

Kelin Xia

Associate Professor

School of Physical and Mathematical Sciences

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Educational and Professional Qualifications

- **Michigan State University**
Visiting Assistant Professor *Jan. 2013 – May 2016*
– Mentor: Guo-Wei Wei
- **Michigan State University**
Visiting scholar *Dec. 2009 – Nov. 2012*
– Advisor: Guo-Wei Wei
- **Ph.D. Graduate University of Chinese Academy of Sciences, China**
Ph.D in Applied Mathematics *Jun. 2007 – Jan. 2013*
– Advisor: Meng Zhan and Guo-Wei Wei

Appointments

- **Nanyang Technological University**
Associate Professor *Mar. 2023 – Present*
- **Nanyang Technological University**
Assistant Professor *Jun. 2016 – Feb. 2023*

Journal Editorship

- Associated Editor: Computational Physiology and Medicine - Frontiers (2022-Present)
- Editorial Advisory Board: Journal of Chemical Information and Modeling (2022- Present)
- Editorial Advisory Board: Patterns (2022- Present)
- Topic Editor: "Topology vs. Geometry in Data Analysis/Machine Learning", MDPI (2022-2023)
- Associate Editors: Computational and Mathematical Biophysics (2021-Present)

Grants and Awards

- Co-PI, MOE AcRF Tier 2, "Machine-Learning-Assisted Topological and Geometrical Data Analysis of Extreme Events in Complex Systems", 2023-2026, SGD 398,380.00
- PI, SPMS Collaborative Research Award, "Geometric data analysis (GDA)-based learning models for corrugated 2D perovskites design and discovery", 2023-2024

- PI, MOE AcRF Tier 2, "Ricci curvature based deep learning models for polymer informatics", 2022-2025, SGD 797,689.00
- Co-PI, NMRC, "Indoor air microbiomes as a gateway to exposome-guided precision medicine for respiratory diseases", 2021-2024, SGD 1,410,000.00
- PI, MOE AcRF Tier 2, "Hodge Laplacian based deep learning models for drug design", 2021-2024, SGD 706,800.00
- Co-PI, MOE AcRF Tier 1, "Incorporating Quantum Chemistry Descriptors and Topological Features to Study G-quadruplex-stabilizer Complexes by Machine Learning Models", 2021-2023, SGD 135,000.00
- PI, MOE AcRF Tier 2, "Topology-based featurization for machine learning models in materials informatics", 2021-2024, SGD 606,456.00
- PI, Alibaba-NTU JRI "Artificial intelligence (AI) based drug design and drug discovery", 2020-2021, SGD 136,104.00
- PI, Merlion Program, "Machine learning models based on weighted-persistent-homology for structure-based drug design", 2020-2022, SGD 22,605.00
- Collaborator, MOE AcRF Tier 1 Thematic Grant, "Improving photocatalysts that recycle microplastics to fuels by artificial intelligence", 2020-2022, SGD 200,000.00
- PI MOE AcRF Tier 1, "Bipartite-graph-based machine learning models for biomolecular interaction analysis", 2020-2022, SGD 99,000.00
- Collaborator, ACE, "Artificial intelligence for the prediction of alternative splicing from epigenomics and transcriptomics data in cancer", 2019-2021, SGD 180,000.00
- PI, NTU/NUS-JSPS, "Elucidation of dynamic opening and closing mechanism of giant protein cage vault", 2019-2021, SGD 76,000.00
- PI: MOE AcRF Tier 2, MOE2018-T2-1-033, "Persistent homology based topological approaches for biomolecular data analysis", 2018-2021, SGD 324,576.00
- PI: MOE AcRF Tier 1, RG31/18, "Modeling and analyzing environmental effects and self-assembly mechanism of large-sized biomolecules", 2018-2020, SGD 94,050.00
- PI: MOE AcRF Tier 1, RG126/16, "A Unified Framework for Multiscale Geometric Modeling of Biomolecular Complex", 2017-2019, SGD 80,000.00
- Co-PI: ASPIRE League Research Grant, "Functional Design of Protein Cage for Sustainable Bionanomaterial", 2017-2018, JPY 3,000,000.00
- PI: Nanyang Technological University, SUG-M4081842.110, 2016-2021, SGD 100,000.00

Before joining NTU

- Co-PI (PI: Guo-Wei Wei), National Science Foundation, DMS-1160352, "FRG: Collaborative research: Variational multiscale approaches to biomolecular structure, dynamics and transport" 09/2012-08/2015.
- Co-PI (PI: Guo-Wei Wei), NIH/NIGMS, 3R01GM090208-04S1, "Geometric flow approach to implicit solvation modeling" 07/2014-06/2015.

