

Curriculum Vitae: Ting Liang

Born in 1994, Guangxi province, China

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Research Interests

Computational Materials Physics and Chemistry

1. Thermal transport and development of advanced computational methodologies
2. Molecular dynamics and DFT calculations of phononic properties
3. Machine learning interatomic potentials and development of foundational models
4. AI for Science (AI4S) applications in multi-functional material systems

Education

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|-------------------|---|
| 08/2021 – Present | The Chinese University of Hong Kong – Hong Kong SAR, China
Doctor of Philosophy in Electronic Engineering, Department of Electronic Engineering
Supervisor: Prof. Jianbin Xu |
| 09/2017 – 06/2020 | Guilin University of Electronic Technology – Guilin, China
Master of Engineering in Mechanical Engineering, Department of Mechanics |
| 09/2013 – 06/2017 | Hefei University of Technology – Hefei, China
Bachelor of Engineering in Process Equipment and Control Engineering, Department of Mechanics |

Working Experience

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|-------------------|---|
| 06/2020 – 06/2021 | Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences – Shenzhen, China
Assistant Engineer in Thermal Characterization Techniques
Advisors: Prof. Xiaoliang Zeng and Prof. Meng Han |
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Primary Honors and Scholarships

- 2020 **National Scholarship for Graduate Students** (Ministry of Education of China, Top 2.5%)
- 2018 **Third-class Academic Excellence Scholarship** (Guilin University of Electronic Technology)
- 2017 **First-class Academic Excellence Scholarship** (Guilin University of Electronic Technology, Top 15%)
- 2016 **National Motivational Scholarship** (Ministry of Education of China)
- 2016 **Third-class Merit Scholarship** (Hefei University of Technology)
- 2015 **Third-class Merit Scholarship** (Hefei University of Technology)

Teaching Experience

- 09/2021 – 11/2024 **The Chinese University of Hong Kong** – Hong Kong SAR, China
Graduate Teaching Assistant for ELEG 3301: Principles of Semiconductor Devices
(Instructor: Prof. Jianbin Xu)
- 01/2023 – 05/2025 **The Chinese University of Hong Kong** – Hong Kong SAR, China
Graduate Teaching Assistant for ENGG 5282: Nanoelectronics
(Instructor: Prof. Jianbin Xu)

Selected Research Projects (Participant)

- 2023 – 2026 Phonon Hydrodynamics in One-dimensional Crystals Towards High Thermal Conduction
General Research Fund (GRF), Hong Kong RGC
PI: Prof. Jianbin Xu
- 2023 – 2028 Nanoscale Heat Transport Mechanisms and Structured Thermal Interface Materials
National Key R&D Program of China, Ministry of Science and Technology (MOST)
PI (HK side): Prof. Jianbin Xu

Selected Invited Talks

- 10/2024 Highly efficient machine learning potential toward thermal transport: from amorphous to heterostructure systems
International Joint Seminar on Mechanical Engineering 2024, Japan (Invited speaker; 30 min; Online)
- 06/2025 NEP89: Universal neuroevolution potential for inorganic and organic materials across 89 elements
The 1st GPUMD Developers Conference and Frontier Seminar on AI Molecular Dynamics, Ningbo, China (Invited speaker; 30 min)

