Lance Kavalsky

Postdoctoral Researcher

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Education & Training

2024–present **Postdoctoral Researcher**, *University of Wisconsin–Madison*, Madison, WI,
Advisor: Professor Manos Mavrikakis.

2023–2024 **PhD Mechanical Engineering**, *University of Michigan*, Ann Arbor, MI,
Advisor: Professor Venkatasubramanian Viswanathan.
Thesis: *Electrochemical Manufacturing: Advances in Design and Accelerated Materials Discovery*
Continued from CMU

2019–2023 **MS Mechanical Engineering**, *Carnegie Mellon University*, Pittsburgh, PA,
Advisor: Professor Venkatasubramanian Viswanathan.

2017–2019 **MASc Materials Science & Engineering**, *University of Toronto*, Toronto, ON,
Advisor: Professor Chandra Veer Singh.
Thesis: *First-principles Investigation of 2D-Phosphorus for Energy Storage Applications*

2013–2017 **HBSc Physics Specialist & Math Minor**, *University of Toronto*, Toronto, ON,
High Distinction.

Research Experience

2024–Present **Postdoctoral Researcher**, *University of Wisconsin-Madison*, Madison, WI.
- Demonstrated presence of high-index facets on Au nanospheres through machine-learned force fields to explain findings of experimental collaborators at Georgia Tech
- Unveiled a phase change in CO occupation on Au surface steps and validated with experimental literature
- Modeled anion poisoning resistance of intermetallic fuel cell cathodes, in close collaboration with experimentalists at Brookhaven National Laboratory

2023–2024 **Graduate Research Assistant**, *University of Michigan*, Ann Arbor, MI.
- Identified a core obstacle to sustainable ironmaking by mapping the electrochemical aqueous iron interface through density functional theory (DFT) calculations
- Developed methodologies for autonomous materials discovery using machine learning and high-throughput computational chemistry

2019–2023 **Graduate Research Assistant**, *Carnegie Mellon University*, Pittsburgh, PA.
- Rigorously benchmarked materials discovery acceleration estimates for closed-loop machine learning frameworks and showed it could accelerate materials discovery by 10-20×
- Proposed a multiobjective scoring scheme for closed-loop discovery and demonstrated it could support electrocatalyst searches that balance activity, cost, and stability
- Open-sourced a software for active-learning guided computational discovery of electrocatalysts, AutoCat

2017–2019 **Graduate Research Assistant**, *University of Toronto*, Toronto, ON.
- Assessed 2D phosphorus electrodes for energy storage through DFT calculations
- Identified strain engineering as an approach to improving 2D phosphorus stability against oxidation via first-principles calculations

Summer 2015 **Research Assistant**, *McMaster University*, Hamilton, ON.
- Built and tested microwell array devices for protoplast fusion

Publications

* indicates equal author contribution

17. **L. Kavalsky** and M. Mavrikakis. "Adsorption and Dissociation of CO on Gold Surfaces: Effect of Coverage and Adatom Clusters" *ChemRxiv*, DOI: 10.26434/chemrxiv-2025-k4d1v (2025) (under review)

16. K.K. Li*, **L. Kavalsky***, M. Figueras-Valls, Y. Ding, M. Mavrikakis, Y. Xia. "What Makes Au Nanospheres Superior to Octahedral and Cubic Counterparts for the Deposition of a Pt Monolayer Shell?" *J. Am. Chem. Soc.*, 147, 29, 25273-25286 (2025)

15. V. Azumah, **L. Kavalsky**, V. Viswanathan. "Lithium Nitride (Li3N) Formation in Lithium-Mediated Electrochemical Ammonia Synthesis Can Be Enhanced with the Right Proton Donor" *J. Catal.*, 450, 116250 (2025)

14. V. Azumah, **L. Kavalsky**, V. Viswanathan. "Proton Donors Influence Nitrogen Adsorption in Lithium-Mediated Electrochemical Ammonia Synthesis" *J. Phys. Chem. C*, 129, 5, 2488-2501 (2025)

