

Yipeng Zhang | Curriculum Vitae

✉ School of Physical and Mathematical Sciences (SPMS)

Nanyang Technological University (NTU), Singapore

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🌐 <https://zhangyipeng01.github.io/>

Research Interests

Geometric Deep learning (GDL), Topological Deep Learning (TDL), Topological Data Analysis (TDA), Mathematical AI.

Education

Nanyang Technological University (NTU)

Singapore

Ph.D. in Mathematics, School of Physical and Mathematical Sciences

Aug 2022 – Present

Research areas: Topological Data Analysis, Topological Deep Learning, Geometric Deep learning.

Fudan University (FDU)

Shanghai, China

M.Sc. in Mathematics, School of Mathematical Sciences

Sep 2019 – Jun 2022

Research area: Toric Topology.

Nankai University (NKU)

Tianjin, China

B.Sc. in Physics, School of Physics

Sep 2015 – Jun 2019

Major: Theoretical Physics.

Nankai University (NKU)

Tianjin, China

Second B.Sc. in Mathematics and Applied Mathematics,

Sep 2015 – Jun 2019

School of Mathematical Sciences

Major: Mathematics and Applied Mathematics.

Publications

Journal Articles

1. Zhang, Y., Shen, C., & Xia, K. (2024). *Multi-Cover Persistence (MCP)-based machine learning for polymer property prediction*. **Briefings in Bioinformatics**, **25**(6), bbae465.
2. Han, B., Zhang, Y., Li, L., Gong, X., & Xia, K. (2025). *TopoQA: A topological deep learning-based approach for protein complex structure interface quality assessment*. **Briefings in Bioinformatics**, **26**(2), bbaf083.
3. Wang, Y., Liu, X., Zhang, Y., Wang, X., & Xia, K. (2025). *Join Persistent Homology (JPH)-based machine learning for metalloprotein–ligand binding affinity prediction*. **Journal of Chemical Information and Modeling**, **65**(6), 2785–2793.
4. Li, L., Zhang, Y. (co-first author), Wang, G., & Xia, K. (2025). *Kolmogorov–Arnold graph neural*

networks for molecular property prediction. **Nature Machine Intelligence**, 7, 1–9.

Conference Papers.....

1. Zhang, Y., Li, L., & Xia, K. (2025). *Rhomboid tiling for geometric graph deep learning*. **Proceedings of the 42nd International Conference on Machine Learning (ICML 2025)**, Proceedings of Machine Learning Research (PMLR), 267, 75392–75412.

Manuscripts Under Review.....

1. Shen, C., Zhang, Y., Er, T. K. G., Han, F., Goto, A., & Xia, K. *Molecular topological deep learning for polymer property prediction*. Under review at **ACS Nano**.
2. Han, B., Zhang, Y., Zheng, M., Gong, X., & Xia, K. *Rhomboid tiling-based topological deep learning (RT-TDL) for quality assessment of protein complex structures*. Under review at **Nature Communications**.

Manuscripts in Preparation.....

1. Zhang, Y., et al. *Diffusion-based positional encoding for Transformer models*.

Academic Presentations

- **Invited Talk.**

the 7th Conference on Computational and Mathematical Bioinformatics and Biophysics (CMBB), Tsinghua Sanya International Mathematics Forum (TSIMF), Sanya, China, Dec 15-19, 2025.

- **Invited Talk.**

IMS–NTU Joint Workshop on “Applied Geometry for Data Sciences, Part II” , Institute for Mathematical Sciences (IMS), Singapore, Jun 2–6, 2025.

- **Oral Presentation.**

2025 Shanghai–Singapore Joint Forum on Mathematical Sciences with Artificial Intelligence, Shanghai Jiao Tong University, China, May 7–9, 2025.

- **Invited Talk.**

ICCM Satellite Workshop on “Applied Geometry and Topology for Data Sciences” , Shanghai Institute for Mathematics and Interdisciplinary Sciences (SIMIS), China, Feb 24–28, 2025.

- **Poster Presentation.**

International Congress of Basic Science (ICBS), Beijing Institute of Mathematical Sciences and Applications (BIMSA), China, Jul 16–28, 2023.

- **Invited Talk.**

Workshop on Geometry and Topology of Spaces with Torus Actions, Xi’ an Jiaotong–Liverpool University (XJTLU), Suzhou, China, Apr 24, 2021.

Honors and Awards

- Best Paper Award, Shanghai–Singapore Forum on AI for Mathematics, May 2025
- NTU Tier 2 Research Scholarship, Aug 2022 –Aug 2026
- Outstanding Graduate Scholarship, Fudan University, Dec 2019
- “Gongneng” Scholarship, Nankai University (×3)
- Merit Student, Nankai University, Nov 2018
- Special Prize, Tianjin Collegiate Mathematics Competition (Top 29), Jul 2016
- First Prize, Nankai University Physics Academic Competition, May 2016