Conference organized

- Organizer (with Jie Wu and Jelena Grbic), "Biomolecular Topology: Modelling and Data Analysis", IMS, NUS, June 24-28, 2024
- Organizer (with Huitao Feng, Fei Han, and Wilderich Tuschmann), "Applied geometry for data sciences", Mathematical Science Research Center, Chongqing, China, July 25-29, 2022
- Organizer (with Jie Wu, Fei Han, and Jelena Grbic), "Applied Topology in Frontier Sciences", IMS, NUS, July 11-22, 2022
- Organizer, special seminar series on "Topologica data analysis (TDA) and its applications", May, 2022
- Associated organizer, "AMSS-YMSC-BIMSA Joint Seminar on Progress of Topology and Its Applications", 2022
- Organizer (with Massimo Ferri, Vidit Nanda, Jie Wu, Guowei Wei), "Beyond TDA—Persistent topology and its applications in data sciences", Online meeting, August 28-30, 2021

Publications

72. Xiang Liu, Huitao Feng, Zhi Lü, **Kelin Xia**, Persistent Tor-algebra for protein-protein interaction analysis, *Briefings in Bioinformatics*, bbado46, <https://doi.org/10.1093/bib/bbado46> (2023)
71. Jian Liu, **Kelin Xia**, Jie Wu, Stephen Shing-Toung Yau, and Guo-Wei Wei. "Biomolecular Topology: Modelling and Analysis." *Acta Mathematica Sinica, English Series* 38(10), 1901-1938 (2022)
70. D. Vijay Anand, Qiang Xu, Junjie Wee, **Kelin Xia**, and Tze Chien Sum, "Topological feature engineering for machine learning based halide perovskite materials design", *npj Computational Materials*, 8 (203) (2022)
69. Leong, Yong Xiang, Emily Xi Tan, Shi Xuan Leong, Charlynn Sher Lin Koh, Lam Bang Thanh Nguyen, Jaslyn Ru Ting Chen, **Kelin Xia**, and Xing Yi Ling, "Where Nanosensors Meet Machine Learning: Prospects and Challenges in Detecting Disease X", *ACS nano* (2022)
68. Xiang Liu, Huitao Feng, Jie Wu, and **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* (2022)
67. 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*, bbac231 (2022).
66. Ronald Koh Joon Wei, Junjie Wee, Valerie Evangelin Laurent, and **Kelin Xia**, "Hodge theory-based biomolecular data analysis", *Scientific Report*, 12(1), 1-16 (2022)
65. Weikang Gong, Junjie Wee, Min-Chun Wu, Xiaohan Sun, Chunhua Li, **Kelin Xia**, "Persistent spectral simplicial complex-based machine learning for chromosomal structural analysis in cellular differentiation", *Briefings in Bioinformatics*, bbac168 (2022)
64. Jelena Grbic, Jie Wu, **Kelin Xia** and Guowei Wei, "Aspects of topological approaches for data science." *Foundations of Data Science*, 4(2), 165 (2022)
63. Xiang Liu, Huitao Feng, Jie Wu, and **Kelin Xia**, "Dowker complex based machine learning (DCML) models for protein-ligand binding affinity prediction." *PLOS Computational Biology* (2022)

62. Chi Seng Pun, Si Xian Lee, and **Kelin Xia**, "Persistent-homology-based machine learning: a survey and a comparative study." *Artificial Intelligence Review* (2022)
61. JunJie Wee and **Kelin Xia**, "Persistent spectral based ensemble learning (PerSpect-EL) for protein-protein binding affinity prediction." *Briefings In Bioinformatics*, 23(2), bbaco24 (2022)
60. Jiajie Peng, Jinjin Yang, D. Vijay Anand, Xuequn Shang, and **Kelin Xia**, "Flexibility and rigidity index for chromosome packing, flexibility and dynamics analysis." *Frontiers of Computer Science*, 16 (4), 1-11 (2022)
59. Peiran Jiang, Ying Chi, Xiao-Shuang Li, Xiang Liu, Xian-Sheng Hua, and **Kelin Xia**, "Molecular persistent spectral image (Mol-PSI) representation for machine learning models in drug design." *Briefings in Bioinformatics*, 23 (1), bbab527 (2022)
58. Jinghao Peng, Jiajie Peng, Haiyin Piao, Zhang Luo, **Kelin Xia**, and Xuequn Shang, "Predicting chromosome flexibility from the genomic sequence based on deep learning neural networks." *Current Bioinformatics* 16 (10), 1311-1319 (2021)
57. Jayanth Kumar Narayana, Micheál Mac Aogáin, Wilson Wen Bin Goh, **Kelin Xia**, Krasimira Tsaneva-Atanasova, and Sanjay H. Chotirmall, "Mathematical-based microbiome analytics for clinical translation." *Computational and Structural Biotechnology Journal*, 19, 6272-6281 (2021)
56. Peter Tsung-Wen Yen, **Kelin Xia**, and Siew Ann Cheong, "Understanding Changes in the Topology and Geometry of Financial Market Correlations during a Market Crash." *Entropy* 23.9: 1211 (2021)
55. JunJie Wee and **Kelin Xia**, "Forman persistent Ricci curvature (FPRC) based machine learning models for protein-ligand binding affinity prediction", *Briefings In Bioinformatics*, bbab136 (2021)
54. Zhenyu Meng and **Kelin Xia**, "Persistent spectral based machine learning (PerSpect ML) for protein-ligand binding affinity prediction", *Science advances*, 7(19), eabc5329, (2021)
53. Xiang Liu, Huitao Feng, Jie Wu, and **Kelin Xia**, "Persistent spectral hypergraph based machine learning (PSH-ML) for protein-ligand binding affinity prediction", *Briefings In Bioinformatics*, 22 (5), bbab127 (2021)
52. JunJie Wee and **Kelin Xia**, "Ollivier persistent Ricci curvature (OPRC) based machine learning for protein-ligand binding affinity prediction", *Journal of Chemical Information and Modeling*, 61 (4), 1617-1626 (2021)
51. Duan Chen, Shaoyu Li, Xue Wang, and **Kelin Xia**, "Fast random algorithms for manifold based optimization in reconstructing 3D chromosomal structures." *Communications in Information and Systems*, 21 (1), 1-29 (2021)
50. Xiang Liu, Xiangjun Wang, Jie Wu, and **Kelin Xia**, "Hypergraph based persistent cohomology (HPC) for molecular representations in drug design", *Briefings In Bioinformatics*, 22 (5), bbaa411 (2021)
49. Jinyin Zha, Yuwei Zhang, **Kelin Xia**, and Fei Xia, "Coarse-grained simulation of mechanical properties of single microtubules with micrometer length." *Frontiers in Molecular Biosciences*, 7, 517 (2020)
48. Chi Seng Pun, Brandon Yung Sin Yong, and **Kelin Xia**, "Weighted-persistent-homology-based machine learning for RNA flexibility analysis", *PLOS ONE*, 15 (8), e0237747 (2020)
47. Chengyuan Wu, Shiquan Ren, Jie Wu, **Kelin Xia**, "Weighted fundamental group", *Bulletin of the Malaysian Mathematical Sciences Society*, 43 (6), 4065-4088 (2020)

