

Aoyan Liang

aoyanliang@gmail.com · [Portfolio](#) · [LinkedIn](#)

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EDUCATION

University of Southern California, Los Angeles Ph.D. in Materials Science	8/2020-Present GPA: 4.0/4.0
University of Southern California, Los Angeles M.S. in Computer Science (Data Science)	1/2022-5/2024 GPA: 4.0/4.0
University of Southern California, Los Angeles M.S. in Materials Science	8/2018-5/2020 GPA: 4.0/4.0
Southwest Jiaotong University, China B.Eng. in Materials Science	9/2014-6/2018 GPA: 3.64/4.0

INTERNSHIP EXPERIENCE

Seagate Technology, Fremont, CA 5/2025-8/2025
Advanced Material Modeling and Media Physics Research Engineering Summer Intern | Mentor: Dr. Pin-Wei Huang & Dr. Ganping Ju

- **FePt Atomic Ordering for Heat-assisted Magnetic Recording (HAMR) Applications:** Developed and performed molecular dynamics (MD) and Monte Carlo (MC) simulations to quantify L1₀ ordering in FePt grains under varied size, composition, strain, and temperature conditions. Provided key insights into ordering behavior that informed experimental validation and guided material design strategies for high-density magnetic recording media.
- **Dopant Effects on FePt Ordering and Segregation:** Applied machine learning (ML) interatomic potentials to screen dopants across the periodic table; identified promising candidates for experimental validation to improve atomic ordering and grain boundary stability.

Lawrence Livermore National Laboratory, Livermore, CA 6/2024-8/2024
Computational Chemistry and Materials Science (CCMS) Intern | Mentor: Dr. Vasily Bulatov

- **Solid Solution Strengthening in Complex Concentrated Alloys:** Conducted extensive large-scale MD simulations to investigate the fundamental alloy strengthening mechanisms under deformation through "alchemical" modifications of embedded atom method (EAM) potentials.

RESEARCH EXPERIENCE

University of Southern California, Los Angeles, CA 8/2020-Present
Graduate Research Assistant | Advisor: Prof. Paulo Branicio

Main Projects:

- **Machine Learning-Driven Analysis of Glass Motifs in Amorphous Metal:** Developed and applied an energy sampling framework to analyze activation energy in metallic glasses. Leveraged local atomic environment descriptors to tokenize metallic glass structures and designed machine learning models to accurately identify and characterize glass-glass interfaces.
- **Optimizing Superalloy Thin Films Nanostructure:** Conducted MD simulations to investigate alloy thin film deposition and use density functional theory (DFT) to analyze defect energetics. Integrate ML with experimental characterization data to identify key processing parameters that govern microstructure evolution.

- **Colloid Transport in Nanoporous Media:** Performed dissipative particle dynamics (DPD) simulations to uncover key mechanisms governing colloid transport and retention behavior in complex nanoporous systems. Analyzed the role of colloid concentration, flow rates, and physiochemical interaction to provide insights into transport efficiency.
- **Hot-press Sintering for Nanoceramics:** Conducted MD simulations using Fortran+MPI to explore the effects of temperature, pressure, and particle size on the densification process. Elucidated mechanisms driving microstructural evolution in AlN nanoceramics during sintering.

Southwest Jiaotong University, China

4/2016-6/2018

Research Assistant | Advisor: *Prof. Xiaosong Jiang*

- **Graphene Reinforced Copper Matrix Composites:** Synthesized graphene-reinforced copper composites using a Cu-Ti₃SiC₂-C system and applied high-pressure torsion to enhance mechanical properties. Explored fine grain strengthening mechanisms and published a review on graphene dispersion methods and their applications.

PROJECT EXPERIENCE

Large-Scale Recommendation System for Yelp Review Dataset 2023

USC Data Mining Competition | University of Southern California

- Designed and implemented a recommendation system to predict user-business ratings from Yelp review data, earning 1st place with an RMSE of 0.968.
- Developed and embedded a graph with 65 million edges and 13 million nodes using PyTorch BigGraph, optimizing distributed training across 64 CPUs to handle large-scale data efficiently.
- Enhanced model accuracy through Bayesian hyperparameter tuning (Optuna) and integrated advanced feature engineering with XGBoost to improve prediction reliability.

Modeling Earthquake Damage in Nepal Using Geographic Embedding

2023

DrivenData Competition

- Built machine learning models to predict building damage levels from the 2015 Gorkha earthquake, achieving an F1 score of 0.7541 with a weighted average ensemble approach.
- Incorporated spatial information via geographic embeddings, paired with engineered features, to optimize a LightGBM model, resulting in an F1 score of 0.7524.
- Explored and deployed advanced ensemble techniques (e.g., soft voting, hard voting, neural networks, and weighted averages) to enhance model robustness and predictive accuracy.

SKILLS

Programming Languages: Python, Fortran (MPI), C/C++ (MPI/OpenMP), SQL (MySQL), R.

Software: VASP, LAMMPS, OVITO, VESTA, Origin, Visual Studio, Microsoft Office.

Computational Methods: Density Functional Theory, Molecular Dynamics, Monte Carlo.

Operating Systems: Linux, MacOS, Windows.

Machine Learning Frameworks: Scikit-learn, TensorFlow, PyTorch, Optuna, XGBoost, LightGBM.

