# 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*

- Investigating the interfacial stability of lithium (Li) and sodium (Na) metal anodes in solid-state batteries, focusing on decomposition mechanisms, dendritic growth, and solid-electrolyte interphase (SEI) formation using a combination of Density Functional Theory (DFT), Machine Learning (ML), and Molecular Dynamics (MD).
- Developing and engineering Machine-Learned Interatomic Potentials (MLIPs) by designing validation metrics, generating first-principles datasets, and implementing active learning to enhance model accuracy, stability, and scalability for complex systems, including interfacial reactivity and correlated transport phenomena.
- Designing and deploying high-throughput DFT and MD workflows on High-Performance Computing (HPC) infrastructures to optimize data curation and scalability for ML applications, including the development of MLIPs and foundation models in collaboration with the Materials Project.
- Managing and organizing large-scale DFT and MD data (simulations up to millions of atoms over nanoseconds) via MongoDB across multiple HPC infrastructures; processing extensive datasets to evaluate transport, reactivity, and morphological changes.
- Leading the group's Machine Learning subgroup to coordinate collaborative development and training efforts. Managing NREL compute resources for the DOE BMR program and representing the group in the DOE ESRA consortium.

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

- Investigated Pd channel formation in Pt–Pd nanoparticle electrocatalysts for fuel cell applications using multiscale simulation techniques (DFT, CE, Monte Carlo), funded by the U.S. Department of Energy.
- Performed over 700 DFT calculations using Quantum ESPRESSO in vacuum and solvent environments to determine cluster energies for Pt–Pd surfaces, analyzing the viability of core-shell nanoparticle structures.

- Built cluster basis sets with the ICET software for cluster expansion fitting and conducted grand canonical and canonical Monte Carlo simulations to model nanoparticle thermodynamics.
- Developed Python scripts for automated data extraction, processing, and management from large-scale simulation datasets, improving data processing efficiency.

**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.

## EDUCATION 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.

**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, including optical microscopy, SEM, EDX, and XRD.
- Assisted in grading lab reports and providing constructive feedback to improve technical writing and data analysis skills.

## TECHNICAL SKILLS

**High-Throughput Computing & Workflows:** VASP, LAMMPS, Quantum ESPRESSO, Atomate2, FireWorks, Jobflow, Pymatgen, ASE, Custodian, ICET.

**Machine Learning & Data Science:** M3GNet, CHGNet, MACE, NequIP, DeepMD-kit, pythonACE (PaceMaker/GraceMaker), TensorFlow, PyTorch, Scikit-learn, Pandas, NumPy, SciPy.

**Programming & Software:** Python, MATLAB, LaTeX, Command-Line Interface (CLI), Git/GitHub, MongoDB, Docker, SLURM, VESTA, OVITO Pro.

**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** *2025–2026*
*Awarded for developing a machine learning framework to study reactive surface reconstruction and passivation films. The active learning framework enhances computational analysis of non-equilibrium*

*surface dynamics, providing insights into corrosion resistance and setting new benchmarks in materials and corrosion studies.*

**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

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