

Aoyan Liang

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EDUCATION

University of Southern California	Los Angeles, CA
Ph.D. in Materials Science, GPA: 4.0/4.0	8/2020-12/2025
<i>Dissertation Title: Computational Insights into Processing-Structure-Property Relationships in Complex Nanoscale Materials</i>	
<ul style="list-style-type: none"> Awards: Nanohub AI4science challenge 2nd Prize (2025); MFD Presentations Award (2024) 	
M.S. in Computer Science (Data Science), GPA: 4.0/4.0	1/2022-5/2024
M.S. in Materials Science, GPA: 4.0/4.0	8/2018-5/2020
<ul style="list-style-type: none"> Awards: Master's Student Achievement Award (2020) 	
Southwest Jiaotong University	Chengdu, China
B.Eng. in Materials Science and Engineering, GPA: 3.64/4.0	9/2014-6/2018
<ul style="list-style-type: none"> Awards: Outstanding Graduate (2018); China National Scholarship (Top 1%, 2017); Grand Comprehensive Scholarship (2017); First-Class Comprehensive Scholarship (4x, 2014-16) 	

PROFESSIONAL EXPERIENCE

Seagate Technology	Fremont, CA
<i>Senior Engineer</i>	01/2026-Present
<ul style="list-style-type: none"> Develop and apply computational simulations to support HAMR media design, analyzing grain formation, composition, and processing conditions to inform R&D strategies. Optimize modeling parameters and troubleshoot simulation workflows, improving predictive accuracy and enabling more efficient development of advanced materials and processes. 	
<i>Research Engineering Intern</i>	05/2025-08/2025
<ul style="list-style-type: none"> Developed and performed MD (Molecular Dynamics) and MC (Monte Carlo) simulations, providing key insights into ordering behavior that guided material design strategies and informed experiments for high-performance HAMR thin film. Applied ML (Machine Learning) interatomic potentials (M3GNet & CHGNet) for high-throughput dopant screening, identifying candidates that accelerate ordering kinetics and stabilize grain boundaries, accelerating materials discovery and enabling targeted experimental validation. 	
Lawrence Livermore National Laboratory	Livermore, CA
<i>Computational Research Intern</i>	06/2024-08/2024
<ul style="list-style-type: none"> Generated and analyzed large-scale MD simulation datasets by modifying interatomic potentials to study alloy strengthening mechanisms, isolating the effects of size and stiffness mismatches. Optimized data workflows and on-the-fly analyses to process massive outputs efficiently on HPC systems, improving scalability and enabling faster insight generation. 	
University of Southern California	Los Angeles, CA
<i>Graduate Research Assistant</i>	8/2020-12/2025

- Developed an energy-sampling framework for rare-event activation processes in metallic glasses, combining statistical mechanics with ML interatomic potentials (NequIP, Allegro) to map free-energy landscapes and characterize glass–glass interfaces.
- Integrated DFT, MD, and ML workflows to optimize alloy thin-film nanostructures, analyzing defect energetics, deposition mechanisms, and composition–processing–structure relationships to guide experimental design.
- Partnered with experimental teams to translate computational results into testable hypotheses that guide real-world materials design and validation.

SKILLS

- **Programming:** Python, Fortran (MPI), Bash, C/C++ (MPI/OpenMP), SQL, R
- **Simulation:** VASP, LAMMPS, ASE, Pymatgen, DFT, MD, MC, DPD
- **Machine Learning:** PyTorch, TensorFlow, Scikit-learn, Hugging Face, Weights & Biases, Optuna, XGBoost, LightGBM, NLP, LLMs
- **Data Analysis & Visualization:** Pandas, NumPy, Matplotlib, Plotly, Seaborn, Jupyter
- **Tools & Platforms:** Git, Linux, HPC (High Performance Computing), MPI/OpenMP

CERTIFICATIONS

- Natural Language Processing Specialization** (DeepLearning.AI) 11/2024
- Built summarization and multilingual QA models using Hugging Face Transformers, including fine-tuning BERT on TyDiQA to improve cross-lingual performance.
- AI for Science on Supercomputers** (Argonne National Laboratory) 12/2022
- Applied distributed training and HPC workflows (MPI, GPU acceleration) to scale neural networks across supercomputers, gaining hands-on experience in deploying AI at scientific scale.
- Fundamentals of Deep Learning** (NVIDIA) 6/2021
- Accelerated data science workflows using GPU-optimized libraries (CuPy, RAPIDS cuDF, Numba), achieving significant speedups in array computations and large-scale data processing

