# Yipeng Zhang | Curriculum Vitae

⚲ School of Physical and Mathematical Sciences (SPMS)

Nanyang Technological University (NTU), Singapore

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## Research Interests

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.

**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, Yipeng**, Cong Shen, and Kelin Xia. *Multi-Cover Persistence (MCP)-based Machine Learning for Polymer Property Prediction*. **Briefings in Bioinformatics**, 25(6): bbae465, 2024.

2. Han, Bingqing, **Yipeng Zhang**, Longlong Li, Xinqi Gong, and Kelin Xia.
   *TopoQA: A Topological Deep Learning-based Approach for Protein Complex Interface Quality Assessment*.
   **Briefings in Bioinformatics**, 26(2): bbaf083, 2025.

3. Wang, Yaxing, Xiang Liu, **Yipeng Zhang**, Xiangjun Wang, and Kelin Xia.
   *Join Persistent Homology (JPH)-based Machine Learning for Metalloprotein–Ligand Binding Affinity Prediction*.
   **Journal of Chemical Information and Modeling**, 2025.

4. Longlong Li, **Yipeng Zhang** (co-first author), Guanghui Wang, and Kelin Xia.

*Kolmogorov–Arnold Graph Neural Networks (KA-GNNs) for Molecular Property Prediction*.
**Nature Machine Intelligence**, 7, 1–9, 2025.

## Conference Papers

1. **Zhang, Yipeng**, Longlong Li, and Kelin Xia.
   *Rhomboid Tiling for Geometric Graph Deep Learning*.
   **Proceedings of the 42nd International Conference on Machine Learning (ICML 2025)**.

## Manuscripts Under Review

1. Cong Shen, **Yipeng Zhang**, Tze Kwang Gerald Er, Fei Han, Atsushi Goto, and Kelin Xia.
   *Molecular Topological Deep Learning for Polymer Property Prediction*.
   Under review at **ACS Nano**.
2. Han, Bingqing, **Yipeng Zhang**, Mei Zheng, Xinqi Gong, Kelin Xia.
   *Rhomboid Tiling-based Topological Deep Learning (RT-TDL) for Quality Assessment of Protein Complex Structures*.
   Under review at **Science Advances**.

## Manuscripts in Preparation

1. **Yipeng Zhang**, 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