Bryant Y. Li
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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*

Experience

- **Lawrence Berkeley National Laboratory @ Persson Group** — Berkeley, California
  Computational Materials Scientist / Graduate Student Researcher — *Aug 2021 - Present*
  - **AI/Machine Learning**: Expert in atomic cluster expansion based feature descriptors, linear/graph-based machine learning interatomic potentials (PACE, MACE, GRACE), with practical experience using equivariant-feature models GNNs (NequIP, Allegro, M3GNET, CHGNet, QET) for MLMD simulations. Specialized in reactive MLIPs for bespoke chemical systems, with practical knowledge in distilling foundational models.
  - **High-throughput Workflow Developer for HPCs**: Developer and maintainer of high-throughput scientific workflows on 'atomate2' codebase for NVIDIA GPU HPCs (Perlmutter, Kestrel). Developed modular library for DFT/MLIP workflows for modeling amorphous/disordered materials, with design features for CUDA enabled parallelization for DFT and Kokkos enabled MLIP-LAMMPs.
  - ***ab initio* Framework**: Architect for DFT datasets encapsulating relevant scientific investigations (surfaces/interfaces, reactivity, phase disordering) intended for bespoke MLIPs, with pipelines involving inverse design from Materials Project, MaxVol-based active learning strategies, experimental validation metric design.
  - **Solid State Batteries**: Specialist in interfacial stability of Li/Na metal anode solid-state batteries, focusing on solid-electrolyte interphase (SEI) formation and morphological characterization of solid-state reactivity via atomistic modeling and reaction pathway prediction, validated against in situ SEM, XPS, EIS experimental data.
  - **Team Responsibilities**: Coordinator of group's AI/ML subgroup for collaborative research and training efforts. Managed NREL compute resources for DOE BMR program and lead representative in the ESRA consortium.
  - **Software Roles**: Architected core "MPMorph" modules on 'atomate2' that solved a previously impossible recursive MD simulation challenge, creating a new capability now adopted by 5+ researchers. Developed using software practices including version control, code review, and unit testing (90% coverage) to stablize performance.
- **PSU Materials Research Institute @ Dabo Group** — University Park, Pennsylvania
  Computational Materials Researcher — *Oct 2019 - May 2021*
  - **Multiscale Simulation Engineer**: Executed over 1000 DFT calculations using Quantum ESPRESSO in vacuum and solvent environments for cluster energies for Pt–Pd surfaces. Developed cluster basis sets with ICET for cluster expansion fitting and performed grand canonical and canonical Monte Carlo simulations. Designed Python scripts for the automation of data extraction, processing, and management from extensive simulation datasets.
  - **Scientific Project**: Investigated Pd channel formation in Pt–Pd nanoparticle electrocatalysts for fuel cell applications, funded by the U.S. Department of Energy.

Selected Publications & Presentations

- **Li, B.,** Karan, V., Kaplan, A.D., Persson, K.A. **(2025).** ***An Atomistic Study of Reactivity in Solid-State Electrolyte Interphase...***: **The Journal of Physical Chemistry C**
- Ganose, A.M., . . . , **Li, B.**, . . . , et al. **(2025).** ***Atomate2: Modular Workflows...***: **Digital Discovery**
- Gallant, M.C., . . . , **Li, B.**, . . . , et al. **(2025).** ***A Cellular Automaton Simulation...***: **Chemistry of Materials**
- **Invited Talks**: AI4X Singapore 2025, MRS Seattle Spring 2025; **Awards**: MSE Dept. Corrosion Award (FY25-26)

Skills

- **High Throughput Workflow Stack:** VASP, LAMMPs, atomate2, fireworks, pymatgen, ASE, jobflow, custodian, mp-api, Quantum ESPRESSO, ICET, PySCF, emmet, Q-Chem, MatBench Discovery, MatterGen
- **Python/Data Science Stack:** PyTorch, TensorFlow, Pandas, NumPy, SciPy, Matplotlib, scikit-learn
- **Software:** Git, Anaconda, Jupyter Notebooks, SLURM, Visual Studio Code, MongoDB, MATLAB, Ovito, VESTA, Robo3T, Docker, uv