BRYANT Y. LI

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EDUCATION

The University of California, Berkeley, *Ongoing* — *August 2021 - Anticipated May 2026*
Ph.D. Materials Science and Engineering — *Berkeley, CA*
Advisor: Prof. Kristin A. Persson

The University of California, Berkeley, *3.80 GPA* — *August 2021 - December 2023*
M.S. Materials Science and Engineering — *Berkeley, CA*
Graduate Certificate - Applied Data Science

The Pennsylvania State University, *3.87 GPA* — *August 2017 - May 2021*
B.S. Materials Science and Engineering, *magna cum laude* — *University Park, PA*
Minor - Applied Mathematics
Dean's List (all semesters)

RESEARCH EXPERIENCE

Graduate Student Researcher, Persson Group — *Aug 2021 – Present*
University of California, Berkeley, Berkeley, CA

- Investigating solid-electrolyte interphase (SEI) formation in solid-state batteries using machine-learned and universal interatomic potentials (MLIPs/UIPs).
- Developed and deployed high-throughput DFT workflows (PBEsol/r2SCAN) to generate datasets for modeling bulk, amorphous, disorder, and interfacial reactivity.
- Applied advanced MLIP frameworks — M3GNet, CHGNet, MACE, NequIP, DeepMD-kit, pyACE — for force field development and molecular dynamics simulations.
- Developed and curating a high-throughput R2SCAN dataset comprising [150,000+] materials entries, expanding the scope and precision of the next-generation Materials Project database for accelerated materials design.
- Designed and implemented `MPMorph` code in Atomate2 for automated amorphous and non-equilibrium structure generation.
- Managing NREL compute resources and leading the group's ML-subgroup; coordinating collaborative development and training efforts.

Undergraduate Research Assistant, Dabo Group — *Sept 2018 – May 2021*
Pennsylvania State University, University Park, PA

- Optimized Pd channel formation in Pt–Pd nanoparticle electrocatalysts for fuel cell applications, funded by the U.S. Department of Energy.
- Performed 700+ DFT calculations using Quantum ESPRESSO in both vacuum and solvent environments to determine cluster energies for Pt–Pd surfaces.
- Built cluster basis sets with ICET for cluster expansion fitting; conducted grand canonical and canonical Monte Carlo simulations.
- Developed Python scripts for automated data extraction, processing, and management from large-scale simulations.

- Collaborated with Dr. James Goff and Prof. Ismaila Dabo; presented progress in weekly research meetings.

Research Assistant, Lemke Group *Sept 2016 – Dec 2017*
The University of Hong Kong, Hong Kong

- Modeled catalytic ammonia production on Fe–Ni alloy clusters (Awaruite, Tetrataenite) to study the origins of life in the Archean Era.
- Performed classical modeling of cluster thermodynamic stability using Finnis–Sinclair, Lennard–Jones, and Sutton–Chen potentials for systems up to $n = 24$ atoms.
- Generated theoretical predictions of magic cluster stability and adsorption behavior for nitrogen and hydrogen species.
- Presented partial findings as a poster at the 2017 American Geophysical Union Fall Meeting.

TEACHING EXPERIENCE

Mathematics Tutor (100–200 Level), Penn State Learning *Aug 2020 – May 2021*
Penn State University, University Park, PA

- Provided one-on-one and group tutoring for 11 hours/week in Calculus I–III, Ordinary and Partial Differential Equations, and Linear Algebra.
- Adapted teaching methods to diverse learning styles, improving student comprehension and problem-solving skills.
- Facilitated collaborative learning sessions, encouraging peer-to-peer problem solving.

Teaching Assistant, Introduction to Materials Laboratory *Aug 2020 – May 2021*
Penn State University, University Park, PA

- Led undergraduate laboratory sessions on standard materials characterization techniques.
- Instructed students in optical microscopy, scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), and X-ray diffraction (XRD).
- Assisted in grading lab reports and providing constructive feedback to improve technical writing and data analysis skills.

TECHNICAL SKILLS

Computational Methods: Density Functional Theory (DFT), Atomic Cluster Expansion (ACE), Machine-Learned Interatomic Potentials (MLIP), Foundational Models, *Ab initio* Molecular Dynamics (AIMD), Molecular Dynamics (MD), Cluster Expansion (CE) Method, Monte Carlo Simulations (canonical, grand canonical), High-throughput Workflow Automation (Atomate2, Jobflow, FireWorks), Machine Learning (ML).