46. D Vijay Anand, Zhenyu Meng, **Kelin Xia**, Yuguang Mu, "Weighted persistent homology for osmolyte molecular aggregation and hydrogen-bonding network analysis", *Scientific Report*, 10, 9685 (2020)
45. Chengyuan Wu, Shiquan Ren, Jie Wu, **Kelin Xia**, "Discrete Morse Theory for Weighted Simplicial Complexes", *Topology and its Applications*, 270, 107038 (2020)
44. Zhenyu Meng, D Vijay Anand, Yunpeng Lu, Jie Wu, **Kelin Xia**, "Weighted persistent homology for biomolecular data analysis", *Scientific Report*, 10, 2079 (2020)
43. **Kelin Xia**, D Vijay Anand, Shikhar Saxena, Yuguang Mu, "Persistent homology analysis of osmolyte molecular aggregation and their hydrogen-bonding networks", *Physical Chemistry Chemical Physics*, 21, 21038-21048 (2019)
42. Zhenliang Wu, Yuwei Zhang, John Zenghui Zhang, **Kelin Xia**, and Fei Xia, "Determining Optimal Coarse-Grained Representation for Biomolecules Using Internal Cluster Validation Indexes", *Journal of Computational Chemistry*, Accepted (2019)
41. Chengyuan Wu, Shiquan Ren, Jie Wu, **Kelin Xia**, "Magnus Representation of Genome Sequences", *Journal of Theoretical Biology*, 480(7), 104-111 (2019)
40. Liangzhen Zheng, **Kelin Xia**, and Yuguang Mu. "Ligand binding induces agonistic-like conformational adaptations in helix 12 of progesterone receptor ligand binding domain." *Frontiers in Chemistry*, 7(315) (2019)
39. Yuwei Zhang, **Kelin Xia**, Zexing Cao, Frauke Gräter, and Fei Xia, "A New Multiscale Method for Construction of Coarse-Grained Models of Large Biomolecules from Low Resolution Data of Cryo-Electron Microscopy", *Physical Chemistry Chemical Physics*, 21, 9720-9727 (2019) (PCCP HOT Articles)
38. Manchugondanahalli S. Krishna, Desiree-Faye Kaixin Toh, Zhenyu Meng, Alan Ann Lerk Ong, Zhenzhang Wang, Yunpeng Lu, **Kelin Xia**, Mookkan Prabakaran, and Gang Chen, "Sequence- and structure-specific probing of RNAs by short nucleobase-modified dsRNA-binding PNAs (dbPNAs) incorporating a fluorescent light-up uracil analog", *Analytical Chemistry*, 91(8):5331-5338 (2019)
37. Alan Ann Lerk Ong, Desiree-Faye Kaixin Toh, Kiran M. Patil, Zhenyu Meng, Zhen Yuan, Manchugondanahalli S. Krishna, Gitali Devi, Phensinee Haruehanroengra, Yunpeng Lu, **Kelin Xia**, Katsutomo Okamura, Jia Sheng, and Gang Chen, "General Recognition of U-G, U-A, and C-G Pairs by Double-Stranded RNA-Binding PNAs Incorporated with an Artificial Nucleobase", *Biochemistry*, 58(10), 1319-1331 (2019)
36. D Vijay Anand, Zhengyu Meng, **Kelin Xia** "Complex multiscale virtual particle model based elastic network model (CMVP-ENM) for normal mode analysis of biomolecular complexes", *Physical Chemistry Chemical Physics*, 21, 4359-4366 (2019)
35. **Kelin Xia**, "Persistent similarity for biomolecular structure comparison", *Communications in Information and Systems*, 18 (4), 251-280 (2018)
34. **Kelin Xia**, "Persistent homology analysis of ion aggregation and hydrogen-bonding network", *Physical Chemistry Chemical Physics*, 20, 13448-13460 (2018)
33. **Kelin Xia**, "Sequence-based Multiscale Modeling for high-throughput Chromosome Conformation Capture (Hi-C) Data Analysis", *PLOS ONE*, 13 (2), e0191899, 2018
32. **Kelin Xia**, "Multiscale virtual particle based elastic network model (MVP-ENM) for biomolecular normal mode analysis", *Physical Chemistry Chemical Physics*, 20 (1), 658-669, 2018

