Xi Wang

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Education

New York University PhD Student 2025.8 - 2030.5

- Program: Courant Computer Science

Shanghai Jiao Tong University Bachelor of Science 2019.9–2023.6

- Computer Science and Bioinformatics

Work Experience

New York University Research Associate 2024.5–2025.5

- Main work: Language model fine-tuning, AI for Science.

Microsoft Research Asia Part-time Researcher 2023.10–2025.5

- Main work: Generative Models for molecules and catalysis.

DP Technology Researcher 2022.5–2025.3

- Main work: Language model design and pre-training, DNA & RNA structure and function prediction, Antibody Design, RNA Secondary Structure Prediction, mRNA Sequence Optimization.

University of Michigan Research Associate 2022.1–2022.9

- Main work: Protein structure prediction.

Publications

- **Xi Wang**, Shengjie Wang, et al., "RapTB: Rooted Absorbed Trajectory Balance with Submodular Replay for Stable Autoregressive GFlowNet Training.", **ICML 2026**. Under review.
- **Xi Wang**, Yang Zhang, et al., "3DCS: Datasets and Benchmark for Evaluating Conformational Sensitivity in Molecular Representations.", **ICLR 2026**.
- **Xi Wang**, et al. "A Unified Pre-Trained RNA Foundation Model for RNA Molecule Dissection and Engineering." **Nature**, Under review.
- Letian Chen, **Xi Wang**, et al. "AtropDiff: Data-Scarce Atropisomer Generation via Multi-Task Pretrained Classifier-Guided Diffusion." **ICLR 2025 DeITa**, Outstanding paper award.
- Gufen Yu, Kaiwen Yu, **Xi Wang**, et al. "CLC-DB: an open source online database of chiral ligands and catalysts." **Journal of Cheminformatics**.
- **Xi Wang**, et al. "Machine Learning for Reaction Performance Prediction in Allylic Substitution enhanced by Automatic Extraction of Substrate-aware Descriptor." **Journal of Chemical Information and Modeling**, (2025), 10.1021/acs.jcim.4c02120.
- **Xi Wang**, et al. "Synergistic catalysis for stereocontrol of prochiral nucleophiles in palladium-catalyzed asymmetric allylic substitution." **Science China Chemistry** 66.8 (2023): 2238-2255.
- Xiaohong Huo, G Li, **Xi Wang**, Wanbin Zhang*, et al. "Bimetallic catalysis in stereodivergent synthesis." **Angewandte Chemie International Edition** 61.45 (2022): e202210086.

Skills

- Coding: Python, C/CPP, R
- Pytorch, Sci-kit learn
- Graphic Design, Guitar