Haitao Lin

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Education Background

College of Material Science and Engineering, Sichuan University ***Sep. 2015 - Jun.2019***

- Major: Solid State Physics Degree: Bachelor GPA: 3.81 (91.04/100) Ranking: 1/74

School of Engineering, Westlake University & Zhejiang University ***Sep. 2021 - Present***

- Major: Computer Science Degree: Doctor Supervisor: Stan. Z. Li

Selected Publication

- [1] **H Lin**, P Hu, M Ren, Z Gao, G Ke, T Wu, SZ Li, On the Design of One-step Diffusion via Shortcutting Flow Paths, ICLR 2026
- [2] **H Lin,** G Zhao, O Zhang, Y Huang, L Wu, Z Liu, C Tan, Z Gao, SZ Li, CBGBench: Fill in the Blank of Protein-Molecule Complex Binding Graph, ICLR 2025 (spotlight)
- [3] **H Lin,** Y Huang, O Zhang, S Ma, M Liu, X Li, S Ji, T Hou, SZ Li, DiffBP: Generative Diffusion of 3D Molecules for Target Protein Binding, Chemical Science, Royal Society of Chemistry, 2024
- [4] **H Lin,** O Zhang, H Zhao, D Jiang, L Wu, Z Liu, Y Huang, SZ Li, PPFlow: Target-aware Peptide Design with Torsional Flow Matching, ICML 2024
- [5] **H Lin,** L Wu, H Yufei, Y Liu, O Zhang, Y Zhou, R Sun, SZ Li, GeoAB: Towards Realistic Antibody Design and Reliable Affinity Maturation, ICML 2024
- [6] **H Lin**, Y Huang, Odin Zhang, L Wu, S Li, Z Chen, SZ Li, Functional-Group-Based Diffusion for Pocket-Specific Molecule Generation and Elaboration, NeurIPS 2023
- [7] **H Lin**, Z Gao, Y Xu, L Wu, L Li, SZ Li, Conditional Local Convolution for Spatio-temporal Meteorological Forecasting, AAAI 2022
- [8] **H Lin,** L Wu, G Zhao, P Liu, SZ Li, Exploring Generative Neural Temporal Point Process, Transactions on Machine Learning Research 2022
- [9] **H Lin**, C Tan, L Wu, Z Liu, Z Gao, SZ Li, An Extensive Survey with Empirical Studies on Deep Temporal Point Process, IEEE TKDE 2024

For more, see the Google Scholar (https://scholar.google.com/citations?user=o5A23qIAAAAJ&hl=en).

Working Experience

AI for Science Institute & DP Tech., Beijing ***supervisor: Guolin Ke*** ***Apr. 2024-Aug.2025***

- Establish Models on electron-cloud-based protein-molecule interaction models.
- Lead projects on fundamental machine-learning method about few-step diffusion model.

Laboratory of Brain and Intelligence, Tsinghua University, Beijing ***supervisor: Quan Wen*** ***Aug. 2019***

- Form deep insights of computational neuroscience, worked on ML-combined neural science.

School of Humanities & Social Science, Hong Kong University of Science and Technology ***Jul. 2017***

- Complete two weeks' immersion in Anthropology study and field research, having a basic knowledge in relevant fields.

Honors & Scholarships

- **National Scholarship** Academic Rank 1st in the College (2016 – 2017)
- **National Scholarship** Academic Rank 1st in the College (2015 – 2016)
- **Suwu Scholarship** (Dec. 2025)
- **The 1st Prize** in 2017 National Academic English Competition (May.2017)
- **The 2nd Prize** in 2016 National Academic Mathematics Competition (Nov.2016)

Language

- IELTS(7.5), GRE(326)