

# 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

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

## Education

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### 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

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### 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

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- **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

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- 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