BRYANT Y. LI

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EDUCATION

The University of California, Berkeley, *Ongoing* — *August 2021 - May 2026 (Expected)*
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*
Lawrence Berkeley National Laboratory / University of California, Berkeley, CA

- **AI/Machine Learning:** Expert in atomic cluster expansion based descriptors and graph-based machine learning interatomic potentials (PACE, MACE, M3GNet, CHGNet). Specialized in developing reactive MLIPs for bespoke chemical systems and distilling foundational models for targeted applications in solid-state batteries.
- **High-throughput Workflow Developer:** Developer of modular DFT/MLIP workflows on the 'atomate2' codebase for NVIDIA GPU-accelerated HPCs (Perlmutter, Kestrel). Engineered scalable data pipelines with MongoDB and parallelization features using CUDA and Kokkos-enabled LAMMPs.
- **Software Engineering & Impact:** Architected core "MPMorph" modules for 'atomate2' that solved a previously intractable recursive MD simulation challenge, creating a new capability now adopted by 5+ researchers. Developed using best practices including version control (Git), code review, and unit testing (90% coverage).
- **Solid State Batteries:** Specialist in interfacial stability of Li/Na metal anode batteries, modeling solid-electrolyte interphase (SEI) formation and degradation mechanisms. Validated atomistic modeling and reaction pathway predictions against in-situ SEM, XPS, and EIS experimental data.
- **Team Leadership:** Coordinate the group's AI/ML subgroup for collaborative research and training. Manage NREL compute resources for the DOE BMR program and serve as the group's lead representative in the DOE ESRA consortium.

Computational Electrocatalysis Researcher @ Dabo Group — *Sept 2018 – May 2021*
Pennsylvania State University, University Park, PA

- Modeled the thermodynamic stability and reaction pathways of Pt–Pd nanoparticle electrocatalysts for electrochemical energy conversion systems (e.g., fuel cells). The fundamental methods are directly applicable to catalyst design for water electrolysis (OER/HER).
- Employed a multiscale modeling approach, using DFT (Quantum ESPRESSO) to determine surface energies and Cluster Expansion (ICET) with Monte Carlo simulations to predict nanoparticle phase stability under reaction conditions.

- Analyzed the viability of core-shell nanoparticle structures to enhance catalytic activity and durability, a key challenge in designing next-generation electrolyzer catalysts.
- Developed automated Python workflows to manage and process large-scale simulation data, establishing a reusable framework for high-throughput catalyst screening.

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.

TECHNICAL SKILLS

High-Throughput Computing: VASP, LAMMPS, Quantum ESPRESSO, Atomate2, FireWorks, Pymatgen, ASE, ICET.
Machine Learning & Data Science: PyTorch, TensorFlow, M3GNet, CHGNet, MACE, NequIP, python-ACE, Scikit-learn, Pandas, NumPy.
Software & DevOps: Python, Git/GitHub, MongoDB, Docker, SLURM, CLI, LaTeX, MATLAB, OVITO Pro.
Materials Characterization: SEM, EDX, XRD, Optical Microscopy.
Languages: English (fluent), Mandarin (fluent), Cantonese (fluent).

HONORS & AWARDS

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, setting new benchmarks in computational corrosion analysis.
DOE Energy Storage Research Alliance (ESRA) *2023–Present*
DOE Advanced Battery Materials Research (BMR) Program *2021–Present*

PRESENTATIONS AND PUBLICATIONS

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.
   Introduced a novel computational framework using high-throughput DFT and MLIPs to simulate

kinetic growth mechanisms of the SEI at the $Li/Li_7P_3S_{11}$ interface, predicting stable products and dynamics.

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., . . . , **Li, B.**, . . . , Jain, A.
   Digital Discovery, **4**(7), 1944–1973 (2025). DOI: 10.1039/D5DD00019J.
   Introduced Atomate2, an enhanced, modular framework for high-throughput DFT calculations that supports multiple electronic structure packages and promotes interoperability to accelerate materials screening.

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.
   Developed a cellular automaton simulation framework to predict phase evolution in solid-state reactions, optimizing synthesis recipes based on precursor choice and reaction conditions.

9. Quantifying Multipoint Ordering in Alloys
   Goff, J., **Li, B.**, Sinnott, S., Dabo, I.
   Physical Review B **104**, 054109 (2021). DOI: 10.1103/PhysRevB.104.054109.
   Introduced cluster order parameters to systematically quantify multipoint ordering in multicomponent lattice systems, elucidating the impact of four-point chemical ordering on Pt-Pd nanocage stability.

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