First-author Publications

- 2026 NEP89: Universal neuroevolution potential for inorganic and organic materials across 89 elements
T. Liang, K. Xu, E. Lindgren, Z. Chen, R. Zhao, J. Liu, E. Berger, B. Tang, B. Zhang, Y. Wang, K. Song, P. Ying, N. Xu, H. Dong, S. Chen, P. Erhart, Z. Fan, T. Ala-Nissila, and J. Xu
Nature Computational Science (revision submitted), 2026.
- 2026 Probing the ideal limit of interfacial thermal conductance in two-dimensional van der Waals heterostructures
T. Liang, K. Xu, P. Ying, W. Jiang, M. Han, X. Wu, W. Ouyang, Y. Yao, X. Zeng, Z. Ye, Z. Fan, and J. Xu
npj Computational Materials 12, 11 (2026).
- 2025 PYSED: A tool for extracting kinetic-energy-weighted phonon dispersion and lifetime from molecular dynamics simulations
T. Liang, W. Jiang, K. Xu, H. Bu, Z. Fan, W. Ouyang, and J. Xu
Journal of Applied Physics 138, 075101 (2025).
- 2023 Mechanisms of temperature-dependent thermal transport in amorphous silica from machine-learning molecular dynamics
T. Liang, P. Ying, K. Xu, Z. Ye, C. Ling, Z. Fan, and J. Xu
Physical Review B 108, 184203 (2023).
- 2022 Abnormally high thermal conductivity in fivefold twinned diamond nanowires
T. Liang, K. Xu, M. Han, Y. Yao, Z. Zhang, X. Zeng, J. Xu, and J. Wu
Materials Today Physics 27, 100705 (2022).
- 2020 Multilayer in-plane graphene/hexagonal boron nitride heterostructures: Insights into the interfacial thermal transport properties
T. Liang, M. Zhou, P. Zhang, P. Yuan, and D. Yang
International Journal of Heat and Mass Transfer 151, 119395 (2020).

- 2019 A molecular dynamics study on the thermal conductivities of single-and multi-layer two-dimensional borophene
T. Liang, P. Zhang, P. Yuan, S. Zhai, and D. Yang
Nano Futures **3**, 015001 (2019).
- 2018 In-plane thermal transport in black phosphorene/graphene layered heterostructures: a molecular dynamics study
T. Liang, P. Zhang, P. Yuan, and S. Zhai
Physical Chemistry Chemical Physics **20**, 21151-21162 (2018).

Co-first Author Publications (#: co-first author)

- 2025 Observation of giant dipole moments of interlayer excitons via layer engineering
 J. Zhu[#], **T. Liang[#]**, F. Shen[#], Z. Chen, and J. Xu
Nature Communications **16**, 10661 (2025).
- 2025 Strain-engineered anisotropic thermal transport in layered MoS₂ structures
 W. Jiang[#], **T. Liang[#]**, J. Xu, and W. Ouyang
ACS Applied Materials & Interfaces **17**, 34833 (2025).
- 2025 Accurate modeling of interfacial thermal transport in van der Waals heterostructures via hybrid machine learning and registry-dependent potentials
 W. Jiang[#], H. Bu[#], **T. Liang[#]**, P. Ying, Z. Fan, J. Xu, and W. Ouyang
arXiv preprint arXiv:2505.00376 (2025).
- 2024 Correlating Young's modulus with high thermal conductivity in organic conjugated small molecules
 J. Zeng[#], **T. Liang[#]**, J. Zhang, D. Liu, S. Li, X. Lu, M. Han, Y. Yao, J. Xu, R. Sun, and C.-P. Wong
Small **20**, 2309338 (2024).
- 2024 Design of soft/hard interface with high adhesion energy and low interfacial thermal resistance via regulation of interfacial hydrogen bonding interaction
 X. Zeng[#], **T. Liang[#]**, X. Cheng, J. Fan, Y. Pang, J. Xu, R. Sun, X. Xia, and X. Zeng
Nano Letters **24**, 6386 (2024).
- 2024 Poly(ionic liquid)s: A promising matrix for thermal interface materials
 J. Zeng[#], **T. Liang[#]**, B. Yang, T. Rao, M. Han, Y. Yao, J. Xu, L. Li, and R. Sun
ACS Applied Materials & Interfaces **16**, 45563 (2024).
- 2023 Twist-dependent anisotropic thermal conductivity in homogeneous MoS₂ stacks
 W. Jiang[#], **T. Liang[#]**, J. Xu, and W. Ouyang
International Journal of Heat and Mass Transfer **217**, 124662 (2023).

- 2021 Optimization of effective thermal conductivity of thermal interface materials based on the genetic algorithm-driven random thermal network model
Y. Su[#], Q. Ma[#], **T. Liang[#]**, Y. Yao, Z. Jiao, M. Han, Y. Pang, L. Ren, X. Zeng, J. Xu, and R. Sun
ACS Applied Materials & Interfaces **13**, 53239-53249 (2021).

Corresponding Author Publications (*: corresponding author)

- 2025 Critical size transitions in silicon nanowires: Amorphization, phonon hydrodynamics, and thermal conductivity
K. Xu, Y. Li, D. Ding, **T. Liang***, J. Wu*, and J. Xu*
The Journal of Physical Chemistry Letters **16**, 8580 (2025).

