Lance Kavalsky

Postdoctoral Researcher

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Education

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

2019–2023 **MS Mechanical Engineering**, *Carnegie Mellon University*, Pittsburgh, PA,
Advisor: Professor Venkatasubramanian Viswanathan.
GPA: 4.0/4.0

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*
GPA: 4.0/4.0

2013–2017 **HBSc Physics Specialist & Math Minor**, *University of Toronto*, Toronto, ON,
High Distinction.
GPA: 3.83/4.00

Employment

2024–Present **Postdoctoral Researcher**, *University of Wisconsin-Madison*, Madison, WI.
- Developing mechanistic models of active site formation for heterogeneous catalysis
- Advisor: Professor Manos Mavrikakis

2023–2024 **Graduate Research Assistant**, *University of Michigan*, Ann Arbor, MI.
- Probed the electrochemical aqueous interface of Fe110 for iron electrowinning 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.
- Developed software for high-throughput DFT calculations and integrated it into a sequential-learning materials discovery framework as part of the ARPA-E DIFFERENTIATE program
- Open-sourced and developed a software for active-learning guided computational discovery of electrocatalysts, AutoCat
- Rigorously calculated materials discovery acceleration estimates for closed-loop frameworks with machine learning surrogatization over the traditional search paradigm
- Proposed a multiobjective scoring scheme for closed-loop discovery and applied it to search for single-atom alloy electrocatalysts balancing activity, cost, and stability

2017–2019 **Graduate Research Assistant**, *University of Toronto*, Toronto, ON.
- Performed density functional theory calculations to study 2D materials for novel battery technologies (including Na-ion, K-ion, and Li-air batteries)
- Investigated methods of improving ambient stability of phosphorene and identified substrate engineering as a promising approach

Summer 2015 **Research Assistant**, ***McMaster University***, Hamilton, ON.
- Responsible for building and testing of microwell array devices for protoplast fusion
- Worked towards optimizing the building process of these devices

Publications

* indicates equal author contribution

12. **L. Kavalsky** and V. Viswanathan. "Electrowinning for room-temperature ironmaking: Mapping the electrochemical aqueous iron interface" *The Journal of Physical Chemistry C*, 2024, 128, 35, 14611-14620 (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*, 2024, 3, 999-1010

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*, 2023, 2, 1112-1125

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 Advances*, 2023, 2, 1500-1511

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

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

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

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*, 2020, 161, 570-576

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

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

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

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

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*.

Teaching Experience

Spring 2023 **TA: 24-703 Numerical Methods in Engineering**, *Carnegie Mellon University*, Pittsburgh, PA.
- Held office hours and project progress meetings
- 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
- Provided support for developing course materials (lecture handouts, midterm questions, code demos, etc..)
- 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

Talks

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

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)

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

Academic Service

Reviewing

ACS Applied Energy Materials, Journal of Open Source Software

Computational Skills

Density Functional Theory: GPAW, VASP, Quantum Espresso, DFTK.jl

General Purpose Coding: python, MATLAB, LaTeX, bash, git

Machine Learning