

Miao-Jiong Tang

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CPC member | CET-6
Integrated M.S.-Ph.D. student in chemistry
• Department of Chemistry, Zhejiang University • data-driven chemistry / chemical AI



Integrated M.S.-Ph.D. student in chemistry at Zhejiang University, working on data-driven organic synthesis reaction modeling and computational acceleration. My research connects asymmetric catalysis, molecular/reaction data infrastructure, quantum-chemical computation, and graph representation learning; first-author papers in Angew. Chem., Int. Ed., Sci. Data, and Chem. Asian J., with contribution to the Nat. Mach. Intell. RXNGraphormer framework.

Education

Zhejiang University • Chemistry, Integrated M.S.-Ph.D. 2022.09 - 2027.06 expected
Department of Chemistry | Research: data-driven organic synthesis reaction modeling and computational acceleration | Advisor: Prof. Xin Hong Hangzhou, China

Zhejiang University • B.S. in Chemistry 2018.09 - 2022.06
Chu Kochen Honors College, Qiushi Chemistry Program | GPA 3.77/4.0 | Advisor: Prof. Xin Hong Hangzhou, China

Honors, Awards, and Funding

2026 Graduate	Zhejiang University Qiushi Rising Star doctoral funding	Funding Award
Undergraduate	Zhejiang University Outstanding Graduate Student; NHU Innovation Scholarship	Award
Undergraduate	Zhejiang University Outstanding Graduate; Outstanding Communist Youth League Member; MCM Meritorious Winner twice	Award
Undergraduate	Academic scholarships (Second Class once, Third Class twice); Chu Kochen Honors College Elite Student Scholarship; provincial SRTF project; National Chemistry Experiment Innovation Design Competition Third Prize	Scholarship

Internship Experience

Fudan Qingpu Institute of Future Technology 2026.07 - present
Research intern

- Designed topological-reaction transition-state generation algorithms and optimized Ascend-based training and inference.

Shanghai Academy of AI for Science • Matter Science Department 2024.07 - 2025.03
Algorithm intern

- Designed fictitious reaction generation algorithms for reaction embeddings, yield/selectivity prediction, and synthesis planning.

Project Experience

MolGR molecular graph reconstruction toolkit 2025.12 - present
XYZ-to-RDKit molecular graph reconstruction Python package Lead developer

- Developed a C++/Python XYZ-to-RDKit toolkit with bond orders, 3D conformers, optional dative bonds, and stereochemistry; optimized candidate enumeration, scoring, and post-processing for millisecond-level reconstruction and improved metal/spin handling.

N,N'-dioxide asymmetric Michael addition modeling platform 2024.10 - 2025.08
First-author paper: Angew. Chem., Int. Ed. 2026 First author / lead

- Curated N,N'-dioxide/metal-catalyzed Michael addition reactions and built mechanism-aware GNN and similarity-weighted extrapolation workflows for catalyst selection and selectivity prediction.

MolOP molecular computation log parser and data engine 2023.10 - present
Computational chemistry data parsing and automation toolkit Lead developer

- Developed a type-aware, unit-aware, parallelizable parser and data engine for molecular computation logs, supporting quantum-chemical data production and automated workflows.

Tianchi Scientific Intelligence Competition: molecular property prediction 2023.08 - 2023.10
Quantum-chemical energy and force prediction for organic molecules Team member

- Used graph neural networks to predict quantum-chemical energies and forces of organic molecules, with model and training-strategy optimization.

QM9star molecular dataset and qm9star_query platform 2023.03 - 2024.06
First-author paper: Sci. Data 2024 First author / lead

- Built a DFT-optimized dataset for ions, radicals, and neutral molecules, plus database queries, API services, GNN examples, and tutorials.

Spectrum-based molecular representations for reaction performance prediction

2022.04 - 2023.02

First-author paper: Chem. Asian J. 2023

First author / lead

- Parsed molecular NMR spectrum images with image-recognition workflows and applied spectrum-derived vectors to reaction performance prediction.

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Professional Skills

- Machine learning:** Proficient in Python-based research data mining, scripting, and model experimentation; familiar with supervised learning, GNNs, Transformer/pre-training models, and image-processing workflows for molecular property prediction, reaction selectivity, synthesis planning, and spectrum-based representations.
- Computational chemistry:** Experienced with Gaussian, xTB, and related tools; able to combine Python scripts with computation software for mechanism studies, batch optimization, log parsing, and data production; understands electronic structure, transition states, atomic/bond properties, and 3D conformations for molecular representation and model interpretation.
- Ascend and operator optimization:** Experienced with the Huawei Ascend platform and operator optimization; able to deploy and profile workloads, locate performance bottlenecks, and improve operator implementations and data flow for Ascend hardware.
- Cheminformatics:** Experienced with RDKit, OpenBabel, and molecular toolkit extension; able to build molecular and reaction data infrastructure from XYZ/SMILES, computation logs, literature reactions, spectrum images, and quantum-chemical outputs.
- Research engineering:** Experienced in chemical databases, API services, command-line tools, and reproducible data pipelines; familiar with backend development, Linux, CI/CD, containers, and virtualization for maintainable research software and automated workflows.
- GitHub:** <https://github.com/gentle1999>
- Google Scholar:** https://scholar.google.com/citations?user=86_ftaAAAAAJ
- ORCID:** <https://orcid.org/0000-0003-2075-366X>

Publications

Currently 3 first-author SCI papers and 8 co-authored papers. Publications are listed with representative works first.

