

# 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

- |                      |                                                                                                                                                                                                           |
|----------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 08/2021 –<br>03/2026 | <b>The Chinese University of Hong Kong</b> – Hong Kong SAR, China<br>Doctor of Philosophy in Electronic Engineering, Department of Electronic Engineering<br>Supervisor: <a href="#">Prof. Jianbin Xu</a> |
| 09/2017 –<br>06/2020 | <b>Guilin University of Electronic Technology</b> – Guilin, China<br>Master of Engineering in Mechanical Engineering, Department of Mechanics                                                             |
| 09/2013 –<br>06/2017 | <b>Hefei University of Technology</b> – Hefei, China<br>Bachelor of Engineering in Process Equipment and Control Engineering, Department of Mechanics                                                     |

## Working Experience

- 06/2020 – **Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences** –  
06/2021 Shenzhen, China  
Assistant Engineer in Thermal Characterization Techniques  
Advisors: Prof. Xiaoliang Zeng and Prof. Meng Han
- 04/2026 – **The Chinese University of Hong Kong** – Hong Kong, China  
present Postdoctoral Researcher  
Advisors: Prof. Jianbin Xu

### 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 – **The Chinese University of Hong Kong** – Hong Kong SAR, China  
11/2024 Graduate Teaching Assistant for ELEG 3301: Principles of Semiconductor Devices  
(Instructor: Prof. Jianbin Xu)
- 01/2023 – **The Chinese University of Hong Kong** – Hong Kong SAR, China  
05/2025 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)*
- 06/2026      Highly Efficient Machine Learning Potentials toward Thermal Transport and Beyond  
*The 2st GPUMD Developers Conference and Frontier Seminar on AI Molecular Dynamics, Changchun, China (Invited speaker; 25 min)*
- 07/2026      Highly Efficient Machine Learning Potentials toward Thermal Transport and Beyond  
*Joint Conference of The 5th International Conference on Phononics and Thermal Energy Science & The 10th Workshop on Thermal Transport, Harbin, China (Invited speaker; 25 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, 1-13, 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)

- 2026 Accurate modeling of interfacial thermal transport in van der Waals heterostructures via hybrid machine learning and registry-dependent potentials  
W. Jiang<sup>#</sup>, H. Bu<sup>#</sup>, **T. Liang<sup>#</sup>**, P. Ying, Z. Fan, J. Xu, and W. Ouyang  
*Journal of Chemical Theory and Computation* **22**, 9 (2026).
- 2025 Observation of giant dipole moments of interlayer excitons via layer engineering  
J. Zhu<sup>#</sup>, **T. Liang<sup>#</sup>**, F. Shen<sup>#</sup>, Z. Chen, and J. Xu  
*Nature Communications* **16**, 10661 (2025).
- 2025 Strain-engineered anisotropic thermal transport in layered MoS<sub>2</sub> structures  
W. Jiang<sup>#</sup>, **T. Liang<sup>#</sup>**, J. Xu, and W. Ouyang  
*ACS Applied Materials & Interfaces* **17**, 34833 (2025).

- 2024 Correlating Young's modulus with high thermal conductivity in organic conjugated small molecules  
J. Zeng<sup>#</sup>, **T. Liang<sup>#</sup>**, 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<sup>#</sup>, **T. Liang<sup>#</sup>**, 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<sup>#</sup>, **T. Liang<sup>#</sup>**, 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 MoS<sub>2</sub> stacks  
W. Jiang<sup>#</sup>, **T. Liang<sup>#</sup>**, J. Xu, and W. Ouyang  
*International Journal of Heat and Mass Transfer* **217**, 124662 (2023).
- 2022 Thermal transport in planar sp<sup>2</sup>-hybridized carbon allotropes: A comparative study of biphenylene network, pentaheptite and graphene  
P. Ying<sup>#</sup>, **T. Liang<sup>#</sup>**, Y. Du, J. Zhang, X. Zeng, and Z. Zhong  
*International Journal of Heat and Mass Transfer* **183**, 122060 (2022).
- 2021 Optimization of effective thermal conductivity of thermal interface materials based on the genetic algorithm-driven random thermal network model  
Y. Su<sup>#</sup>, Q. Ma<sup>#</sup>, **T. Liang<sup>#</sup>**, 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

- 2026 Sulfonium-ligand-regulated crystallization interfacial dynamics enables near-infrared perovskite light-emitting diodes with 27% EQE  
X. Sun, J. Li, **T. Liang**, D. Liu, W. Tang, Y. Huang, Z. Chen, B. Wu, B. Chen, J. Xu, and M. Long  
*ACS Energy Letters* (2026).
- 2026 A phase-change-enabled thermal interface material with the competitive thermal resistance of  $0.03^{\circ}\text{C}\cdot\text{cm}^2\cdot\text{W}^{-1}$  for electronic devices thermal management in AI era  
G. Lv, Y. Pang, **T. Liang**, Y. Qiao, J. Xu, R. Sun, and X. Zeng  
*Advanced Functional Materials* 36, e00063 (2026).
- 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).