BRYANT Y. LI

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EDUCATION

University of California, Berkeley *Berkeley, CA*
Ph.D. Materials Science and Engineering
Advisor: Prof. Kristin A. Persson

University of California, Berkeley, *3.80 GPA* *Berkeley, CA*
M.S. Materials Science and Engineering
Graduate Certificate – Applied Data Science

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

RESEARCH EXPERIENCE

Graduate Student Researcher, Persson Group *Aug 2021 – Present*
Lawrence Berkeley National Laboratory / University of California, Berkeley

- **AI/ML Algorithm Development:** Developed and benchmarked machine-learned interatomic potentials (MACE, ACE, NequIP, M3GNet, CHGNet, DeepMD-kit) for reactive disordered systems. Identified that ACE-based descriptors outperform spherical-harmonic architectures for amorphous morphology prediction, achieving 100× faster inference on CPUs while maintaining accuracy for million-atom simulations. Modeled inorganic and organic in amorphous/disordered systems via MLIP-MD.
- **Interface & Surface Reaction Modeling:** Discovered a 4-layer heterogeneous solid-electrolyte interphase (SEI) morphology—Li_xP | nanocrystalline Li_2S (∼2nm) | disordered Li_xP-Li_2S | amorphous electrolyte—invisible to in-situ XPS/SEM characterization. Explained passivation mechanisms via electronic bandgap analysis: Li_2S acts as insulating barrier while Li_xP phases are semiconducting (1.1–1.8 eV). Distinguished SEI (passivating) from mixed-conductor interphase (MCI) based on Na_xP percolation pathways (0.4–1.0 eV, conductive) driven by correlated Na-P ionic mobility.
- **Million-Atom Reactive Simulations:** Executed 1-million-atom, 10-nanosecond reactive interface simulations using bespoke ACE potentials—equivalent to millions of CPU-hours of AIMD compute time—to characterize SEI vs. MCI formation kinetics and validate against experimental benchmarks (XPS, SEM, EIS).
- **Simulation Platform Development (MPMorph):** Architected core MPMorph module in `atomate2` for automated melt-quench molecular dynamics, enabling simulation of amorphous and disordered morphologies applicable to organic thin-film and molecular systems. Integrated Packmol backend for molecular packing with short-range order and long-range disorder. Adopted by 50+ researchers across NERSC matgen allocation; maintained with 90% unit test coverage and CI/CD practices.
- **Active Learning Framework:** Developed active learning pipeline combining structural generation (MPMorph + polyhedra-based selection) with MaxVol and DIRECT sampling strategies. Outperformed generative models (MatterGen, ChgGEN) for discovering interface reactivity intermediates, amorphous configurations, and solid-state crystallization pathways.

- **High-Throughput Data Analytics:** Designed and managed scalable data pipelines across 3 MongoDB databases (50k+ entries each), implementing strategic metadata tagging and UUID-workflow integration for optimized query operations. Contributed 15k entries to the Materials Project R2SCAN database (public release v2025.09.25), now integrated into phase diagram, interface reaction, and Pourbaix diagram applications.
- **HPC Workflow Engineering:** Lead developer of modular DFT/MLIP workflows on `atomate2` for GPU-accelerated HPCs (NERSC Perlmutter, NREL Kestrel). Compiled Kokkos-enabled LAMMPS adaptable to MACE, GRACE, and ACE potentials; deployed as group-wide software for 50+ collaborators. Integrated CUDA-enabled parallelization for electronic structure calculations.
- **Technical Leadership:** Lead group representative for DOE BMR and ESRA consortiums; present quarterly progress to multi-institutional teams and author quarterly reports. Mentored 5+ PhD students and postdocs across 5 consortiums (ESRA, BMR, LiSA, Materials Project, Volkswagen) on MLIP development, training procedures, and deployment best practices.

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

- **Surface & Interface Simulation:** Executed 1000+ DFT calculations using Quantum ESPRESSO in vacuum and implicit solvent environments to model surface adsorption sites and charge transfer kinetics for Pt–Pd nanoparticle electrocatalysts (HER/ORR applications), funded by the U.S. Department of Energy.
- **Multiscale Modeling:** Developed cluster basis sets with ICET for cluster expansion fitting; performed grand canonical and canonical Monte Carlo simulations (MCHammer) to predict surface morphology and phase stability. Introduced cluster order parameters to quantify multipoint ordering effects on Pd clustering and nanocage formation.
- **Workflow Automation:** Designed Python scripts for automated data extraction, processing, and management from large-scale simulation datasets, establishing reusable framework for high-throughput catalyst screening.
- **Publication:** First-author contribution demonstrating thermodynamic favorability of Pd channel formation on Pt-Pd surfaces, enabling chemical leaching strategies for hollow nanocage synthesis. Published in *Physical Review B*.

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 investigate prebiotic nitrogen fixation and 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 findings at the 2017 American Geophysical Union Fall Meeting.