31. **Kelin Xia**, Zhiming Li, Lin Mu, "Multiscale persistent functions for biomolecular structure characterization", *Bulletin of Mathematical Biology*, 80(1),1-30, 2018
30. Yin Cao, Bao Wang, **Kelin Xia** and Guo-Wei Wei, "Finite volume formulation of the MIB method for elliptic interface problems", *Journal of Computational and Applied Mathematics*, 321, 60-77, 2017
29. Lin Mu, **Kelin Xia** and Guowei Wei, "Geometric and electrostatic modeling using molecular rigidity functions", *Journal of Computational and Applied Mathematics*, 313, 18-37, 2016
28. Duc D Nguyen, **Kelin Xia** and Guo-Wei Wei, "Generalized flexibility-rigidity index", *Journal of Computational Chemistry*, 144, 234106, 2016
27. Kristopher Opron, **Kelin Xia** , Zachary F. Burton and Guo-Wei Wei, "Flexibility-Rigidity index for protein-nucleic acid flexibility and fluctuation analysis", *Journal of Computational Chemistry*, 37, 1283-1295, 2016

Before joining NTU

26. Zixuan Cang, Lin Mu, Kedi Wu, Kristopher Opron, **Kelin Xia** and Guo-Wei Wei, "A topological approach to protein classification", *Molecular Based Mathematical Biology*, 3, 140-162, 2015
25. **Kelin Xia**, Kristopher Opron and Guo-Wei Wei, "Multiscale Gaussian network model (mGNM) and multiscale anisotropic network model (mANM)", *Journal of Chemical Physics*, 143, 204106, 2015
24. **Kelin Xia**, Zhixiong Zhao and Guo-Wei Wei, "Multiresolution persistent homology for excessively large biomolecular datasets", *Journal of Chemical Physics*, 143, 134103, 2015
23. **Kelin Xia** and Guo-Wei Wei, "Multiresolution topological simplification", *Journal of Computational Biology*, 22(9), 1-5, 2015
22. **Kelin Xia** and Guo-Wei Wei, "Multidimensional persistence in biomolecular data", *Journal of Computational Chemistry*, 36, 1502-1520, 2015
21. **Kelin Xia** and Guo-Wei Wei, "Persistent homology for cryo-EM data analysis", *International Journal for Numerical Methods in Biomedical Engineering*, 31(8), e02719, 2015
20. Jinkyong Park, **Kelin Xia** and Guo-Wei Wei, "Atomic scale design and three dimensional simulations of nanofluidic systems", *Microfluidics and Nanofluidics*, 19(3), 665-692, 2015
19. Kristopher Opron, **Kelin Xia** and Guo-Wei Wei, "Communication: Capturing protein multiscale thermal fluctuations", *Journal of Chemical Physics*, 142, 211101, 2015
18. Bao Wang, **Kelin Xia** and Guo-Wei Wei, "Second order method for solving 3D elasticity equations with complex interfaces", *Journal of Computational Physics*, 294, 405-438, 2015
17. **Kelin Xia**, Xin Feng, Yiyong Tong and Guo-Wei Wei, "Persistent homology for the quantitative prediction of fullerene stability", *Journal of Computational Chemistry*, 36, 408-422, 2015
16. Bao Wang, **Kelin Xia** and Guo-Wei Wei, "Matched interface and boundary method for elasticity interface problems", *Journal of Computational and Applied Mathematics*, 285, 203-225, 2015
15. **Kelin Xia** and Guo-Wei Wei, "A Galerkin formulation of the MIB method for three dimensional elliptic interface problems", *Computers and Mathematics with Applications*, 68, 719-745, 2014
14. **Kelin Xia** and Guo-Wei Wei, "Persistent homology analysis of protein structure, flexibility and folding", *International Journal for Numerical Methods in Biomedical Engineering*, 30, 814-844, 2014