- [Tang, M.-J.](#); Zhang, T.; Huang, Q.; Li, S.; Liu, R.; Li, H.; Chen, X.; Dong, S.; Liu, X.; Feng, X.; Hong, X. Data - Driven Modeling of N,N' - Dioxide/Metal - Catalyzed Asymmetric Michael Additions. *Angew. Chem., Int. Ed.* **2026**, 65(12), e18560. DOI: <https://doi.org/10.1002/anie.202518560> (2024 JIF: 17.0)
- [Tang, M.-J.](#); Zhu, T.-C.; Zhang, S.-Q.; Hong, X. QM9star, two Million DFT-computed Equilibrium Structures for Ions and Radicals with Atomic Information. *Sci. Data* **2024**, 11(1), 1158. DOI: <https://doi.org/10.1038/s41597-024-03933-6> (2024 JIF: 6.9)
- [Tang, M.-J.](#); Xu, L.-C.; Zhang, S.-Q.; Hong, X. Exploring Spectrum - based Molecular Descriptors for Reaction Performance Prediction. *Chem. Asian J.* **2023**, 18(7), e202300011. DOI: <https://doi.org/10.1002/asia.202300011> (2024 JIF: 3.3)
- Xu, L.-C.; [Tang, M.-J.](#); An, J.; Cao, F.; Qi, Y. A unified pre-trained deep learning framework for cross-task reaction performance prediction and synthesis planning. *Nat. Mach. Intell.* **2025**, 7(9), 1561-1571. DOI: <https://doi.org/10.1038/s42256-025-01098-4> (2024 JIF: 23.9)
- Xu, G.-X.; Liu, J.-R.; Gao, Z.; [Tang, M.-J.](#); Sun, Y.-Z.; Li, Z.-L.; Liu, X.-Y.; Zhang, S.-Q.; Hong, X. Unveiling mechanistic patterns of copper-catalyzed radical bond formation through linear free energy relationship. *Nat. Commun.* **2025**, 17(1), 1027. DOI: <https://doi.org/10.1038/s41467-025-67770-w> (2024 JIF: 15.7)
- Xu, L.-C.; Zhang, S.-Q.; Li, X.; [Tang, M.-J.](#); Xie, P.-P.; Hong, X. Towards Data - Driven Design of Asymmetric Hydrogenation of Olefins: Database and Hierarchical Learning. *Angew. Chem., Int. Ed.* **2021**, 60(42), 22804-22811. DOI: <https://doi.org/10.1002/anie.202106880> (2024 JIF: 17.0)
- Xu, L.-C.; Zhu, D.-X.; [Tang, M.-J.](#); Liu, T.-T.; Liu, Y.-Z.; Ma, C.-H.; Li, Z.-X.; Zhang, S.-Q.; Hong, X. Transforming Molecular Synthesis With Large Language Models. *Chem. Eur. J.* **2026**, 32(31), e71074. DOI: <https://doi.org/10.1002/chem.71074> (2024 JIF: 3.7)
- Wang, X.; [Tang, M.-J.](#); Yang, Z.; Xiong, A.; Hong, X.; Feng, X.; Liu, X. Asymmetric Desymmetrization of para - Quinamines via (3+2) Cycloaddition With 1,3,5 - Triazinanes. *Chem. Eur. J.* **2026**, 32(36), e71220. DOI: <https://doi.org/10.1002/chem.71220> (2024 JIF: 3.7)
- Chen, Z.; [Tang, M.](#); Chen, X.; Ding, D.; Gao, J.-K.; She, Y.; Yang, Y.-F. Using machine learning methods to predict the diabatic bond dissociation energy of non-heme iron complexes. *Org. Biomol. Chem.* **2025**, 23(19), 4758-4767. DOI: <https://doi.org/10.1039/d5ob00007f> (2024 JIF: 2.8)
- Sun, Y.-Z.; [Tang, M.-J.](#); Zhang, S.; Hong, X. 数据驱动的有机分子理化性质预测. *Chin. Sci. Bull.* **2024**, 70(4-5), 492-507. DOI: <https://doi.org/10.1360/tb-2024-0812> (2024 JIF: 1.2)
- Zhang, S.-Q.; Hong, X.; Xu, L.-C.; Li, X.; [Tang, M.-J.](#); Yuan, L.-T.; Zheng, J.-Y. A Molecular Stereostructure Descriptor Based On Spherical Projection. *Synlett* **2021**, 32(18), 1837-1842. DOI: <https://doi.org/10.1055/s-0040-1705977> (2024 JIF: 1.4)