Xin Hong

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Research Interests

My research focuses on AI4Science, particularly on AI-driven approaches for drug discovery. Key areas of interest include protein structure prediction, virtual screening, molecular affinity prediction, and de novo drug design.

Education

University of Chinese Academy of Sciences *2016 - 2023*
Ph.D. student in Institute of Computing Technology, Chinese Academy of Sciences
Advisors: Prof. Hong Hu & Prof. Zhongzhi Shi & Prof. Shuo Bai & Prof. Yanyan Lan

Beijing University of Technology *2012 - 2016*
Undergraduate student in School of Software Engineering

Work Experience

Institute for AI Industry Research (AIR), Tsinghua University *July 2023 - present*
Postdoc
Advisor: Prof. Yanyan Lan, Prof. Weiying Ma
- **DrugCLIP:** Find Ligands for All Human Proteins.

Institute for AI Industry Research (AIR), Tsinghua University *June 2021 - June 2023*
Research Intern
Advisor: Prof. Yanyan Lan
- **AIRFold:** ranked first in the CAMEO 3D structure prediction challenge for 4 weeks (2022.07.23-2022.08.20).
- Protein Language Model for Multiple Sequence Alignment Generation.

Beijing Academy of Artificial Intelligence (BAAI) *October 2020 - July 2021*
Research Intern
- **WenLan:** a Chinese version large scale vision and language pretrained model.
- Zhiyanpianyu: a one-say and one-guess game based on WenLan.

Megvii Research *June 2018 - March 2019*
Research Intern
Advisors: Pengfei Xiong & Haoqiang Fan
- image inpainting, 3D album, annotation tool for human segmentation based on superpixel.

IBM China System and Technology Development Center *October - December, 2015*
Development Intern

Mafengwo *August - October, 2015*
Front-end Development Intern

Publications

- **Deep contrastive learning enables genome-wide virtual screening.**
  Yinjun Jia† , Bowen Gao† , Jiaxin Tan† , Jiqing Zheng† , **Xin Hong**† , Wenyu Zhu, Haichuan Tan, Yuan Xiao, Liping Tan, Hongyi Cai, Yanwen Huang, Zhiheng Deng, Xiangwei Wu, Yue Jin, Yafei Yuan, Jiekang Tian, Wei He, Weiying Ma, Yaqin Zhang, Wei Zhang* , Lei Liu* , Chuangye Yan* , Yanyan Lan*.
  Science, 2026.
- **Learning Protein-Ligand Binding in Hyperbolic Space.**
  Jianhui Wang†, Wenyu Zhu†, Bowen Gao†, **Xin Hong**, Ya-Qin Zhang, Wei-Ying Ma, Yanyan Lan.
  Proceedings of the AAAI Conference on Artificial Intelligence (AAAI), 202s6.
- **How Good is AlphaFold3 at Ranking Drug Binding Affinities?**
  Xin Hong†, Bowen Gao†, Yinjun Jia†, Wenyu Zhu, Qixuan Chen, Xiaohe Tian, Zhenyi Zhong, Jianhui Wang, Yanyan Lan.
  Proceedings of the ICML 2025 Generative AI and Biology (GenBio) Workshop, 2025.
- **Pre-training with fractional denoising to enhance molecular property prediction.**
  Yuyan Ni†, Shikun Feng†, **Xin Hong**, Yuancheng Sun, Wei-Ying Ma, Zhi-Ming Ma, Qiwei Ye, Yanyan Lan.
  Nature Machine Intelligence, 2024.
- **Visual Reasoning: from State to Transformation.**
  Xin Hong, Yanyan Lan, Liang Pang, Jiafeng Guo, Xueqi Cheng.
  IEEE Transactions on Pattern Analysis and Machine Intelligence, 2023.

- **Transformation Driven Visual Reasoning.**
  Xin Hong, Yanyan Lan, Liang Pang, Jiafeng Guo, Xueqi Cheng.
  2021 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR), 2021.
- **Deep Fusion Network for Image Completion**
  Xin Hong, Pengfei Xiong, Renhe Ji, Haoqiang Fan.
  Proceedings of the 27th ACM International Conference on Multimedia (ACMMM), 2019.
  Stats as of October 2022: ★ 204.
- **Attention-driven Factor Model for Explainable Personalized Recommendation**
  Jingwu Chen, Fuzhen Zhuang, **Xin Hong**, Xiang Ao, Xing Xie, Qing He.
  The 41st International ACM SIGIR Conference on Research and Development in Information Retrieval (SIGIR), 2018.

Selected Awards and Honors

- Recipient, NSFC Young Scientists Fund (Class C), 2025.
- Huiyan Scholar of Tsinghua University, 2023.
- National Funding Plan for Postdoctoral Researchers, 2023.
- Ranked first in the CAMEO 3D structure prediction challenge, 2022.
- The 1st Place of *Fake News Detection on the Internet during the COVID-19, Big Data Charity Challenge*, 2020.
- IBM Student Innovation Lab Program Award, 2014.

Skill

- **Programming Languages:** Python, HTML, CSS, Javascript, Java, C++, C#.
- **Tools:** Docker, Vim, Git; PyTorch, FAISS; Vue.js, TailwindCSS, FastAPI; Illustrator, Photoshop.