ADDITIONAL EXPERIENCE

- **Teaching Assistant:** Supported 5 USC courses including Deep Learning, Atomistic Simulation, Thermodynamics, Materials Science Labs (2021–24).
- **Conference Presentations:** Delivered 8 oral and poster presentations at international conferences (TMS, MRS).
- **Peer Reviewer:** Completed 85 reviews across 20 international journals, including *Acta Materialia*, *Computational Materials Science*, and *Computer Physics Communications*.

PUBLICATIONS

[ORCID](#) · [Google Scholar Profile](#) · [Web of Science Profile](#)

2026

1. **Liang, A.**, Gurniak, E. J., & Branicio, P. S. (2026) From surface segregation to glass-glass interfaces: composition, activation-energy landscapes and strength in CuZr nanoglasses (*Under review*)
2. Yazdani, M. H., **Liang, A.**, Otero, A. J. M., Liu, Y., Farkas, D., Hodge, A. M., Rupert, T. J., Beyerlein, I. J., & Branicio, P. S. (2026) Composition-driven nanotwin engineering in sputtered

Ni-Fe and Ni-Cr films: linking fault energetics to twin thickness. *Acta Materialia*, 306, 121890.

2025

3. **Liang, A.**, Zhou, X., Aubry, S., Bertin, N., & Bulatov, V. V. (2025) Computational alchemy clarifies origins of alloy strengthening. *npj Computational Materials*.
4. Bulatov, V. V., Bertin, N., Aubry, S., Zepeda-Ruiz, L. A., Zhou, X., **Liang, A.**, Ooppelstrup, T., & Sadig, B. (2025) Network aspects of single crystal plasticity. *Journal of Materials Research and Technology*, 36, 5611.
5. Carvalho, A. P., **Liang, A.**, Kawasaki, Cupertino-Malheiros, L., Branicio, P. S., & Figueiredo, R. B. (2025) Dynamic recovery as a strengthening mechanism in nanostructured metals. *Journal of Materials Research and Technology*, 35, 754.

2024

6. **Liang, A.**, Liu, C., & Branicio, P. S. (2024). Colloid Transport in Bicontinuous Nanoporous Media. *Langmuir*, 40(21), 10868.
7. Alwen, A., **Liang, A.**, Branicio, P. S., & Hodge, A. M. (2024). Combinatorial and high-throughput investigation of growth nanotwin formation. *Acta Materialia*, 270, 119839.

2023

8. Yuan, S., **Liang, A.**, Liu, C., Tian, L., Mousseau, N., & Branicio, P. S. (2023). The effect of heat treatment paths on the aging and rejuvenation of metallic glasses. *Physical Review Materials*, 7(12), 123603.
9. Yuan, S., **Liang, A.**, Liu, C., Nakano, A., Nomura, K., & Branicio, P. S. (2023). Uncovering hidden vacancy-like motifs in metallic glasses with machine learning. *Materials & Design*, 233, 112185.
10. **Liang, A.**, Goodelman, D. C., Hodge, A. M., Farkas, D., & Branicio, P. S. (2023). CoFeNiTi_x and CrFeNiTi_x high entropy alloy thin films microstructure formation. *Acta Materialia*, 257, 119163.

2022

11. Guan, X., **Liang, A.**, & Branicio, P. S. (2022). High pressure shear induced microstructural evolution in nanocrystalline aluminum. *Computational Materials Science*, 203(15), 111105.

2021

12. **Liang, A.**, Liu, C., & Branicio, P. S. (2021). Hot-press sintering of aluminum nitride nanoceramics. *Physical Review Materials*, 5(9), 096001.

2018

13. **Liang, A.**, Jiang, X., Hong, X., Jiang, Y., Shao, Z., & Zhu, D. (2018). Recent developments concerning the dispersion methods and mechanisms of graphene. *Coatings*, 8(1), 33.