Yipeng Zhang | Curriculum Vitae

School of Physical and Mathematical Sciences (SPMS)

Nanyang Technological University (NTU), Singapore

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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