

# Bryant Y. Li

LinkedIn, Google Scholar, Github

Email : bryantli@lbl.gov /bryant.li@berkeley.edu

Mobile : 2018513233

## SUMMARY

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*Ph.D. level AI/ML Research Engineer with 5+ years of experience architecting and deploying novel machine learning models for complex scientific problems on high-performance computing (HPC) systems. Expertise in Graph Neural Networks (GNNs), equivariant models, and foundation model distillation. Proven leader in guiding research initiatives, mentoring teams, and implementing robust, scalable software solutions with a focus on end-to-end model development, from data generation and active learning to deployment and validation.*

## EDUCATION

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

## EXPERIENCE

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- **Lawrence Berkeley National Laboratory** Berkeley, California  
*AI/ML Research Engineer / Graduate Student Researcher* Aug 2021 - Present
  - **AI/ML Model Development:** Architected and trained novel physics-informed machine learning models, including equivariant Graph Neural Networks (GNNs) and transformer-based architectures (e.g., NequIP, MACE), to simulate complex reactive systems. Specialized in fine-tuning and distilling large-scale foundational models for domain-specific applications.
  - **HPC Workflow Engineering:** Developed and maintained scalable, high-throughput scientific ML workflows for large-scale NVIDIA GPU-based HPCs (Perlmutter). Engineered a modular library for parallelized model training and inference, leveraging CUDA and Kokkos to optimize performance on distributed systems.
  - **Software Architecture & Best Practices:** Architected and delivered core modules for the ‘atomate2’ workflow library that solved a critical recursive simulation challenge, enabling new research capabilities now adopted by multiple teams. Championed software engineering best practices, including version control (Git), rigorous code review, and CI/CD, achieving over 90% unit test coverage.
  - **Active Learning & Data Generation:** Designed and implemented a novel framework for generating high-quality training datasets, incorporating inverse design principles and MaxVol-based active learning strategies. Developed robust metrics to validate model predictions against real-world experimental data (SEM, XPS, EIS).
  - **Leadership & Collaboration:** Led the AI/ML research subgroup, coordinating collaborative projects and mentoring junior researchers on advanced machine learning techniques. Managed HPC resource allocation for a multi-institutional Department of Energy program.
- **Pennsylvania State University, Materials Research Institute** University Park, Pennsylvania  
*Computational Researcher* Oct 2019 - May 2021
  - **Scientific Computing Automation:** Developed Python scripts to automate data extraction, processing, and management for over 1000 large-scale quantum mechanics (DFT) and Monte Carlo simulations. Built cluster expansion models to analyze thermodynamic properties of complex alloy systems.

## SELECTED PUBLICATIONS & PRESENTATIONS

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- **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

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- **AI/ML & Data Science:** PyTorch, TensorFlow, scikit-learn, Pandas, NumPy, SciPy, Matplotlib
- **HPC & Scientific Computing:** Python, LAMMPS, atomate2, pymatgen, ASE, fireworks, jobflow, SLURM, CUDA
- **Software & Tools:** Git, Docker, MongoDB, Anaconda, Jupyter Notebooks, Visual Studio Code, CI/CD