

Wenye Xiong

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RESEARCH INTEREST

Multimodal Machine Learning, Computer Vision, AI for Healthcare & Life Science.
Generative AI, Scene Understanding.

EDUCATION

ShanghaiTech University

Shanghai, CHN

B.E. in Computer Science and Technology

September 2023 - June 2027 (expected)

- Overall GPA: 3.8/4.0 (rank 13/172 in CS major, 19/267 in school)
- Relevant Coursework: Introduction to Information Science and Technology(A+), Introduction to Programming(A), Algorithms and Data Structures(A), Introduction to Machine Learning(A-), Artificial Intelligence in Medical Imaging(A), Computational Science and Engineering(A+), Computer Architecture(A-) & Project(A), Protein Design(A+), Game Theory(A)

AWARDS & HONORS

- **MERIT STUDENT**(Top 2% in school), ShanghaiTech University, 2023-2024
- **AI HONOR CLASS**(Honors Degrees), ShanghaiTech University, 2024-2027(expected)
- **GOLD MEDAL**, International Genetically Engineered Machine Competition (iGEM), 2024
- **2023 OUTSTANDING MENTOR ASSISTANT**, ShanghaiTech University, 2023

EXPERIENCE

Virtual Reality and Visual Computing Center (VRVC), ShanghaiTech

June 2024 - Oct. 2024

Undergraduate Research Assistant, Supervisor: Dr. Minzhang Li

- Exploring the application of Deep Learning and latest Diffusion Model in Protein Structure Prediction
- Contributed to the development of ShanghaiTech Fold, a diffusion-based model for all-atom biomolecular assembly

Perception, Learning and UnderStAnding (PLUS) Lab, ShanghaiTech

Jan. 2025 - present

Undergraduate Research Assistant, Supervisor: Prof. Xuming He

- Exploring the cutting-edge methods of Layout and Scene Graph based Diffusion Model, and applying it to the task of Medical Image Generation.
- Implementing the Scene Graph Diffusion Model with newest Training-free Method.

PACIFY project for iGEM 2024 [\[wiki\]](#)

Dec. 2023 - Oct. 2024

Team Member

- Performed homology modeling to obtain the structure of $\beta_{10} - E5 - \beta_{11} - K5$, and used AlphaFold 2 to predict the structure of $\beta_1 - \beta_9$
- Operated protein preparation and molecular dynamics simulation
- Developed devices based on PID algorithm to address the issue of itchiness without doing harm to the skin

MakeSense, ShanghaiTech First SensUs Team

Aug. 2024 - present

Co-Founder & Leader of Data Analysis Team

- Developing a wearable device based on biosensors to continuously monitor acute kidney injury (AKI) biomarkers.
- Investing in an enzyme-based creatinine sensor and QCM (Quartz Crystal Microbalance) platform.
- Leading the data analysis team to develop a machine learning model to predict the AKI risk.

PUBLICATIONS

No publications yet.

COURSE PROJECTS

De Novo Design of Odorant Binding Proteins for Breast Cancer Detection

Dec. 2024 - Jan. 2025

Course Project, Supervisor: Prof. Jiayi Dou

- Designed three novel Odorant Binding Proteins (OBPs) to specifically recognize Volatile Organic Compounds (VOCs)—hexanal, octanal, and nonanal—that serve as biomarkers for breast cancer.
- Executed a complete de novo computational design pipeline, generating protein backbones with RFDiffusionAA and designing amino acid sequences using LigandMPNN.
- Validated designs using AutoDock, PyRosetta, and ESMFold, demonstrating that the engineered proteins achieved significantly higher binding affinity and stability compared to their natural counterparts.

Neural Olfactory Sensing and Evaluation (NOSE)

May. 2025 - June. 2025

Course Project for Introduction to Machine Learning, Supervisor: Prof. Yujiao Shi

- Fine-tuned **MolFormer**, a large chemical language model, on the GS-LF olfactory dataset to adapt its generalized representations for specialized odor prediction tasks.
- Evaluated the model against the state-of-the-art **OpenPOM** on the Keller-2016 dataset, performing odor label classification and pleasantness rating prediction.
- Achieved state-of-the-art performance, with the fine-tuned model matching or surpassing OpenPOM on key metrics, demonstrating the efficacy of fine-tuning for machine olfaction.

TECHNICAL STRENGTHS

Programming Languages

Matlab, Python, C&C++, RISC-V

Framework & Toolchain

PyTorch, Git, Docker, Linux, Rosetta

Misc

L^AT_EX, Markdown, IELTS 7.5(6.5)