Mengyi Chen

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Education

National University of Singapore — Singapore
Ph.D. in Mathematics (Expected Aug. 2027) — *Aug. 2023 – Present*

- Supervisor: Qianxiao Li
- Research Interests:
  - Machine learning methods for mesoscale and macroscale modeling of materials from microscopic data
  - Thermodynamics of complex materials, computing free energy and entropy for phase stability and synthesis
  - Ab initio phase-field modeling of phase transformations and microstructure evolution at realistic experimental scales and conditions

Columbia University — New York, USA
Visiting Student, Department of Applied Physics and Applied Mathematics — *Jan. 2022 – May 2022*

University of Chinese Academy of Sciences — Beijing, China
B.Sc. in Mathematics and Applied Mathematics — *Sep. 2019 – Jun. 2023*

Publications

[1] **Mengyi Chen**, Peichen Zhong, Zihan Zhang, Qianxiao Li. "Learning Ab Initio Phase-Field Models." *arXiv preprint* arXiv:2610.01432, 2026.

[2] Zihan Zhang*, **Mengyi Chen***, Qianxiao Li, Peichen Zhong. "Interfacial Melting as a Thermodynamic Indicator of Solid-State Synthesizability." *Nature Communications*, in press, 2026. arXiv:2606.22885.

[3] Zhichao Han, **Mengyi Chen**, Qianxiao Li. "Learning Permutation-Invariant Macroscopic Dynamics." *International Conference on Machine Learning (ICML)*, PMLR 306:39655–39671, 2026.

[4] **Mengyi Chen**, Pengru Huang, Kostya S. Novoselov, Qianxiao Li. "Scalable Learning of Macroscopic Stochastic Dynamics." *Physical Review Materials*, 10(3):033805, 2026.

[5] **Mengyi Chen**, Qianxiao Li. "Learning Macroscopic Dynamics from Partial Microscopic Observations." *Advances in Neural Information Processing Systems (NeurIPS)*, 37:48996–49021, 2024.

[6] Sheng Gong, Yumin Zhang, Zhenliang Mu, Zhichen Pu, Hongyi Wang, Xu Han, Zhiao Yu, **Mengyi Chen**, Tianze Zheng, Zhi Wang, Lifei Chen, Zhenze Yang, Xiaojie Wu, Shaochen Shi, Weihao Gao, Wen Yan, Liang Xiang. "A Predictive Machine Learning Force-Field Framework for Liquid Electrolyte Development." *Nature Machine Intelligence*, 7(4):543–552, 2025.

**Equal contribution.*

Work Experience

ByteDance AML Research Intern — Dec. 2022 – Jul. 2023
Beijing, China

- Contributed to developing equivariant graph neural network models for machine learning force fields in the ByteDance AI Molecular Simulation Booster (BAMBOO) project

Honors & Awards

NUS Faculty of Science PhD Conference Award	2026
NUS Graduate Tutor Merit Award (Semester 2, AY2025/26)	2026
NeurIPS 2024 Travel Award	2024
NUS Faculty of Science Dean's Graduate Fellowship	2023
UCAS Overseas Graduate Studies Fellowship (Top 5%)	2023
UCAS Second-Class Scholarship	2022

Professional Service

Co-organizer, *ICLR 2025 Workshop on Machine Learning Multiscale Processes (MLMP)*, Singapore — 2025

Skills & Interests

Languages: Chinese (native), English (fluent)
Interests: Rock climbing, violin