Co-author Publications

- 2025 Moiré-driven interfacial thermal transport in twisted transition metal dichalcogenides
W. Jiang, **T. Liang**, H. Bu, J. Xu, and W. Ouyang
ACS Nano **19**, 16287 (2025).
- 2025 NEP-MB-pol: a unified machine-learned framework for fast and accurate prediction of water's thermodynamic and transport properties
K. Xu, **T. Liang**, N. Xu, P. Ying, S. Chen, N. Wei, J. Xu, and Z. Fan
npj Computational Materials **11**, 275 (2025).
- 2025 Phonon coherence and minimum thermal conductivity in disordered superlattices
X. Wu, Z. Wu, **T. Liang**, Z. Fan, J. Xu, M. Nomura, and P. Ying
Physical Review B **111**, 085413 (2025).
- 2025 Poly(ionic liquid) matrices embedded with liquid metal particles: A versatile solution for high-power density thermal management
J. Zeng, T. Rao, **T. Liang**, Y. Yao, C. Wang, J. Xu, L. Li, and R. Sun
Composites Part A: Applied Science and Manufacturing **199**, 109221 (2025).
- 2025 Inhomogeneous interfacial layer: A hidden cause of high thermal contact resistance in polymer-based thermal interface materials with spherical fillers
H. Shi, X. Li, **T. Liang**, Z. Wen, L. Ren, M. Han, Y. Yao, X. Zeng, J. Xu, and R. Sun
ACS Applied Materials & Interfaces **17**, 70984 (2025).

- 2025 Device-scale atomistic simulations of heat transport in advanced field-effect transistors
K. Xu, G. Wang, **T. Liang**, Y. Xiao, D. Ding, H. Guo, X. Gao, L. Tong, X. Wan, G. Zhang, and J. Xu
arXiv preprint arXiv:2511.18915 (2025).
- 2025 Phonon coherence and minimum thermal conductivity in disordered superlattices
X. Wu, Z. Wu, **T. Liang**, Z. Fan, J. Xu, M. Nomura, and P. Ying
Physical Review B **111**, 085413 (2025).
- 2024 Deformable and highly adhesive poly(ionic liquid)/liquid metal visco-elastomers for thermal management
B. Yang, J. Zeng, **T. Liang**, M. Han, C. Zhang, J. Xu, Y. Yao, and R. Sun
Journal of Materials Chemistry A **12**, 22233-22247 (2024).
- 2023 Variable thermal transport in black, blue, and violet phosphorene from extensive atomistic simulations with a neuroevolution potential
P. Ying, **T. Liang**, K. Xu, J. Zhang, J. Xu, J. Wu, Z. Fan, T. Ala-Nissila, and Z. Zhong
International Journal of Heat and Mass Transfer **202**, 123681 (2023).
- 2023 Methoxy functionalization of phenethylammonium ligand for efficient perovskite light-emitting diodes
X. Sun, **T. Liang**, K. H. Ngai, Z. Nie, K. Fan, S. Li, C. C. S. Chan, K. S. Wong, X. Lu, J. Xu, and M. Long
Advanced Optical Materials **11**, 2300464 (2023).
- 2023 Sub-micrometer phonon mean free paths in metal-organic frameworks revealed by machine-learning molecular dynamics simulations
P. Ying, **T. Liang**, K. Xu, J. Zhang, J. Xu, Z. Zhong, and Z. Fan
ACS Applied Materials & Interfaces **15**, 40682 (2023).
- 2023 Accurate prediction of heat conductivity of water by a neuroevolution potential
K. Xu, Y. Hao, **T. Liang**, P. Ying, J. Xu, J. Wu, and Z. Fan
The Journal of Chemical Physics **158**, 204114 (2023).
- 2022 Gradient nano-grained graphene as 2D thermal rectifier: A molecular dynamics based machine learning study
K. Xu, **T. Liang**, Y. Fu, Z. Wang, Z. Fan, N. Wei, J. Xu, Z. Zhang, and J. Wu
Applied Physics Letters **121**, 133501 (2022).