ODIN ZHANG

(HAOTIAN ZHANG)

Paul G. Allen School of Computer Science & Engineering
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EDUCATION

Chinese University of Hong Kong — Hong Kong, China
Ph.D. in Computer Science, advised by **Pheng Ann Heng**, **David Baker**, **Gaurav Bhardwaj** — 2025.9-2027.9

- Vice-Chancellor Scholarship (only 1 in CS Department)
- ODesign Group Leader

University of Washington — Seattle, U.S.
Master (Ph.D. Transferred) in Computer Science, Paul G. Allen School, advised by **David Baker** — 2024.9 –2025.9

Zhejiang University — Hangzhou, China
M.M. in Pharmaceutical science, advised by **Tingjun Hou** and **Changyu Hsieh** — 2022.9 –2024.6

- National Scholarship (Top 1 Graduate Student in Pharmacy Department)

Zhejiang University — Hangzhou, China
Dual B.S in Pharmaceutical science & Physics, advised by **Tingjun Hou** — 2018.9 –2022.6

- GPA: 3.85/4.00
- First Prize in China Undergraduate Physics Tournament (Top 0.1%)
- Top Ten College Students in the College of Pharmacy (TOP 0.8%)
- Four First Prize in the 16th University Sports Games of Zhejiang Province

AWARDS

Baidu AI Talent Scholarship (10 Worldwide), Chu Kochen Scholarship. (Top 10 Graduate Student at ZJU)

RESEARCH INTERESTS

AI-aided Protein Design; AI-aided Small Molecule Design; LLM-Agent for Pharmaceutic Purpose

GRANTS

2025 LinGang Lab Key Project, project manager, 3 million￥; NSFC Basic Research Scheme (PhD), 300,000￥

INDUSTRY EXPERIENCE

LinGang Laboratory — Shanghai, China
Group Leader, AI Mol Design — 2025.06– present

- Led the AI-powered molecule design method development (ODesign Team).
- Organize the 10 target RNA/DNA/peptide/mini-protein design campaigns.

Pledge Therapeutics — Greater Boston, U.S.
Structure-based AIDD consultant — 2024.03– 2024.09

- Applied the Gen-AI to two test cases (internal) and two test cases (External).
- Refined Gen-AI platform based on crystallographer, structural biologist, and medicinal chemist insight.
- Performed Lead optimization of a viral capsid targeting small molecule
- Performed Hit expansion against a viral protein based on existing fragment co-crystal structure data

Carbon Silicon AI — Hangzhou, China
Senior DL-Engineer, leading a 10-people group — 2022.05– 2024.03

- Developed molecular conformation generation algorithms, the main product is **SDEGen.**
- Developed 3D pocket-aware drug design models, the main products are **ResGen** and **SurfGen.**
- Developed the first unified deep lead optimization framework, the main product is **Delete.**
- Developed protein-ligand binding conformation prediction model, the main product is **KarmaDock**
- Responsible for the molecular generation direction.

