018) *Minneapolis, MN*

Graduate Student Representing Kulik Group *November 2018*

- Presented an oral presentation regarding collaborative work for machine learning in single-site catalysis reaction energetics.

American Institute of Chemical Engineers Annual Meeting (2018) *Pittsburgh, PA*

Graduate Student Representing Kulik Group *November 2018*

- Presented an oral presentation regarding current research work in session titled "Data Science in Catalysis."

Service

Committee Service for: Dean Alissa Park's Ad Hoc GPU Committee (UCLA)
Journal Peer Review for: Chemistry of Materials (1), ACS Catalysis (1), Chemical Communications (1), ACS Omega (2), Journal of Chemical Information and Modeling (4), The Journal of Computational Chemistry (2), Chem (2), Nature Computational Science (2), Nature Communications (3), JACS Au (1), npj Computational Materials (3), Digital Discovery (Data: 3, Article: 1), The Journal of Physical Chemistry Letters (1), The Journal of Physical Chemistry B (2), Computational Materials Science (7), Scientific Data (1), Chemical Science (4), Industrial Engineering and Chemistry Research (1), The Journal of Chemical Physics (2), Matter (2), Biomechanics and Modeling in Mechanobiology (1), Energy and Environmental Science Catalysis (1).
Proposal Peer Review for: DOE Funding for Accelerated, Inclusive Research [FAIR; BES] (2023: 1), DOE Energy Earthshot Research Centers [EERC; BES] (2023: 2), NSF ENG/CBET Adhoc/Virtual (2024: 1), ARPA-E Vision OPEN (2024: 1).
Seminar Organization for: AI in Science Seminar Series @ UChicago (invited/hosted: Andrew Ferguson, Arthi Jayaraman, Muhammed Shuaibi, Bryce Meredig); Greater Boston Area Theoretical Chemistry Seminar Series @ MIT (invited/hosted: Teresa Head-Gordon, Berend Smit, Shaama Sharada, Francesco Evangelista, Jason Goodpaster, Eugene Koonin, Laura Gagliardi, William Jorgensen)
Conference Organization for: Computational Materials Science and Engineering Gordon Research Seminar (GRS) Co-Chair

Certifications and Skills

2017 **Engineer-in-Training**, FE - Chemical, National Council of Examiners for Engineering and Surveying *Sacramento, CA*
2016 **First-Aid/CPR Certification**, American Red Cross *Fremont, CA*

Skills:
(advanced): LaTeX, Microsoft Office, MATLAB, Python, HTML/CSS, NMR Spectroscopy, Density Functional Theory, Machine Learning (Keras, TensorFlow), Software Development (Including Continuous Integration/Continuous Deployment), Docker, System Adminstration (RedHat), Continuum Modeling, Molecular Dynamics
(basic): SolidWorks, UV-Vis Spectroscopy, FTIR Spectroscopy, HPLC, DSC, DLS, DSF, Instron Compression, Powder X-Ray Diffraction, Basic MOF Synthesis, Machining (Lathe and Mill), Soldering

Extracurricular Activities and Outreach

South Side Science Festival of Chicago
Chicago, IL

Demonstration Volunteer — *Sept 2023*

- In charge of a science demonstration for the South Side Science Festival (over 1,000 attendees).

Greater Boston Area Theoretical Chemistry Seminar (Hosted by Graduate Students of BU, Harvard, and MIT)
Cambridge, MA

Primary Host (2018/2019) — *June 2018 - Apr. 2023*

- Responsible for inviting and hosting Professor Berend Smit (initially at UC Berkeley, now at EPFL in Switzerland), Professor Francesco Evangelista (Emory University), Dr. Eugene Koonin (NIH, NAS Member), Jason Goodpaster (UMn), Laura Gagliardi (UMn), Shaama Sharada (USC), Teresa Head-Gordon (UC Berkeley), and William Jorgensen (Yale).
- In charge of coordinating meetings with faculty and graduate students over a three day visit. Also responsible for planning housing, meals, and events during seminar visit. In charge of orchestrating visit over three schools (MIT, Harvard, BU) with $>$ 80 graduate students and 30 faculty.

Massachusetts Institute of Technology, Department of Chemical Engineering
Cambridge, MA

Graduate Student — *Oct. 2018 - Apr. 2023*

- Presented poster presentations and demonstrations at MIT Energy Night, a viewing at the MIT museum for the general public, with an estimated 2500 attendees. Created interactive demonstration to make complicated concepts more visual and easy to understand.

Massachusetts Institute of Technology, ACCESS Program
Cambridge, MA

Presenter — *Sept. 2019*

- Gave general presentations regarding computational chemistry to under represented minority students interested in attending graduate school.

University of California, Berkeley Club Figure Skating
Berkeley, CA

Safety Officer (2013), Treasurer (2014), Webmaster (2014-2016), President (2015 and 2016) — *Aug. 2013 - Jan. 2017*

- Raised $10,000 in funds by hosting a local competition.
- Managed a team of $\sim$50 students (undergraduate and graduate) from diverse backgrounds.
- Independently built and implemented team website using HTML and CSS (figureskating.berkeley.edu).
- Weekly volunteer for "Special Skaters" at Oakland Ice Center, a disability-inclusive figure skating camp that provides free figure skating lessons.

Regents' Overnight Host Program (ROHP)
Berkeley, CA

Committee Member (2013 and 2014), Coordinator (2015) — *Aug. 2013 - May. 2016*

- Planned four overnight host programs during Spring 2014/2015/2016 for 300 prospective freshmen Regents' Scholars.
- Developed an Out-of-State Regents' Overnight Host Program.
- Coordinated with the University of California, Berkeley, Scholarship Office to manage a budget of $20,000 for the overnight host programs.
- Obtained high profile speakers (including Nobel Laureates Randy Schekman, Saul Perlmutter, and George Smoot).
- Coordinated the development of a website using HTML and CSS (rohp.berkeley.edu).

Teaching, Tutoring, and Demonstrations - College of Chemistry
Berkeley, CA

Tutor (2014 and 2015), Undergraduate Student Instructor (2016) — *Aug. 2014 - Dec. 2016*

- Tutored student-athletes in chemistry and mathematics ($\sim$ 20 students over 3 years).
- Taught a laboratory section of 30 undergraduate students. Received a rating of 6.9/7, the highest of all instructors (graduate or undergraduate).
- Developed website for College of Chemistry Peer Advising Blog (http://www.cchem.berkeley.edu/peer-advising-blog/).
- Performed science demonstrations and lessons at Oakland Technical High School.