Machine Learning for Materials Science: Development and training of MLIPs (PaceMaker, GraceMaker, M3GNet, CHGNet, MACE, NequIP, DeepMD-kit), Feature Engineering, Model Deployment for HPC Pipelines.

Programming & Data Science: Python (Pandas, ASE, Matplotlib, NumPy, SciPy), Command-Line Interface (CLI), Git/GitHub, MongoDB, Materials Project API, LaTeX, MATLAB.

High-Performance Computing (HPC): Parallel computing (MPI, OpenMP), CPU and GPU architectures, NERSC Perlmutter, NREL Kestrel, Job Scheduling (SLURM, PBS).

Visualization & Analysis: VESTA, OVITO Pro, Electronic Structure Visualization (band structures, DOS), Trajectory Analysis.

Languages: English (fluent), Mandarin (fluent), Cantonese (fluent).

Certifications: International Baccalaureate (IB) Bilingual Diploma.

HONORS, AWARDS, AND RESEARCH GRANTS

DOE - Energy Storage Research Alliance (ESRA)	*2023–Present*
DOE VTO program - Advanced Battery Materials Research (BMR)	*2021–Present*
UCB MSE Corrosion Award	*2025–Present*
Sam Zerfoss Memorial Scholarship	*2019–2021*
Matthew J. Wilson Honors Scholarship	*2020–2021*
The Sobota Family Scholarship	*2020*
Edward S. Sproles, Jr. Scholarship Fund	*2020*
John and Elizabeth Holmes Teas 18–19 Merit Scholarship Fund	*2019*
Virginia S. and Phillip L. Walker, Jr. Scholarship	*2018*

PRESENTATIONS AND PUBLICATIONS

Google Scholar — ORCID: 0000-0001-5482-509X

1. Machine Learning-Aided Prediction of Na Solid-State Interfaces **Li, B.**, Jeon, H., Persson, K.A. *In preparation.*
2. The Role of Machine Learning Interatomic Potentials in Developing the Next Generation of Solid-State Batteries Phuthi, M.K., Wei, G., **Li, B.**, Majumdar, S., Kolluru, V.S.C., Kumar, N., Blau, S., Canepa, P., Chan, M.K.Y., Gomez-Bombarelli, R., Persson, K.A., Ceder, G., Ong, S.P. *In preparation.*
3. Towards an Atomistic Understanding of Solid-State Reaction Interfaces Using Machine-Learned Interatomic Potentials **Li, B.**, Karan, V., Persson, K.A. *arXiv*, (2025) DOI: arxiv.2511.20976.
4. An Atomistic Study of Reactivity in Solid State Electrolyte Interphase Formation for $Li/Li_7P_3S_{11}$ **Li, B.**, Karan, V., Kaplan, A.D., Wen, M., Persson, K.A. *The Journal of Physical Chemistry C*, Accepted (2025). DOI: 10.1021/acs.jpcc.5c03589.
5. Machine Learning Aided Atomistic Modeling of Solid State Electrolyte Interphase Formation for $Li/Li_7P_3S_{11}$ **Li, B.**, Persson, K. *AI4X 2025 International Conference* (2025). [Oral Presentation] Presentation Link
6. An Atomistic Study of Reactivity in Solid State Electrolyte Interphase Formation for $Li/Li_7P_3S_{11}$ Systems **Li, B.**, Karan, V., Kaplan, A., Persson, K. *Materials Research Society (MRS) Spring Meeting*, Seattle, WA, April 2025. [Oral Presentation] Presentation Link
7. Atomate2: Modular Workflows for Materials Science Ganose, A.M., Sahasrabuddhe, H., Asta, M., Beck, K., Biswas, T., Bonkowski, A., . . . , **Li, B.**, . . . , Jain, A. *Digital Discovery*, **4**(7), 1944–1973 (2025). DOI: 10.1039/D5DD00019J
8. A Cellular Automaton Simulation for Predicting Phase Evolution in Solid-State Reactions Gallant, M.C., McDermott, M.J., **Li, B.**, Persson, K.A. *Chemistry of Materials*, **37**(1), 210–223 (2024). DOI: 10.1021/acs.chemmater.4c02301
9. Quantifying Multipoint Ordering in Alloys Goff, J., **B. Li**, Sinnott, S., Dabo, I., *Physical Review B* **104**, 054109 (2021). DOI: 10.1103/PhysRevB.104.054109
10. Awaruite and Tetrataenite Driven NH_3 Synthesis **Li, B.**, Lemke, K. *American Geophysical Union (AGU) Fall Meeting*, 2015, Abstract ID: ED41A-0827. [Poster Presentation] Abstract Link