

# Ying Li

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## Summary

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I obtained my Ph.D. and bachelor's degrees from Peking University and Nanjing University, respectively. I have extensive research experience in high-performance computing (HPC) and deep learning. I have published papers in prestigious journals and conferences such as EMNLP, Physical Review Letters, Advanced Functional Materials, and Physical Review Applied, with a total citation of 966 and an H-index of 16. My current research interests focus on enhancing the reasoning capabilities of large language models (LLMs) and multimodal foundation models, with applications to mathematical reasoning and AI for Science.

## Education and Awards

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| Peking University, PhD, Computational Physics                                                                                                                                                                                                                                                                                                                                       | 2019.10 – 2024.07 |
| <ul style="list-style-type: none"><li>• <b>China International College Students' Innovation Competition</b>, Bronze Award of Beijing Province, Intelligent Agent for Mental Health Monitoring and Emotional Companionship.</li><li>• <b>Amazon DeepRacer College Challenge</b>, second place of Peking University, representing Peking University in the national finals.</li></ul> |                   |
| Peking University, PhD, Physics                                                                                                                                                                                                                                                                                                                                                     | 2016.09 - 2019.10 |
| Nanjing University, Bachelor in Physics                                                                                                                                                                                                                                                                                                                                             | 2012.09 - 2016.06 |
| <ul style="list-style-type: none"><li>• <b>Mathematical Contest in Modeling</b>, Meritorious Winner</li><li>• <b>National Mathematical Modeling Competition</b>, First Prize of Jiangsu Province</li><li>• <b>Outstanding Graduate of Nanjing University</b></li></ul>                                                                                                              |                   |
| Chongqing Nankai Middle School                                                                                                                                                                                                                                                                                                                                                      | 2009.09 - 2012.06 |

## Research Experience

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| Tsinghua University, YMSC and BIMSA                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | 2025.03 - Present |
| <ul style="list-style-type: none"><li>• <b>Latent Reasoning</b><br/>Enhancing the reasoning capabilities of large language and multimodal foundation models by enabling parallel reasoning-path exploration and compressed computation within a unified latent space.</li><li>• <b>LLM for Math Proof</b><br/>Integrating LLMs with formal languages to achieve automated mathematical theorem proving through methods such as fine-tuning, reinforcement learning, prompt engineering, and data engineering.</li><li>• <b>Agent Based Modeling (ABM)</b><br/>Introducing multi-agent reinforcement learning (MARL) algorithms into the study of social behavior.</li></ul> |                   |
| Peking University, School of Computer Science                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | 2024.06 – 2025.03 |
| <ul style="list-style-type: none"><li>• <b>Distributed and Heterogeneous Acceleration of LLMs</b><br/>Training and inference acceleration of LLMs on heterogeneous platforms (GPU + NPU) through parallelism and memory management.</li><li>• <b>AI Tutorials</b><br/>I authored a series of AI tutorials (<a href="#">Link</a>) for the <b>Ministry of Education's Large Model Public Service Platform</b>. These tutorials cover neural network fundamentals, CNNs, LLM, and text-to-image generation.</li></ul>                                                                                                                                                          |                   |

- **Collaborative Projects**

I completed a series of projects related to LLMs as the Primary developer. The clients for these projects are the **Ministry of Education, China Unicom (Guangdong Branch), and a national research institute.**

Peking University, Laboratory of Computational Physics

2019.10 – 2024.07

- **NLP-Based Extraction of Psychological Indicators**

Fine-tuning Transformer-based embedding models via an indirect supervised contrastive learning approach in Siamese network architecture to extract psychological indicators from historical corpora.

- **Predicting Hamiltonians with Graph Neural Networks (GNNs)**

Treating atoms as nodes and interatomic interactions as edges, GNNs are used to iteratively update node and edge embeddings to predict the elements of periodic Hamiltonians.

- **Automated Density Functional Theory (DFT) Workflow**

Developed an automated DFT workflow integrating geometric structure processing, script generation, automated job submission with error correction, and data post-processing.

- **Development and Application of DFT Methods**

Developed DFT methods to address interface formation, defects, disorder, and other phenomena in interfaces and transport systems.

## Media Coverage

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- Co-corresponding Author work: Yuqi Chen, Sixuan Li, Ying Li, et al., EMNLP main, 2024. Covered by [DeepTech](#) and [MIT Technology Review China](#).
- Co-first Author Work: Hong Li, Qiuhui Li, Ying Li (co-first author), et al., Advanced Functional Materials, 34(38): 2402474, 2024. Covered by [Physics Department of Peking University](#).
- First Author Work: Ying Li, et al. Physical Review Applied, 20(6):064044, 2023. Covered by [Fermi Technology](#).