13. Kristopher Opron, **Kelin Xia** and Guo-Wei Wei, "Fast and anisotropic flexibility-rigidity index for protein flexibility and fluctuation analysis", *Journal of Chemical Physics*, 140, 234105, 2014
12. **Kelin Xia**, Meng Zhan and Guo-Wei Wei, "MIB Galerkin method for elliptic interface problems", *Journal of Computational and Applied Mathematics*, 272, 195-220, 2014
11. **Kelin Xia** and Guo-Wei Wei, "Molecular nonlinear dynamics and protein thermal uncertainty quantification", *Chaos*, 24, 013103, 2014
10. **Kelin Xia** and Guo-Wei Wei, "Stochastic model for protein flexibility analysis", *Physical Review E*, 88, 062709, 2013
9. **Kelin Xia**, Kristopher Opron and Guo-Wei Wei, "Multiscale multiphysics and multidomain models—Flexibility and rigidity", *Journal of Chemical Physics*, 139, 194109, 2013.
8. **Kelin Xia**, Xin Feng, Zhan Chen, Yiyong Tong and Guo-Wei Wei, "Multiscale geometric modeling of macromolecules I: Cartesian representation", *Journal of Computational Physics*, 257, 912-936, 2014
7. Xin Feng, **Kelin Xia**, Zhan Chen, Yiyong Tong and Guo-Wei Wei, "Multiscale geometric modeling of macromolecules II: Lagrangian representation", *Journal of Computational Chemistry*, 34, 2100-2120, 2013
6. Xin Feng, **Kelin Xia**, Yiyong Tong and Guo-Wei Wei, "Geometric modeling of subcellular structures, organelles, and multiprotein complexes", *International Journal for Numerical Methods in Biomedical Engineering*, 28(12), 1198-1223, 2012
5. Guo-Wei Wei, Qiong Zheng, Zhan Chen and **Kelin Xia**, "Variational multiscale models for charge transport", *SIAM Review*, 54(4), 699-754, 2012
4. **Kelin Xia**, Meng Zhan, Decheng Wan and Guo-Wei Wei, "Adaptively deformed mesh based interface method for elliptic equations with discontinuous coefficients", *Journal of Computational Physics*, 231(4), 1440-1461, 2012
3. **Kelin Xia**, Meng Zhan and Guo-Wei Wei, "MIB method for elliptic equations with multi-material interfaces", *Journal of Computational Physics*, 230(12), 4588-4615, 2011
2. Ming Yi, **Kelin Xia** and Meng Zhan, "Theoretical study for regulatory property of scaffold protein on MAPK cascade: a qualitative modeling", *Biophysical Chemistry*, 147(3), 130-139, 2010
1. Qi Zhao, Ming Yi, **Kelin Xia** and Meng Zhan, "Information propagation from IP₃ to target protein: a combined model for encoding and decoding of Ca²⁺ signal", *Physica A*, 388, 4105-4114, 2009

Conference papers

2. Xiang Liu, and 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 (2022)
1. Xiang Liu, and Kelin Xia, "Neighborhood complex based machine learning (NCML) models for drug design." In Interpretability of Machine Intelligence in Medical Image Computing, and Topological Data Analysis and Its Applications for Medical Data, pp. 87-97. Springer, Cham (2021).

Conferences and Presentations

- Invited speaker: "Topological Data Analysis and Applications", Dagstuhl Seminar, Germany, May 07-12, 2023
- Invited speaker: "Dirac equation between discrete and continuous: new trends and applications", Online, QMUL, May 3-4, 2023
- Invited speaker: CDSML Seminar Series, NUS, Feb 16, 2023
- Invited speaker: Spring School on Geometric Methods in Data Science, Braude College of Engineering, Karmiel, Israel, February 12-17, 2023
- Invited speaker: "Workshop on topological data analysis: mathematics, physics and beyond", KIAS, Seoul, South Korea, February 08-10, 2023
- Invited speaker: ICMMA 2022 International Conference on "Topology and its Applications to Engineering and Life Science", Meiji Institute for Advanced Study of Mathematical Sciences, Tokyo, Japan, November 28, 2022
- Invited speaker: Seminar at Queen Mary University of London, UK, November 16, 2022
- Invited speaker: Seminar at University of Liverpool, UK, November 15, 2022
- Invited speaker: Mini-sumposiums "Special Session on Applied Knot Theory" at 2022 Fall Southeastern Sectional Meeting, University of Tennessee at Chattanooga, Chattanooga, US, October 15-16, 2022
- Invited speaker: Seminar at Karlsruhe Institute of Technology, Germany, September 30, 2022
- Invited speaker: Seminar at University of Bologna, Italy, September 28, 2022
- Invited speaker: Seminar at University of Milan, Italy, September 26, 2022
- Invited speaker: Seminar at Naikai University, China, September 23, 2022
- Invited speaker: "The Second Workshop on Topological Data Analysis for Biomedical Imaging", Singapore, September 22, 2022
- Invited speaker: Seminar at School of Mathematics, Hangzhou Normal University, China, September 21, 2022 (Online meeting)
- Invited speaker: Seminar at Korea Institute for Advanced Study, Korea, August 17, 2022 (Online meeting)
- Invited speaker: Seminar at Xiamen University, China, August 04, 2022 (Online meeting)
- Invited speaker: Minisymposium "Molecular Biosciences: Advances in Molecular Property and Structure Predictions" on 2022 SIAM Conference on the Life Sciences, Pennsylvania, US, July 11, 2022 (Hybrid)
- Invited speaker: Seminar at International Laboratory of Algebraic Topology and Its Applications, HSE, Russia, May 20, 2022 (Online meeting)
- Invited speaker: Workshop on "The Mathematics of Soft Matter", Institute for Mathematical and Statistical Innovation (IMSI), Chicago, US, February 28-March 4, 2022 (Online meeting)
- Invited speaker: DKU-NUSRI Joint Workshop on Pure and Applied Mathematics, January 6-9, 2022 (Online meeting)

