

Yize Zhou

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SUMMARY

I am currently a research intern at Peking University Chengdu Academy for Advanced Interdisciplinary Biotechnology, focusing on generative-AI driven peptide and biomolecular design. Previously, I worked as a Research Assistant at Wave Intelligence Lab, CUHK, supervised by 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

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| Wuhan University, Wuhan, China | Sep. 2022 – Jun. 2025 |
| <ul style="list-style-type: none">• 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 |
| <ul style="list-style-type: none">• 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>

RESEARCH EXPERIENCE

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| Project 1: Geometric Transformer for Chromosome Modeling. | Jul. 2025 – Sep. 2025 |
| <i>Research Assistant</i> , Wave Intelligence Lab, CUHK CSE (HongKong, China). | |
| <ul style="list-style-type: none">• 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.