## Selected Publications

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- [1] Sixuan Li, **Ying Li**, et al. Scalable Memory-Guided Framework for Consistent Ultra-High-Resolution Segmentation. *In preparation*. 2026
- [2] Sixuan Li, **Ying Li**, et al. AnaX: Anatomy-Aware Hybrid Network for ADHD fMRI Diagnosis. *submitted*. 2026
- [3] **Ying Li**, et al. Quantum transport simulation of sub-1-nm gate length monolayer MoS<sub>2</sub> transistors. *arXiv:2404.13801, IEEE Transactions on Electron Devices (under review)*, 2026.
- [4] Mohammad Atari, Yuqi Chen, **Ying Li**, et al. PsyEmbedding: Fine-tuning Pre-trained Transformer Models for Quantifying Psychological Similarity in Text. *In preparation*. 2026
- [5] Yuqi Chen, Sixuan Li, **Ying Li (co-corresponding author)**, et al. Surveying the dead minds: Historical-psychological text analysis with contextualized construct representation (CCR) for classical Chinese. *EMNLP main*, 2024.
- [6] **Ying Li**, et al. Electrical contacts in monolayer MoSi<sub>2</sub>N<sub>4</sub> transistor. *ACS Applied Materials & Interfaces*, 16(37): 49496–49507, 2024.
- [7] **Ying Li**, et al. Monolayer WSi<sub>2</sub>N<sub>4</sub>: A promising channel material for sub-5-nm-gate homogeneous CMOS

devices. *Physical Review Applied*, 20(6):064044, 2023.

[8] **Ying Li**, *et al.* Ballistic MoS<sub>2</sub> transistors with ultra-high on-state current. *Science China Materials*, 67(10): 3083-3086, 2024.

[9] Hong Li, Qiuhui Li, **Ying Li (co-first author)**, *et al.* Recent experimental breakthroughs on 2D transistors: Approaching the theoretical limit. *Advanced Functional Materials*, 34(38): 2402474, 2024.

[10] **Ying Li**, *et al.* Review on quantum advantages of sampling problems. *Acta Physica Sinica*, 70(21): 210201, 2021.

[11] Xinyue Yang, Shibo Fang, **Ying Li**, *et al.* Ab-Initio Quantum Transport Simulation of Sub-1 nm Gate Length Monolayer and Bilayer WSe<sub>2</sub> Transistors: Implications for Ultra-Scaled CMOS Technology. *ACS Applied Nano Materials*, 8(7): 3460-3470, 2025.

[12] Benchuan Lin, Shuo Wang, Anqi Wang, **Ying Li**, *et al.* Electric control of fermi arc spin transport in individual topological semimetal nanowires. *Physical Review Letters*, 124(11):116802, 2020.

[13] Xingyuan Wang, Huazhou Chen, **Ying Li**, *et al.* Microscale vortex laser with controlled topological charge. *Chinese Physics B*, 25(12): 124211, 2016.

[Google Scholar Link](#)

## Internship

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**Huawei Technologies Co., Ltd.** 2012 Lab, Data Center 2021.01-2021.06

- **Quantum Machine Learning**

Integrating quantum circuits with machine learning, including quantum convolutional neural networks, quantum-classical hybrid neural networks, and variational quantum circuits.

- **Classic Simulator for Random Quantum Circuits**

Using tensor networks to compute sampling probabilities of random quantum circuits, and reducing practical simulation time by incorporating read and write operation counts into the loss function.

**China Merchants Securities Co., Ltd.** Information and Communications Team 2020.08-2020.11

- Industry data analysis, research report writing, IPO prospectus review.

## Technology Stack

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### Coding

- Programming Languages: Python (proficient), bash (proficient), C++, C, Matlab, Mathematica
- Tools: git, docker
- Frameworks: PyTorch, HuggingFace (Transformers, Accelerate, Diffuser, Gradio, etc.), DeepSpeed, TensorFlow, vLLM, LangChain, Langgraph, MindIE, LLaMA-Factory
- HPC Platforms: HPC Platform of Tsinghua University, Peking University; National Supercomputing Shenzhen Center, Guizhou Center; In-house Server Cluster
- Computational software and packages: VASP, QuantumATK, Quantum ESPRESSO, SIESTA, Pymatgen, ASE, GPAW, Qiskit, Cirq, etc.

### Operations & Maintenance Experience

- Administrator: Data Center for Laboratory of Computational Physics
- Executive AP (committee member) of Linux Club of Peking University (LCPU)

## Fundings

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Beijing Science and Technology Rising Star Program, Team Member 2025

## Teaching Experience

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For 8 universities including PKU, BJTU, etc: XSCOW Platform Training, Lecturer ([Link](#)) 2024

Peking University: Programming Language Series Lectures, Lecturer 2021

Peking University: Solid State Physics, Teaching Assistant 2017

Mentoring:

Fall 2017, Jia Yu, BS Physics (Peking University '18)

Fall 2017, Jianwei Wang, BS Physics (Peking University '18)

## Talks and Meetings

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The Rise of Latent Reasoning: From Chain-of-Thought to Silent Inference 2025.11.07

- Hong Kong Laureate Forum, Hong Kong

Automated Formalization and Theorem Proving via Large Language Models 2025.05.27

- Postdoc Workshop III 2025, Yau Mathematical Sciences Center, Tsinghua University

An Introduction to Large Language Models: Foundations and Applications 2025.03.28

- Invited by Shenzhen Institute for Quantum Science and Engineering of Southern University of Science and Technology

## Activities

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Peking University, AI for Science Salon 2023.10.28

- Planned and co-organized a salon themed “AI for Science”. Invited researchers from ByteDance Research, DP Technology, and Microsoft Research Asia to share their insights, with over 100 participants.

## Service

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- Reviewer of ICLR, AAAI, ACL, Advanced Materials Interfaces, Physica B: Condensed Matter
- Chair of three AI Science and Machine Learning sessions of the International Congress of Basic Science (ICBS) 2025