PUBLICATIONS

1. Zhang, H., Zhang, X., Lin, H., et al. ODesign: A World Model for Biomolecular Interaction Design. [2510.22304] ODesign: A World Model for Biomolecular Interaction Design
2. **Zhang, H**., Lin, H., Zhang, X., Wang, X., et al. Graph Neural Networks in Modern AI-aided Drug Discovery, ***Chemical Reviews***, 2025, 125, 20, 10001–10103. (IF=55.8)
3. Zhao, H., **Zhang, H.**, RAPiDock: Pushing the Boundaries of Protein-peptide Docking with Rational and Accurate Diffusion Generative Model. ***Nature Machine Intelligence***, 1308–1321 (2025). (通讯)
4. **Zhang, H.**, et al. ResGen is a pocket-aware 3D molecular generation model based on parallel multiscale modelling, ***Nature Machine Intelligence***, *5*, 1020–1030 (2023). Code
5. **Zhang, H.***, Wang T.*, et al. Learning on topological surface and geometric structure for 3D molecular generation, ***Nature Computational Science***,3.10 (2023): 849-859. Code
6. **Zhang, H.*,** Jin J.*, ECloudGen: Access to Broader Chemical Space for Structure-based Molecule Generation. ***Nature Computational Science***, *(*2025*).*
7. Zhang, X.*, **Zhang, H.***, et al. Efficient and accurate large library ligand docking with KarmaDock. ***Nature Computational Science***, *3*, 739–740 (2023). Code
8. Chen, S., **Zhang, H.*,** et al. Deep lead optimization enveloped in protein pocket and its application in designing potent and selective ligands targeting LTK protein. ***Nature Machine Intelligence****,7, 448–458 (2025).* Code
9. Wu, Z., **Zhang, H.**, Wang, X., et al. Leveraging Language Model for Advanced Multi-Property Molecular Optimization via Prompt Engineering. ***Nature Machine Intelligence***, 6, 1359-1369 (2024). Code
10. **Zhang, H.***, Huang, Y.*, Chen, S.*, et al. FragGen: towards 3D geometry reliable fragment-based molecular generation. ***Chemical Science*** 15.46 (2024): 19452-19465. Code
11. **Zhang, H.***, Lin, H*. et al, Deep Lead Optimization: Leveraging Generative AI for Structural Modification. ***Journal of the American Chemical Society*** 146.46 (2024): 31357-31370.
12. **Zhang, H.**, Li, S., Zhang, J., Wang, Z., Wang, J., Jiang, D., ... & Hou, T. (2023). SDEGen: learning to evolve molecular conformations from thermodynamic noise for conformation generation. ***Chemical Science***, *14*(6), 1557-1568. Code
13. Huang, Y.*, **Zhang, H**.*, Wu, L., Tan, C., Lin, H., Gao, Z., ... & Li, S. (2024). Re-Dock: Towards Flexible and Realistic Molecular Docking with Diffusion Bridge. ***ICML 2024***.
14. Lin, H.*, **Zhang, H.***, Zhao, H., Jiang, D., Wu, L., Liu, Z., ... & Li, S. Z. (2024). PPFlow: Target-aware Peptide Design with Torsional Flow Matching. ***ICML 2024***.
15. Wang, T.*, Zhang, X.*, **Zhang, H.***, et al. Highly accurate and efficient deep learning paradigm for full-atom protein loop modeling with KarmaLoop. ***Research*** *7 (2024): 0408*. Code
16. Zhang, J.*, **Zhang, H.*,** Qin, Z., Kang, Y., Hong, X., & Hou, T. (2023). Quasiclassical Trajectory Simulation as a Protocol to Build Locally Accurate Machine Learning Potentials**.** ***Journal of Chemical Information and Modeling***. *63(4),* 1133-1142
17. Lin, H. **Zhang, H.** …, Li, S. Tokenizing Electron Cloud in Protein-Ligand Interaction Learning, arxiv.
18. Weng, G., **Zhang, H.**, Nie, D., Zhang, H., Liu, L., Hou, T., & Kang, Y. (2024). Rediscmol: Benchmarking molecular generation models in biological properties. ***Journal of Medicinal Chemistry,*** 67(2), 1533-1543.
19. Wang, Y., **Zhang, H**., Wang, J., Tang, G., & Bai, H. (2023). An Engineered Design of Self-Assembly Nanomedicine Guided by Molecular Dynamic Simulation for Photodynamic and Hypoxia-Directed Therapy. ***Molecular Pharmaceutics*** *20(4),* 1543-8384.
20. Zhang, X., Shen, C., **Zhang, H.**, Kang, Y., Hsieh, C. Y., & Hou, T. (2024). Advancing Ligand Docking through Deep Learning: Challenges and Prospects in Virtual Screening. ***Accounts of Chemical Research***, 789-804.
21. Wang, M., Li, S., Wang, J., **Zhang., H**., et al. ClickGen: Directed Exploration of Synthesizable Chemical Space via Modular Reactions and Reinforcement Learning. ***Nature Communications****, 15(1), 10127.* Code
22. Lin H, Yufei Huang, **Zhang, H.**, et al. DiffBP: Generative Diffusion of 3D Molecules for Target Protein Binding. ***Chemical Science*** 16.3 (2025): 1417-1431.. Code
23. Lin H, Yufei Huang, **Zhang, H.**, et al. Functional-Group-Based Diffusion for Pocket-Specific Molecule Generation and Elaboration. ***NeurIPS 2024***, arxiv: 2306.13769.
24. Du H.*, Jiang D.*, **Zhang, H.**, et al. A Flexible Data-Free Framework for Structure-Based De Novo Drug Design with Reinforcement Learning. ***Chemical Science****, 14(43), 12166-12181.*. Code
25. Zhao, Y., Zhang, J., **Zhang, H.**, Gu, S., Deng, Y., Tu, Y., ... & Kang, Y. (2023). Sigmoid Accelerated Molecular Dynamics: An Efficient Enhanced Sampling Method for Biosystems. ***The Journal of Physical Chemistry Letters***, *14*(4), 1103-1112.

26. Jia, L., Feng, Z., **Zhang, H.**, Song, J., Zhong, Z., Yao, S., & Song, M. (2022). Explainable Fragment-Based Molecular Property Attribution. ***Advanced Intelligent Systems***, *4*(10), 2200104