- Invited speaker: The fourth conference on Computational and Mathematical Bioinformatics and Biophysics, TSIMF, Sanya, China, December 13-17, 2021 (Online meeting)
- Invited speaker: Topological Data Analysis and its Applications for Medical Data (MICCAI 2021), September 27, 2021 (Spot Light)
- Invited speaker: Asia Pacific Seminar on Applied Topology and Geometry, September 17, 2021
- Invited speaker: Workshop on "Metrics in Multiparameter Persistence 2021", Lorentz Center@Virtual, July 19-22, 2021
- Invited speaker: ILJU POSTECH MINDS Workshop on "Topological Data Analysis and Machine Learning", July 6-9, 2021 (Zoom online meeting)
- Invited speaker: Applied Algebraic Topology Research Network (AATRN) Seminar, June 23, 2021 (Zoom online meeting)
- Invited speaker: Applied Topology Seminar 2021, Dalian University of Technology, June 6-11, 2021 (Online presentation)
- Invited speaker: POSTECH Minds Seminar, Pohang University of Science Technology, South Korea, May 25, 2021 (Zoom online meeting)
- Invited speaker: Nankai Mathematical Seminar, Naikai University, Tianjin, China, April 29, 2021 (Online meeting)
- Invited speaker: ACS spring 2021 symposium "Graph Theory Underpinning New Domains of Physical Chemistry", April 13, 2021 (Zoom online meeting)
- Invited speaker: Deep Learning for Dynamical System (ODE & PDE) Seminar, Duke-Kunshan University, China, March 22, 2021 (Zoom online meeting)
- Invited speaker: Seminar at data science institute, Shangdong Univeristy, China, Jan 15 2021 (Zoom online meeting)
- "The International Consortium of Chinese Mathematicians (ICCM) 2020 Annual Meeting", USTC, Hefei, China, Dec 27-29 (Zoom online meeting) Best Paper Award (distinguished paper)
- Invited speaker: "The third TSIMF Conference on Computational and Mathematical Bioinformatics and Biophysics", Sanya, China, Dec 20-24, 2020 (Zoom online meeting)
- Invited speaker: "The 8th East Asian Conference on Algebraic Topology" (EACAT 8), Vietnam Institute for Advanced Study in Mathematics (VIASM) & Vietnam National University (VNU), Dec 14-18, 2020 (Zoom online meeting)
- Invited speaker: "Applied topology winter school and seminars", Dec 13-16, 2020, Dalian, China (Online and onsite meeting)
- Invited speaker: CCMA Seminar on Mathematics of Data and Computation, Department of Mathematics, PennState, April 17, 2020
- Invited speaker(workshop cancelled): Symposium "Graph Theory Underpinning New Domains of Physical Chemistry" at Spring 2020 National Meeting of the American Chemical Society, Philadelphia, USA, March 22-26, 2020
- Invited speaker(workshop cancelled): Workshop on Geometry of Metric Spaces, Tsinghua Sanya International Mathematics Forum (TSIMF), Sanya, China, March 16-20, 2020

- Invited speaker: Winter School on Topological Data Analysis, Novosibirsk State University, Russia, February 3-8, 2020
- Invited speaker: Conference on "Algebraic Topology and Applied Topology", Chongqing, China, Jan 3-8, 2020
- Invited speaker: "The second conference on Computational and Mathematical Bioinformatics and Biophysics", Tsinghua Sanya International Mathematics Forum (TSIMF), Sanya, China, December 9-13, 2019
- Invited speaker: Singapore University of Technology and Design, Singapore, Sep 27 2019
- Invited speaker: Workshop on Computational Topology at Dalian, Dalian University of Technology, July 21-31, 2019
- Invited speaker: School of Mathematics, South China University of Technology, Guangzhou, June 11, 2019
- Invited speaker: Workshop on "Structure in the Micro-world", TGDA@OSU TRIPODS Center, Ohio State University, USA, May 28-31, 2019
- Invited speaker: "NSF-CBMS Conference: Mathematical Molecular Bioscience and Biophysics", Department of Mathematics, University of Alabama, USA, May 13 - 17, 2019
- Invited speaker: "Computational and Mathematical Approaches for Bioinformatics and Biophysics", Tsinghua Sanya International Mathematics Forum (TSIMF), Sanya, China, December 10-14, 2018
- (Academic Committee, Speaker) The First National Conference on Molecular Biology and Topology, Shijiazhuang, Hebei, China, Oct 26-29, 2018
- Invited speaker: Mini-symposium "Applied and Computational Topology" at SIAM Central States Section Meeting, University of Oklahoma, Norman, OK, Oct 5-7, 2018
- Invited speaker: Complexity community Share session, NTU, Singapore, Sep 25, 2018
- Invited speaker: Strategic Partnership with IIT Madras, IISc and IIT Bombay and Joint Workshops, India, Sep 17-20, 2018
- Invited speaker: Workshop on Algebraic topology and Geometric Topology, Dalian, China, Aug 9-13, 2018
- Invited speaker: (Declines due to time conflict) Mathematics of Drug Design/Discovery, The Fields Institute for Research in Mathematical Sciences, Toronto, Canada, June 4 - 7, 2018
- Invited speaker: Workshop on Algebraic Topology and Applied Topology, NUS, Singapore, Jan 23, 2018
- Invited speaker: School of Life Science and Technology, Tokyo Institute of Technology, Yokohama, Japan, Nov 24, 2017
- Invited speaker: Mini-symposium "Molecular Bioscience and Biophysics: Modeling and Computation" at the 3rd SIAM CSS annual meeting, Fort Collins, Colorado, Sep 29 - Oct 1, 2017
- Invited speaker: Department of Mathematics, National University of Singapore, September 20, 2017
- Invited speaker: NYU-ECNU Center for Computational Chemistry at NYU Shanghai, Shanghai, September 7, 2017