13. M.S. Johnson, D. Farina, **L. Kavalsky**, *et. al.*. "Automatic Generation of Chemical Mechanisms for Electrochemical Systems: Solid Electrolyte Interphase Formation in Lithium Batteries" *J. Phys. Chem. C*, 129, 28, 1266712678 (2025)

12. **L. Kavalsky** and V. Viswanathan. "Electrowinning for room-temperature ironmaking: Mapping the electrochemical aqueous iron interface" *J. Phys. Chem. C*, 128, 35, 14611-14620 (2024) (part of Jens K. Nørskov Festschrift virtual special issue)

11. **L. Kavalsky**, V.I. Hegde, B. Meredig, V. Viswanathan. "A Multiobjective Closed-loop Approach Towards Autonomous Discovery of Electrocatalysts for Nitrogen Reduction" *Digital Discovery*, 3, 999-1010 (2024)

10. **L. Kavalsky***, V.I. Hegde*, E. Muckley, M.S. Johnson, B. Meredig, V. Viswanathan. "By how much can closed loop frameworks accelerate computational materials discovery?" *Digital Discovery*, 2, 1112-1125 (2023)

9. R. Patil, M. Kaur, S. House, **L. Kavalsky**, *et. al.*. "Reversible Alkaline Hydrogen Evolution and Oxidation Reactions Using NiMo Catalysts Supported on Carbon" *Energy Adv.*, 2, 1500-1511 (2023)

8. E. Annevelink*, R.C. Kurchin*, E. Muckley, **L. Kavalsky**, *et. al.*. "AutoMat: Accelerated Computational Electrochemical systems Discovery" *MRS Bulletin*, 47, 1036-1044 (2022)

7. L.M. Tsiverioti, **L. Kavalsky**, V. Viswanathan. "Robust Analysis of $4e^-$ vs $6e^-$ Reduction of Nitrogen on Metal Surfaces and Single-Atom Alloys" *J. Phys. Chem. C*, 126, 31, 12994-13003 (2022)

6. **L. Kavalsky** and V. Viswanathan. "Robust Active Site Design of Single-Atom Catalysts for Electrochemical Ammonia Synthesis" *J. Phys. Chem. C*, 124, 42, 23164-23176 (2020)

5. S. Mukherjee, **L. Kavalsky**, K. Chattopadhyay, C.V. Singh. "Dramatic improvement in the performance of graphene as Li/Na battery anodes with suitable electrolytic solvents" *Carbon*, 161, 570-576 (2020)

4. **L. Kavalsky**, S. Mukherjee, C.V. Singh. "Compression induced resistance of singlet oxygen dissociation on phosphorene" *Phys. Rev. Materials*, 4, 021001 (2020) (Editor's Suggestion highlight)

3. **L. Kavalsky**, S. Mukherjee, C.V. Singh. "Phosphorene as a Catalyst for Highly Efficient Nonaqueous Li–Air Batteries" *ACS Appl. Mater. Interfaces, 11, 1, 499-510 (2019)*

2. S. Mukherjee, **L. Kavalsky**, K. Chattopadhyay, C.V. Singh. "Adsorption and diffusion of lithium polysulfides over blue phosphorene for LiS batteries" *Nanoscale*, 10, 45, 21335-21352 (2018)

1. S. Mukherjee*, **L. Kavalsky***, C.V. Singh. "Ultrahigh storage and fast diffusion of Na and K in blue phosphorene anodes" *ACS Appl. Mater. Interfaces*, 10, 10, 8630-8639 (2018)

Awards

2023 **NAM28 Kokes Award**, *North American Catalysis Society*.
2022 **NAM27 Kokes Award**, *North American Catalysis Society*.
2020 **Alexander Graham Bell CGS-D3 Scholarship**, *NSERC*.
2018 **Haultain Fellowship**, *University of Toronto*.
2017 **Graduate Student Endowment Fund Award**, *University of Toronto*.
2014 **New College In-Course Scholarship**, *University of Toronto*.
2013 **James A Priestly Admission Scholarship**, *University of Toronto*.
2013 **New College Open Admission Scholarship**, *University of Toronto*.

