

Lance Kavalsky

PhD Candidate

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Education

- 2019–Present **PhD 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

Research Experience

- 2019–Present **Graduate Research Assistant**, *Carnegie Mellon University*, Pittsburgh, PA.
- Developed software for high-throughput density functional theory 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 paradigm
 - Developed an uncertainty quantified framework for robustly predicting electrocatalytic activity of single-atom catalysts towards ammonia synthesis
- 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

Awards

- 2022 **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*.

Publications

8. E. Annevelink*, R.C. Kurchin*, E. Muckley, **L. Kavalsky**, *et. al.*. "AutoMat: Accelerated Computational Electrochemical systems Discovery" *MRS Bulletin* (accepted) [arXiv:2011.04426](https://arxiv.org/abs/2011.04426)
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**, 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 LiAir 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

* indicates equal author contribution

Teaching Experience

- 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..)

- 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

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)

Academic Service

Reviewing

since 2021 **Applied Energy Materials**, *American Chemical Society*.

Computational Skills

Density Functional Theory: GPAW, QUANTUM ESPRESSO, VASP, DFTK.JL

General Purpose Coding: python, MATLAB, L^AT_EX, bash, git

Machine Learning