- Invited speaker: Workshop on "Topology of the biomolecular world", American Institute of Mathematics, San Jose, CA, July 24-28, 2017
- Invited speaker: International Symposium on Computational Mathematics, Optimization, and Computational Intelligence (CMOCI 2017), IIT Indore, India, July 17 - 19, 2017
- Invited speaker: "Mathematical Biophysics and Molecular Biosciences", Tsinghua Sanya International Mathematics Forum (TSIMF), Sanya, China, December 19-23, 2016
- Poster: MBI emphasis workshop on "Topological, Geometric, and Statistical Techniques in Biological Data Analysis", Mathematical Biosciences Institute, December 12-December 16, 2016
- Invited speaker: Department of Mathematics, National University of Singapore, August 31, 2016
- Invited speaker: Bioinformatics Institute, A*STAR, August 23, 2016
- Invited speaker: School of Biological Science, Nanyang Technological University, August 15, 2016
- Organizer: Mini-symposium "Molecular Biosciences and Biophysics: Topological and Geometric methods" at SIAM Conference on Life Sciences, Boston, Massachusetts, July 13, 2016 (Co-organizer: Prof. Natasha Jonoska)

Before joining NTU

- Invited speaker: Department of Mathematics and Statistics, University of North Carolina Charlotte, April 25, 2016
- Invited speaker: School of Mathematical Science, Monash University, April 21, 2016
- Invited speaker: School of Physical and Mathematical Science, Nanyang Technological University, March 8, 2016
- Invited speaker: Department of Mathematics, The university of Tennessee at Chattanooga, February 30, 2016
- Invited speaker: Department of Mathematical Science, Georgia Southern University, February 22, 2016
- Invited speaker: Department of Mathematics, North Carolina State University, January 21, 2016
- Invited speaker: MBI emphasis workshop on "Geometric and Topological Modeling of Biomolecules", Mathematical Biosciences Institute, Ohio State University, September 28-October 2, 2015
- Invited speaker: IMA hot topic workshop on "Mathematics of Biological Charge Transport: Molecular and Beyond", Institute for Mathematics and its Applications, Twin Cities, 2015
- Invited speaker: MBI workshop on "Geometric and Topological Modeling of Biomolecules", Mathematical Biosciences Institute, Ohio State University, September 28-October 02, 2015
- Organizer: Workshop on "Persistent homology for biosciences", East Lansing, October 18, 2014 (With Prof. Guo-Wei Wei and Prof. Yiying Tong)
- Organizer: Mini-symposium "Molecular Biosciences: Topological modeling of biomolecules" at SIAM Conference on Life Sciences, Charlotte, North Carolina, August 4-7, 2014 (Co-organizer: Prof. Yuanan Diao)

- Invited speaker: Mini-symposium "Modeling and computation of problems in mathematical biology" at The 38th annual meeting of the SIAM Southeastern Atlantic Section, Florida Institute of Technology in Melbourne, Florida, March 28-30, 2014
- Poster: IMA Annual Program Year Workshop Topological Structures in Computational Biology, December 9-13, 2013
- Poster: 2013 Great Lakes SIAM Conference: Computational Mathematics: Modeling, Algorithms and Applications, Central Michigan University, April 20, 2013
- Invited speaker: Mathematical Challenges in Biomolecular/Biomedical Imaging and Visualization, Mathematical Biosciences Institute, Ohio State University, February 18-22, 2013
- Invited speaker: 12th International Symposium on Mathematical and Computational Biology, Tempe, Arizona, November 7-10, 2012
- Speaker: SMB Annual Meeting and Conference, Knoxville, Tennessee, July 25-28, 2012
- Participation: 2nd Midwest Conference on Mathematical Methods for Images and Surfaces, East Lansing, August 27-28, 2011
- Participation: Modeling and Computation of Biomolecular Structure and Dynamics, Mathematical Biosciences Institute, Ohio State University, April 25-29, 2011
- Poster: Fluid Motion Driven by Immersed Structures, University of Toronto, August 9-13, 2010
- Participation: Workshop on Nano-Bio Mathematics and Mechanics, Michigan State University, August 5, 2010
- Participation: Modeling and Numerical PDEs in Mathematical Biology and Applications, Oakland University, April 16, 2011
- Participation: Frontiers in Mathematical Biology: NSF-NIH PIs Meeting 2010, University of Maryland, College Park, April 26-27, 2010
- Participation: SIAM Great Lakes Conference: Modeling and numerical PDEs in Mathematical Biology, University of Michigan at Dearborn, April 17, 2010

