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+), Introdcution 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)

Harvard University **Cambridge, USA**
Visiting Undergraduate Student *September 2025 - May 2026*

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
- **FIRST PLACE**, Analytical Performance, SensUs Competition, 2025
- **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

- Explored the application of Deep Learning and Diffusion Model in Protein Structure Prediction
- Implemented a SE(3) Equivariant Transformer to build a 3D equivariant structure module
- 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

- Investigated **Compostional Scene Generation** with Scene Graph based Diffusion Model.
- Focused on learning the disentangled representation from the scene graph, enabling flexible control over the generation process.
- Explored Classifier-Free Guidance and Training-Free Method in Image Generation.

PACIFY - 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 - Aug. 2025*
Co-Founder & Leader of Data Analysis Team

- Developed a wearable device based on biosensors to continuously monitor acute kidney injury (AKI) biomarkers.
- Invested in an enzyme-based creatinine sensor and QCM (Quartz Crystal Microbalance) platform.
- Our team won the **First Place** in Analytical Performance.

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	LaTeX, Markdown, IELTS 7.5(6.5)