Patents and Patent Applications

1. US Patent Application PCT/US2024/050004 "Electrochemical Synthesis of Direct Reduced Metal and Metal-derived Compounds" Inventors: **Kavalsky, L.** (Ann Arbor, MI), Viswanathan, V. (Ann Arbor, MI)

Oral Talks

5. **L. Kavalsky**, M. Mavrikakis. "Modeling Au Surfaces in Reactive Environments via Machine-Learned Interatomic Potentials" *2025 MRS Fall Meeting*, Boston, MA (November 2025)

4. **L. Kavalsky**, X. Zhao, K. Sasaki, M. Mavrikakis. "Understanding Anion Adsorption in Low Pt-Loading N-Doped Intermetallic Fuel Cell Cathodes" *248th ECS Meeting*, Chicago, IL (October 2025)

3. (Invited) **L. Kavalsky**, M. Mavrikakis. "Developing Machine-Learned Interatomic Potentials for Au: A Gold Mine for Surface Science Insights" Hougen/CATHEX Symposium, Madison, WI (June 2025)

2. **L. Kavalsky**, V.I. Hegde, V. Viswanathan. "Autonomous Multiobjective Computational Discovery of NRR Electrocatalysts" *The 28th North American Catalysis Society Meeting*, Providence, RI (June 2023)

1. **L. Kavalsky**, V.I. Hegde, E. Muckley, L.M. Tsiverioti, V. Viswanathan. "A Generalizable Closed-Loop Framework for Accelerated Discovery of Electrochemical Nitrogen Reduction Catalysts" *The 27th North American Catalysis Society Meeting*, New York City, NY (May 2022)

Poster Presentations

3. **L. Kavalsky**, X. Zhao, K. Sasaki, M. Mavrikakis. "Investigating Anion Poisoning on N-doped $L1_0$ Intermetallic Fuel Cell Cathodes through First-Principles Modeling" *2025 MRS Fall Meeting*, Boston, MA (November 2025)

2. **L. Kavalsky**, V.I. Hegde, V. Viswanathan. "Accelerated Computational Discovery of Electrocatalysts via an Autonomous Multiobjective Workflow" *Accelerate Conference*, Toronto, ON (August 2023)

1. **L. Kavalsky**, V. Viswanathan. "Unraveling the Iron-Water Interface for Electrochemical Steel Production" *The 28th North American Catalysis Society Meeting*, Providence, RI (June 2023)

Teaching Experience

Spring 2023 **TA: 24-703 Numerical Methods in Engineering**, *Carnegie Mellon University*, Pittsburgh, PA.
- Assisted running hands-on in-class exercises
- Led an introductory C++ coding workshop and ran homework review sessions

Fall 2021 **TA: 24-643 Energy Storage Materials & Systems**, *Carnegie Mellon University*, Pittsburgh, PA.
- Held office hours to address student questions and cover supplementary course content
- Led an introductory Python coding workshop

Fall 2018 **TA: MSE1038H/438H Computational Materials Design**, *University of Toronto*, Toronto, ON.

- Conducted lab sessions which provided senior undergraduate and graduate students hands-on experience with Density Functional Theory and Molecular Dynamics simulation techniques
- Delivered a guest lecture on Ab-Initio Molecular Dynamics and Metadynamics

July 2017 **Counsellor: Da Vinci Engineering Enrichment Program Summer Academy**, *University of Toronto*, Toronto, ON.

- Provided teaching support in the Foundations of Quantum Mechanics course for Grade 11 & 12 students
- Led a session on superconductivity

Academic Service

Reviewing

ACS Applied Energy Materials, *Journal of Open Source Software*

Open-Source Software Contributions

- **AutoCat**: A python package for both electrocatalyst discovery via sequential learning and automated catalyst structure generation for DFT. I have been leading the development of this code
- **dftinputgen**: Tools for automated DFT input script generation. I contributed GPAW support
- **dfttopif**: A package with tools for parsing DFT output and extracting relevant data into the PIF format. I contributed GPAW support