

Yize Zhou

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SUMMARY

I previously worked as a Research Assistant at Wave Intelligence Lab, The Chinese University of Hong Kong, under the supervision of Prof. Shengchao Liu. My research lies at the intersection of AI for Science and biology, with a focus on advancing scientific discovery through geometric deep learning, generative models, and Large Language Model (LLM) reasoning.

EDUCATION

Wuhan University, Wuhan, China Sep. 2022 – Jun. 2025

- M.Sc. in Applied Mathematics, School of Mathematics and Statistics
- GPA: 3.64/4.00; Average: 90.8/100;
- Core Courses: Inverse Problems and Computation (92), Complex Network Theory and Applications (96), Advanced Numerical Analysis (96)
- Honors: First-Class Academic Scholarship of Wuhan University; National Second Prize (2 times), “Huawei Cup” China Graduate Mathematical Modeling Competition;

Hainan University, Haikou, China Sep. 2018 – Jun. 2022

- B.Sc. in Information and Computing Science, School of Mathematics and Statistics
- GPA: 3.72/4.00; Rank: 1/40; Average: 90.11/100;
- Core Courses: Mathematical Analysis (92), Computer Operating System (93), Operations Research and Optimization (95), Mathematical Modeling (96)
- Honors: National Scholarship (TOP 0.2%), First Prize, China Undergraduate Mathematical Contest in Modeling (CUMCM) (TOP 0.5%), Outstanding Winner & SIAM Award, Mathematical Contest in Modeling (MCM/ICM, TOP 0.02%)

PUBLICATIONS

- **Y. Zhou**, H. Li, and S. Liu*. (2026). A Resolution-Agnostic Geometric Transformer for Chromosome Modeling Using Inertial Frame. (*ICLR 2026*)
<https://openreview.net/forum?id=OwLl8Xi6JG>
- J. Li, L. Peng, Y. Li, **Y. Zhou**, H. Cao, C. Tan, and S. Liu*. (2026). Base-and-Sugar Dual-Frame Flow Matching for RNA Co-Design. (*ICML 2026 Workshop GenBio*)
<https://openreview.net/forum?id=6lIWd2AwK6>
- **Zhou, Y.**, Zhang, J., Zhu, C., & Wang, H*. (2022). Modelling and analysis of rumour propagation based on stochastic optimal control. *Alexandria Engineering Journal*, 61(12), 12869-12880. DOI: <https://doi.org/10.1016/j.aej.2022.06.057>
- Zhang, J., **Zhou, Y.**, Wang, Z., & Wang, H*. (2023). Analysis and achievement for fractional optimal control of Hepatitis B with Caputo operator. *Alexandria Engineering Journal*, 70, 601-611. DOI: <https://doi.org/10.1016/j.aej.2023.03.015>

RESEARCH EXPERIENCE

Project 1: Geometric Transformer for Chromosome Modeling. Jul. 2025 – Sep. 2025

Research Assistant, Wave Intelligence Lab, CUHK CSE (HongKong, China).

- Developed InertialGenome, a Transformer-based framework for 3D chromosome

reconstruction, solving limited model expressiveness and generalization issues across varying Hi-C resolutions.

- Implemented a pose canonicalization module to align chromosomes with their inertial frames, achieving a rotation-invariant 3D representation. Designed a geometry-aware positional encoding leveraging Nyström estimation to efficiently capture long-range structural dependencies via low-rank RBF kernel approximation.
- Evaluated the model on single-cell 3D datasets, outperforming 4 baselines and achieving a 5% improvement in cross-resolution transfer learning and functional verification tasks.

Project 2: Reasoning Trace Modeling for Pathway Discovery. Jan. 2026 – Jun. 2026

Research Assistant, Wave Intelligence Lab, CUHK CSE (HongKong, China).

- Developed ChatPathway, a thermodynamics-guided framework that models LLM reasoning traces to eliminate autoregressive semantic drift and causal inconsistencies in symbolic biological pathway generation.
- Constructed a latent phase space via a dual-loss Autoencoder, and integrated a Port-Hamiltonian Neural Network (PHNN) to enforce dissipative energy constraints for fine-tuning regularization and inference steering.
- Evaluated on a curated KEGG graph-text corpus across 6 tasks (e.g., pathway enrichment, counterfactual knockout inference), achieving stable convergence in physical alignment and significantly reducing biologically invalid generations.

Project 3: Drug–Target Affinity (DTA) Prediction

Apr. 2024 – Oct. 2024

AI Algorithm Intern, MetaNovas Biotech (Shanghai, China).

- Created Natural and Synthetic DTA datasets based on the Papyrus database (Homo sapiens subset); applied scaffold splitting for evaluation.
- Trained FusionDTA-based models: the partition model is synthetic, natural, pretrained + fine-tuned, and merged. Achieved Spearman correlations of 0.31, 0.45, 0.53, and 0.78 across the four models, confirming the benefits of pretraining and large-scale integration.
- Deployed a robust API for real-time prediction of unknown drug–target affinities, enabling downstream applications in drug discovery. Project selected for presentation at the 78th Annual Meeting of the Society of Cosmetic Chemists (SCC), USA.

Project 4: Meta-Learning Approach for Low-Data Drug Discovery Sep. 2024 – Oct. 2024

AI Algorithm Intern, MetaNovas Biotech (Shanghai, China).

- Developed a MAML-GAT framework that combines Model-Agnostic Meta-Learning (MAML) with graph attention networks (GAT) for low-resource molecular prediction tasks.
- Created scaffold-based few-shot tasks on skin permeability and sensitization; achieved superior generalization performance on unseen tasks.
- Demonstrated the effectiveness of meta-learning in reducing data dependency while maintaining high accuracy in drug discovery scenarios.

SKILLS & RESEARCH INTERESTS

Languages: Native Chinese; English: CET-6 (503)

Skills: Proficient in Python, MATLAB; skilled in PyTorch for geometric deep learning and generative model development.

Research Strengths: Hands-on experience in AI-driven biomolecular modeling, with independent project design and academic paper writing capabilities.