

# Xiang Liu, Ph.D candidate

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## Education

- 2021/09 – ..... 📌 **Ph.D. Chern Institute of Mathematics, Nankai University**  
supervised by **Prof. Kelin Xia** and **Prof. Huitao Feng**
- 2017/09 – 2020/12 📌 **M.S School of Mathematical Sciences, Nankai University**  
supervised by **Prof. Xiangjun Wang**
- 2013/09 – 2017/06 📌 **B.E College of Software, Jilin University**

## Research Experience

- 2023/11 – ..... 📌 **Joint Phd Student** School of Physical and Mathematical Sciences, Nanyang Technological University. In Prof. **Kelin Xia**'s group.
- 2022/06 – 2023/09 📌 **Visiting scholar** Yanqi Lake Beijing Institute of mathematical sciences and applications (BIMSA). In Prof. **Jie Wu**'s group.
- 2020/09 – 2021/09 📌 **Visiting Research Fellow** Center for Topology and Geometry based Technologies, Hebei Normal University. In Prof. **Jie Wu**'s group.
- 2019/12 – 2020/07 📌 **Visiting student** School of Physical and Mathematical Sciences, Nanyang Technological University. In Prof. **Kelin Xia**'s group.

## Research Interests

Topological/Geometric data analysis

Mathematical AI

Machine/Deep learning

## Research Publications

1. Shuang Wu, **Xiang Liu**, Ang Dong, Claudia Gagnoli, Christopher Griffin, Jie Wu, Shing-Tung Yau, Rongling Wu. The metabolomic physics of complex diseases. *The Proceedings of the National Academy of Sciences (PNAS)*, 120(42), e2308496120 (2023)
2. Jialin Bi, Junjie Wee, **Xiang Liu**, Cunquan Qu, Guanghui Wang, Kelin Xia. Multiscale Topological Indices for the Quantitative Prediction of SARS CoV-2 Binding Affinity Change upon Mutations. *Journal of Chemical Information and Modeling*, 63(13), 4216-4227 (2023)
3. Kelin Xia, **Xiang Liu**, Junjie Wee. Persistent Homology for RNA Data Analysis. *Homology Modeling: Methods in Molecular Biology*, 2627:211-229 (2023)
4. **Xiang Liu**, Huitao Feng, Zhi Lü, Kelin Xia, Persistent Tor-algebra for protein-protein interaction analysis, *Briefings in Bioinformatics*, 24(2) 2023; bbado46, <https://doi.org/10.1093/bib/bbado46>. (2023)

5. Ran Liu, **Xiang Liu**, Jie Wu. Persistent Path-Spectral (PPS) Based Machine Learning for Protein–Ligand Binding Affinity Prediction. *Journal of Chemical Information and Modeling* 63(3), 1066-1075. (2023)
6. **Xiang Liu**, Huitao Feng, Jie Wu, Kelin Xia. Hom-Complex-Based Machine Learning (HCML) for the Prediction of Protein–Protein Binding Affinity Changes upon Mutation. *Journal of Chemical Information and Modeling* 62(17), 3961-3969. (2022)
7. Li Xiao-Shuang, **Xiang Liu**, Le Lu, Xian-Sheng Hua, Ying Chi, and Kelin Xia. Multiphysical graph neural network (MP-GNN) for COVID-19 drug design. *Briefings in Bioinformatics*, 23(4); bbac231, (2022).
8. **Xiang Liu**, Huitao Feng, Jie Wu, Kelin Xia, Dowker complex based machine learning (DCML) models for protein-ligand binding affinity prediction, *Plos Computational Biology*, 18(4), e1009943, (2022)
9. **Xiang Liu**, Kelin Xia, Persistent Tor-algebra based stacking ensemble learning (PTA-SEL) for protein-protein binding affinity prediction, *ICLR 2022 Workshop on Geometrical and Topological Representation Learning*, GTRL 2022 Poster, (2022)
10. Peiran Jiang, Ying Chi, Xiao-Shuang Li, Zhenyu Meng, **Xiang Liu**, Xian-Sheng Hua, Kelin Xia, Molecular persistent spectral image (Mol-PSI) representation for machine learning models in drug design, *Briefings in Bioinformatics*, 23(1); bbab527, (2022)
11. **Xiang Liu**, Kelin Xia. Neighborhood Complex Based Machine Learning (NCML) Models for Drug Design. *Interpretability of Machine Intelligence in Medical Image Computing, and Topological Data Analysis and Its Applications for Medical Data*. Springer, Cham, 87-97. **(Spot Light)** (2021)
12. **Xiang Liu**, Huitao Feng, Jie Wu, Kelin Xia, Persistent spectral hypergraph based machine learning (PSH-ML) for protein-ligand binding affinity prediction, *Briefings in Bioinformatics*, 22(5); bbab127, (2021)
13. **Xiang Liu**, Xiangjun Wang, Jie Wu, Kelin Xia, Hypergraph based persistent cohomology (HPC) for molecular representations in drug design, *Briefings In Bioinformatics*, 22(5); bbaa411, (2021)

## Academic Activities

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- Invited speaker, BIMSA workshop on digraph topology and GLMY theory, BIMSA, November 24-26, 2023
- Invited speaker, TDA Seminar at Mathematical Science Research Center, Chongqing University of Technology, November 16, 2023
- Poster, The first International Congress of Basic Science, BIMSA, July 16-28, 2023
- Invited speaker, Advances in Homotopy Theory IV, BIMSA, June 19-23, 2023
- Invited speaker, Topology and application seminar, Shihezi University, May 20-22, 2023
- Invited speaker, Nankai 2023 Topology and its application Seminar, Nankai University, May 13-15, 2023
- Invited speaker, BIMSA Topology Seminar, BIMSA, December 26, 2022
- Invited speaker, Applied topology seminar, Liaoning Normal University, December 9-11, 2022
- Poster, ICMMA 2022 International Conference on "Topology and its Applications to Engineering and Life Science", November 29, 2022
- Invited speaker, Seminar at Southern University of Science and Technology, Department of Mathematics, September 19, 2022
- Invited speaker, The 2nd Young Topologist Seminar, BIMSA, June 4-8, 2022

- Poster, ICLR 2022 Workshop on Geometrical and Topological Representation Learning, April 29, 2022
- Invited speaker, Topological Data Analysis and its Applications for Medical Data (MICCAI 2021), September 27, 2021 (Spot Light)
- Invited speaker, International Conference and Summer School on Applied Topology, Shijiazhuang, August 1-15, 2021
- Invited speaker, Applied topology seminars, Dalin University of Technology, June 6-11, 2021
- Invited speaker, Applied topology winter school and seminars, Liaoning Normal University (Online meeting), December 13-16, 2020
- Invited speaker, The first Joint workshop on Topology and Data Science, Chongqing University of Science and Technology, August 25-29, 2020.
- Participation, Workshop on Computational Topology at Dalian, Dalian University of Technology, July 21-31, 2019

## **Seminar Organized**

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- Organizer (with Jie Wu, Jingyan Li), BIMSA Math and Biology Seminar, BIMSA, September 23 — December 30, 2022