Aoyan Liang

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Updated on Mar 05, 2025

EDUCATION

University of Southern California, Los Angeles 8/2020-5/2025 (Expected)
Ph.D. in Materials Science GPA: 4.0/4.0

University of Southern California, Los Angeles 1/2022-5/2024
M.S. in Computer Science (Data Science) GPA: 4.0/4.0

University of Southern California, Los Angeles 8/2018-5/2020
M.S. in Materials Science GPA: 4.0/4.0

Southwest Jiaotong University, China 9/2014-6/2018
B.Eng. in Materials Science GPA: 3.64/4.0

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

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 (DFT), Molecular Dynamics (MD).
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).

PROFESSIONAL EXPERIENCE

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

- **Machine Learning-Driven Analysis of Glass Motifs in Metallic Glasses:** Develop and apply an energy sampling framework to analyze activation energy in metallic glasses. Leverage local atomic environment descriptors to tokenize metallic glass structures and design machine learning models to accurately identify and characterize glass-glass interfaces.
- **Optimizing Superalloy Thin Films Nanostructure:** Conduct MD simulations to investigate alloy thin film deposition and use DFT to analyze defect energetics. Integrate machine learning with experimental characterization data to identify key processing parameters that govern microstructure evolution, enhancing the process-structure relationship in superalloy thin films.
- **Colloid Transport in Nanoporous Media**: Performed 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.

Lawrence Livermore National Laboratory, Livermore 6/2024-8/2024

CCMS Graduate Internship, Mentor: Dr. Vasily Bulatov

- **Solid Solution Strengthening in Complex Concentrated Alloys:** Performed large-scale MD simulations (~10^8 atoms) to investigate fundamental alloy strengthening mechanisms. Developed a novel "computational alchemy" approach to customize force fields, uncovering the synergistic and antagonistic effects of size and stiffness misfits on strengthening, offering key insights for high-performance alloy design.

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-Ti_3SiC_2-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.

PROJECTS

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.

PUBLICATIONS

ORCID · Google Scholar Profile · Web of Science Profile

1. **Liang, A.,** Zhou, X., Aubry, S., Bertin, N., Bulatov, V. V. (2025) Atomistic Perspectives on Solid Solution Strengthening: Size versus Stiffness Misfit (*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 (*Under review*)
3. Carvalho, A. P., **Liang, A.,** Kawasaki, Cupertino-Malheiros, L., Branicio, P. S., & Figueiredo, R. B. (2025) Strengthening nanostructured metals through dynamic. *Journal of Materials Research and Technology*, 35, 754.

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.
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.
9. Guan, X., **Liang, A.**, & Branicio, P. S. (2022). High pressure shear induced microstructural evolution in nanocrystalline aluminum. *Computational Materials Science*, 203(15), 111105.
10. **Liang, A.**, Liu, C., & Branicio, P. S. (2021). Hot-press sintering of aluminum nitride nanoceramics. *Physical Review Materials*, 5(9), 096001.
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.**, 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
2. **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
3. **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.
4. **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
5. **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.
6. **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.
7. **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

AWARDS & HONORS

2nd Prize – AI 4 science challenge (NanoHub)	2025
Presentations Award Winner – 2024 USC MFD Symposium	2024
1st Place – USC Data Mining Competition (Link)	2023
Rank 17/6714 – 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
SAS Certified Base Programmer for SAS 9	6/2019
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 (Total: 15 journals, 60 reviews)

Acta Materialia, Applied Surface Science, Chemical Papers**,** Computational Materials Science, Computer Physics Communications, Journal of Alloys and Compounds, Journal of Applied Physics, Journal of Crystal Growth, Journal of Non-Crystalline Solids, Mechanics of Materials, Progress in Materials Science, Scientific Reports, Separation and Purification Technology, Surface and Interface Analysis, Thin Solid Films.