Teaching

- **Instructor**
 - "MH4517 Data Applications in Natural Sciences", MH4517, 2021
 - "Advance Investigation in Linear Algebra II", MH9201, 2021
 - "Calculus I", MH1100, 2021
 - "Advance Investigation in Linear Algebra I", MH9200, 2021
 - "MH4517 Data Applications in Natural Sciences", MH4517, 2020
 - "Advance Investigation in Linear Algebra II", MH921, 2020
 - "Advance Investigation in Linear Algebra I", MH9200, 2020
 - "Calculus I", MH1100, 2020
 - "Advance Investigation in Calculus II", MH9101, 2019
 - "Advance Investigation in Linear Algebra I", MH9200, 2019
 - "Calculus I", MH1100, 2019
 - "Advance Investigation in Calculus I", MH9100, 2018
 - "Calculus I", MH1100, 2018

"Algebraic Topology", MH4600, 2017
 "Calculus I", MH1100, 2017
 "Algebraic topology", MH4600, 2017
 "Advanced Investigations in Linear Algebra I" MH 9200, 2016
 "Calculus 1" MTH 132 (Section 016 and Section 020), 2015;
 "Calculus 1" MTH 132 (Section 014 and Section 033), 2014;
 "Calculus 1" MTH 132 (Section 016 and Section 024), 2013

- **Series of lectures**

"Modeling and Computation of human sensory systems" MTH 995 , 2013

- **Mentor for undergraduates (with Prof. Guo-Wei Wei)**

Archie Brown III, Summer Research Opportunities Program at MSU, 2012;
 Rinaldi Romulus, Summer Research Opportunities Program at MSU, 2013;
 Zhuozhuo Tu, International Exchange Program at Department of Mathematics in MSU, 2013;
 Fengze Cao, International Exchange Program at Department of Mathematics in MSU, 2014

Students and Postdocs

- **Postdoc**

Chuan-Shen HU: 2022- Present
 Min-Chun WU: 2021- 2022
 Bin Liu: 2020-2021
 Zhenyu Meng: 2018-2021
 Vijay Anand:2018-2021

- **Phd students**

Yasharth Bachubhai Yadav (2023.1-Present)
 Xinyu You (2023.1-Present)
 Yipeng ZHANG (2022.8-Present)
 Xiang LIU, 2021-Present (Joint with Prof. Huitao Feng)
 Liang HUANG, 2021-present
 Ronald Koh Joon Wei, 2019-present
 Junjie WEE, 2019-present

- **Final Year Project**

CHOO Hou Yee: 2021-2022
 TAN Zhi en, JOSHUA: 2021-2022
 WANG Zihong: 2021-2022
 TAN Chenhjui: 2020-2022
 TEDJA Erika: 2020-2021
 TI Tze Hong: 2019-2020
 KANG Hwee Young: 2019-2020
 EW Jo EE: 2019-2020
 WU Meixi: 2019-2020
 LAUREN Alerie Evangelin: 2018-2019
 LIM Wen Sheng: 2017-2018
 LEE Si Xian: 2017-2018
 CHU Wee Khong: 2016-2017

Professional services

Guest Editors

- Special issue "Topological modeling and analysis of big data in biomolecules" on Molecular Based Mathematical Biology, 2016

Journal Reviewer

- Applied Mathematics and Computation
- Bioinformatics
- Briefings in Bioinformatics
- Chemical Biology and Drug Design
- Chemical Physics Letters
- Chemical Science
- Communications Biology
- Computational and Structural Biotechnology Journal
- Computational Biology and Chemistry
- Computer Methods in Applied Mechanics and Engineering
- Computers in Biology and Medicine
- Drug Discovery Today
- European Journal of Applied Mathematics
- Genomics
- International Journal for Numerical Methods in Biomedical Engineering
- International Journal of Biomathematics
- Journal of Applied Mathematics
- Journal of Computational and Applied Mathematics
- Journal of Chemical Information and Modeling
- Journal of Chemical Physics
- Journal of Molecular Liquids
- Journal of Theoretical and Computational Chemistry
- Mathematics of Computation
- Molecular Based Mathematical Biology
- Nature Communications
- NeurIPS

- Neurocomputing
- Nonlinearity
- Scientific Report
- Statistical Applications in Genetics and Molecular Biology
- Symmetry
- Transactions on Computational Biology and Bioinformatics