Bryant Y. Li

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Experience

- **Lawrence Berkeley National Laboratory / University of California, Berkeley** — Berkeley, California
  Computational Materials Scientist / Graduate Student Researcher @ Persson Group — *Aug 2021 - Present*
  - **High-throughput Workflow Developer**: Developed and optimized high-throughput DFT and MD workflows on High-Performance Computing (HPC) platforms, engineering scalable data pipelines with MongoDB for large-scale materials informatics and AI/ML applications.
  - **Machine Learning Interatomic Potential Specialists**: Engineered and validated machine learning interatomic potentials (MLIPs) using first-principles data and active learning, optimizing model accuracy and efficiency for simulating complex phenomena like interfacial reactivity and correlated transport in battery systems.
  - **Data Engineering and Scientific Methodologies**: Applied advanced data science techniques and Python libraries to analyze large-scale simulation data (up to 1M atoms), deriving scientific insights by integrating DFT, MD, Neural Networks, and Monte Carlo methods with experimental validation.
- **PSU Materials Research Institute, Millennium Science Complex** — University Park, Pennsylvania
  Computational Materials Researcher @ Dabo Group — *Oct 2019 - May 2021*
  - **Multiscale Simulation Engineer**: Conducted multiscale simulations for a U.S. DOE-funded project on fuel cell electrocatalysts, performing thousands of surface DFT calculations to investigate nanoparticle surface phenomena
  - **Data Management**: Developed Python scripts to automate data management and analysis pipelines for Cluster Expansion (CE) and Monte Carlo simulations, designed for research efficiency.

Education

- **The University of California, Berkeley (UCB)** — Berkeley, California
  Ph.D. & M.S. *- Materials Science and Engineering; Applied Data Science GPA: 3.8* — *Aug. 2021 – May. 2026*
- **The Pennsylvania State University (PSU)** — University Park, Pennsylvania
  B.S. *- Materials Science and Engineering; Minor in Applied Mathematics; GPA: 3.89* — *Aug. 2018 – May. 2021*

Skills

- **High Throughput Workflow Stack:** VASP, LAMMPs, atomate2, fireworks, pymatgen, ASE, jobflow, custodian, mp-api, Quantum ESPRESSO, ICET
- **Python/Data Science Stack:** Pandas, NumPy, SciPy, Matplotlib, scikit-learn, TensorFlow, PyTorch, MongoDB
- **MLIP Stack:** python-ACE, GRACE, MACE, NequIP, QET, M3GNET, CHGNet, DeepMD-kit
- **Software:** Git, Anaconda, Docker, Jupyter Notebooks, Visual Studio Code, MATLAB, Ovito, VESTA, Robo3T, SLURM

Selected Publications

- **Li, B.,** et al. **(2025).** ***An Atomistic Study of Reactivity in Solid-State Electrolyte Interphase....*** **The Journal of Physical Chemistry C**: Led the development of a DFT and MLIP computational framework to successfully predict thermodynamically stable products and reaction dynamics at the $Li/Li_7P_3S_{11}$ solid-state battery interface.
- Ganose, A.M., . . . , **Li, B.**, . . . , et al. **(2025).** ***Atomate2: Modular Workflows for Materials Science.*** **Digital Discovery**: Contributed to the development of atomate2, a next-generation high-throughput computational framework designed to accelerate materials screening and the generation of large-scale property databases for materials informatics.
- Gallant, M.C., . . . , **Li, B.**, et al. **(2025).** ***A Cellular Automaton Simulation for Predicting Phase Evolution....*** **Chemistry of Materials**: Co-developed a novel cellular automaton simulation to predict phase evolution in solid-state reactions, validating the model against experimental synthesis of complex oxides to optimize reaction conditions.
- Goff, J., **Li, B.**, et al. **(2021).** ***Quantifying Multipoint Ordering in Alloys.*** **Physical Review B**: Introduced a method using cluster order parameters to quantify complex chemical ordering in multicomponent alloys, explaining its critical impact on the stability of Pt/Pd nanoparticle electrocatalysts.

Leadership & Project Management

- **Program Management**: Served as lead project manager for the Persson group's DOE Advanced Battery Materials Research (BMR) program, responsible for directing research progress, authoring quarterly stakeholder reports, and managing NRL High-Performance Computing resources.
- **Consortium Representation**: Represented the research group in the multi-institution DOE Energy Storage Research Alliance (ESRA), aligning group strategy with consortium goals for AI/ML applications in sodium and zinc battery systems.
- **Technical Leadership**: Directed the Machine Learning subgroup, leading weekly meetings to coordinate collaborative code development, architect shared computational workflows, and ensure communication across multiple battery research projects.