Other Skills: High-performance Computing (HPC), Natural Language Processing (NLP), Large Language Model (LLM).

PUBLICATIONS

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

2025

1. **Liang, A.**, Zhou, X., Aubry, S., Bertin, N., Bulatov, V. V. (2025) Atomistic Perspectives on Solid

Solution Strengthening: Size versus Stiffness Misfit (*Preprint, Under review*)

2. Bulatov, V. V., Bertin, N., Aubry, S., Zepeda-Ruiz, L. A., Zhou, X., **Liang, A.**, Oppelstrup, T., Sadig, B. (2025) Network aspects of single crystal plasticity. *Journal of Materials Research and Technology*, 36, 5611.
3. 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

4. **Liang, A.**, Liu, C., & Branicio, P. S. (2024). Colloid Transport in Bicontinuous Nanoporous Media. *Langmuir*, 40(21), 10868.
5. 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

6. 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.
7. 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.
8. **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

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

2021

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

2018

11. **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.

CONFERENCE PRESENTATIONS

1. **Liang, A.**, Yazdani, H., Farkas, D., Hodge A., & Branicio, P. S., Twin Boundary Engineering in Ni-based Superalloy Thin Films. Talk presented at: *2025 TMS Annual Meeting & Exhibition* - March 2025 - Las Vegas, NV, USA.
2. **Liang, A.**, Liu, C., & Branicio, P. S., Nanoparticle Transport in Bicontinuous Nanoporous Media. Talk presented at: *2024 MFD Student Research Symposium* - March 2024 - Los Angeles, CA, USA
3. **Liang, A.**, Goodelman, D. C., Hodge, A. M., Farkas, D., & Branicio, P. S., Exploring the Composition-Structure Relationships of High Entropy Alloy Thin Films: Combining Experiments and Atomistic Simulations. Poster presented at: *2023 MFD Student Research Symposium* - March 2023 - Los Angeles, CA, USA
4. **Liang, A.**, Hodge, A. M., Farkas D., & Branicio P. S., Atomistic modeling of physical vapor deposition and melt-quenching of CoCrFeNiTi_x high entropy alloys. Poster presented at: *2023 TMS Annual Meeting & Exhibition* - March 2023 - San Diego, CA, USA.
5. **Liang, A.**, & Branicio, P. S., Atomistic Modeling of Electric-field-assisted Sintering of AlN Nanoceramics. Poster presented at: *2022 MFD Student Research Symposium* - March 2022 - Los

Angeles, CA, USA

6. **Liang, A.**, Liu, C., & Branicio, P. S., Atomistic Modeling of Hot-press Sintering of AlN Nanoceramics. Poster presented at: *2022 TMS Annual Meeting & Exhibition* - February 2022 - Anaheim, CA, USA.
7. **Liang, A.**, Liu, C., & Branicio, P. S., Atomistic Modeling of Hot-Press Sintering of AlN Ceramics. Poster presented at: *2021 MRS Fall Conference* - November 2021 - Boston, MA, USA.
8. **Liang, A.**, & Branicio, P. S., Hot-Press Sintering of Aluminum Nitride Nanoceramics. Poster presented at: *2021 MFD Student Research Symposium* - February 2021 - Los Angeles, CA, USA

CERTIFICATIONS & AWARDS & HONORS

Certifications

Natural Language Processing Specialization (DeepLearning.AI)	11/2024
AI for Science on Supercomputers (Argonne National Laboratory)	12/2022
Fundamentals of Deep Learning (NVIDIA)	6/2021
SAS Certified Base Programmer for SAS 9	6/2019

Awards & Honors

2nd Prize – AI 4 science challenge (NanoHub)	2025
2024 Symposium – MFD Presentations Award Winner	2024
First Place, USC Data Mining Competition (Link)	2023
Rank 17/6714, Modeling Earthquake Damage (DrivenData Competition Leaderboard)	2023
Nominee for 2021 MRS Fall Meeting Best Poster (Materials Research Society)	2021
Master's Student Achievement Award (University of Southern California) (Link)	5/2020
Outstanding Graduate of Southwest Jiaotong University	2018
China National Scholarship (1%)	2016-2017
Grand Comprehensive Scholarship (Southwest Jiaotong University)	2016-2017
First-Class Comprehensive Scholarship (4 times)	2014-2016
Honorable Mention in MCM/ICM	2017
Third Prize in Asia and Pacific Mathematical Contest in Modeling	2016

TEACHING EXPERIENCE

University of Southern California, Los Angeles

Teaching Assistant

Courses:

• MASC 575 - Basics of Atomistic Simulation of Materials	Spring 2022
• MASC 110L - Materials Science (Lab section)	Fall 2022
• MASC 520 - Mathematical Methods for Deep Learning	Spring 2023
• MASC 503 - Thermodynamics of Materials	Fall 2023
• CHE 499 - Confectionary Manufacturing - Science and Technology	Spring 2024

PROFESSIONAL SERVICE

Reviewer for International Journals

69 reviews across 16 journals. Selected journals include:

Acta Materialia, Applied Surface Science, Computational Materials Science, Journal of Alloys and Compounds, Journal of Applied Physics, Progress in Materials Science, Scientific Reports, Thin Solid Films, Surface and Interface Analysis, Computer Physics Communications.