TECHNICAL SKILLS

AI/ML & Algorithm Development: PyTorch, TensorFlow, JAX; Machine-Learned Interatomic Potentials (MACE, ACE, GRACE, NequIP, Allegro, M3GNet, CHGNet, DeepMD-kit); Active Learning (MaxVol, DIRECT); Model Benchmarking (EOS, RDF, diffusivity metrics); GPU/CPU Deployment.

Atomistic Simulation & Electronic Structure: Density Functional Theory (VASP, Quantum ESPRESSO, PBEsol, r2SCAN), *Ab initio* Molecular Dynamics (AIMD), Classical Molecular Dynamics (LAMMPS), Bandstructure & Electronic Structure Calculations, Interface Reactivity Modeling, Amorphous/Disordered Morphology Simulation.

Software Engineering: Python, `atomate2/pymatgen` (core contributor), Git/GitHub, Unit Testing (90% coverage), Code Review & PR Management, Kokkos-enabled LAMMPS Compilation, Docker; AI-Assisted Development (Claude Code, Cursor, Roo).

Data Analytics & High-Performance Computing: MongoDB (150k+ entries across 3 databases), Pandas, NumPy, SciPy, Metadata Schema Design, Query Optimization; SLURM, NERSC Perlmutter, NREL Kestrel; CUDA/Kokkos Parallelization.

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

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

HONORS, AWARDS, AND RESEARCH GRANTS

UCB MSE Corrosion Award *2025–2026*
Awarded for developing a novel machine learning and active learning framework to study reactive surface reconstruction and passivation films.

DOE Energy Storage Research Alliance (ESRA) *2023–Present*

DOE Advanced Battery Materials Research (BMR) Program *2021–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*

PUBLICATIONS AND PRESENTATIONS

Google Scholar — ORCID: 0000-0001-5482-509X — **63 citations, h-index: 3**

1. **Li, B.**, Jeon, H., Persson, K.A. Machine Learning-Aided Prediction of Na Solid-State Interfaces. *In preparation.*
2. 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. The Role of Machine Learning Interatomic Potentials in Developing the Next Generation of Solid-State Batteries. *In preparation.*
3. **Li, B.**, Karan, V., Persson, K.A. Towards an Atomistic Understanding of Solid-State Reaction Interfaces Using Machine-Learned Interatomic Potentials. *arXiv* (2025). DOI: arxiv.2511.20976.
4. **Li, B.**, Karan, V., Kaplan, A.D., Wen, M., Persson, K.A. An Atomistic Study of Reactivity in Solid State Electrolyte Interphase Formation for $Li/Li_7P_3S_{11}$. *The Journal of Physical Chemistry C*, Accepted (2025). DOI: 10.1021/acs.jpcc.5c03589.
5. **Li, B.**, Persson, K. Machine Learning Aided Atomistic Modeling of Solid State Electrolyte Interphase Formation for $Li/Li_7P_3S_{11}$. *AI4X 2025 International Conference* (2025). [Oral Presentation] Link.
6. **Li, B.**, Karan, V., Kaplan, A., Persson, K. An Atomistic Study of Reactivity in Solid State Electrolyte Interphase Formation for $Li/Li_7P_3S_{11}$ Systems. *Materials Research Society (MRS) Spring Meeting*, Seattle, WA, April 2025. [Oral Presentation] Link.
7. Ganose, A.M., Sahasrabuddhe, H., Asta, M., Beck, K., Biswas, T., Bonkowski, A., . . . , **Li, B.**, . . . , Jain, A. Atomate2: Modular Workflows for Materials Science. *Digital Discovery*, **4**(7), 1944–1973 (2025). **49 citations.** DOI: 10.1039/D5DD00019J.

8. Gallant, M.C., McDermott, M.J., **Li, B.**, Persson, K.A. A Cellular Automaton Simulation for Predicting Phase Evolution in Solid-State Reactions. *Chemistry of Materials*, **37**(1), 210–223 (2024). DOI: 10.1021/acs.chemmater.4c02301.

9. Goff, J., **Li, B.**, Sinnott, S., Dabo, I. Quantifying Multipoint Ordering in Alloys. *Physical Review B* **104**, 054109 (2021). DOI: 10.1103/PhysRevB.104.054109.

10. **Li, B.**, Lemke, K. Awaruite and Tetrataenite Driven NH_3 Synthesis. *American Geophysical Union (AGU) Fall Meeting*, 2017, Abstract ID: ED41A-0827. [Poster Presentation] Link.

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 (11 hours/week) in Calculus I–III, Ordinary and Partial Differential Equations, and Linear Algebra.
- Adapted teaching methods to diverse learning styles; facilitated collaborative problem-solving sessions.

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

- Led undergraduate laboratory sessions on materials characterization: optical microscopy, SEM, EDX, and XRD.
- Provided constructive feedback on technical writing and data analysis in lab reports.