



Yuanxi Yu



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Education

2024.03 – Now	Shanghai Jiao Tong University	Postdoctoral Researcher	Supervisor: Prof. Liang Hong
2020.09 -- 2025.03	Shanghai Jiao Tong University	Ph.D. Student	
2016.09 -- 2020.06	Shanghai Jiao Tong University	B.Sc. Student	
2024.03 -- 2024.09	University of Birmingham	Exchange Student	

Awards

- Outstanding graduate of Shanghai in 2024
- Shanghai Jiao Tong University Zhiyuan Honorary Doctorate
- National Scholarship of China in SJTU (2024)
- National Scholarship of China in SJTU (2022)
- Outstanding graduate of Shanghai Jiao Tong University in 2020

Research Interests

AI4Science; Deep learning guided protein design; VAE

Selected Publications

- **Yu Y**, Jiang F, Ma X, et al. Entropy-driven zero-shot deep learning model selection for viral proteins *Neurips*, 2025, Poster
 - Pioneered a matrix-based framework, an architecture compatible with multiple PLMs that boosted inference speed by 10× while maintaining superior accuracy for protein mutant stability prediction
- **Yu Y**, Jiang F, Zhong B, et al. Entropy-driven zero-shot deep learning model selection for viral proteins *Physical Review Research*, 2025, 7(1): 013229
 - Utilized Shannon entropy to select the most suitable protein language model for screening viral protein mutants, significantly improving prediction accuracy on both the public ProteinGym leaderboard and private datasets.
- **Yu Y**, Jin S, Fan X, et al. Emergence of Debye Scaling in the Density of States of Liquids under Nanoconfinement[J]. *ACS nano*, 2024. (Cover article)
 - Employed inelastic neutron scattering techniques and all-atom molecular dynamics simulations to investigate the differences between liquid confined in quasi-two-dimensional conditions compared to bulk states. 1/2

- Zhou Z, Zhang L, **Yu Y (co-first author)**, et al. Enhancing efficiency of protein language models with minimal wet-lab data through few-shot learning[J]. *Nature Communications*, 2024, 15(1): 5566
 - Integrated learning to rank, meta-learning and LoRA to design a few-shot learning tool for directed protein evolution, capable of improving the prediction accuracy of large models by several fold using as few as 20 experimental data points.
- Fan, J, Li, M, Dong, J, **Yu, Y (co-first author)**, et al. A general temperature-guided language model to design proteins of enhanced stability and activity. *Science Advances*. (2024)
 - Utilized the temperature-aware language model PRIME to generate protein mutants with enhanced stability and activity, demonstrating outstanding performance in improving multiple protein fitness through wet-lab validation.
- **Yu Y**, Yang C, Baggioli M, et al. The ω^3 scaling of the vibrational density of states in quasi-2D nanoconfined solids[J]. *Nature Communications*, 2022, 13(1): 3649
 - Combined inelastic neutron scattering techniques and molecular dynamics simulations to measure the vibrational density of states of quasi-two-dimensional confined ice, and performed modeling and analysis based on the Debye model, providing the first analytical solution for the scaling of vibrational density of states in this system.
- Jiang F, **Yu Y***, Hong L, et al. Discovery of Expression-Governing Residues in Proteins[J]. *bioRxiv*, 2025.01.06.631498. (**corresponding author**)
 - Employed a matrix landscape alignment strategy to efficiently achieve zero-shot and few-shot predictions of protein sequence expression levels, demonstrating excellent performance on both public high-throughput datasets and small datasets.

Other Publications and patents

- The evolution of anionic nanoclusters at the electrode interface in water-in-salt electrolytes[J]. *Physical Chemistry Chemical Physics*, 2023, 25(15): 10301-10312. (**co-first author**)
- VenusMutHub: a systematic evaluation of protein mutation effect predictors on small-scale experimental data[J]. *Acta Pharmaceutica Sinica B* doi: 10.1016/j.apsb.2025.03.028
- A Deep Retrieval-Enhanced Meta-learning Framework for Enzyme optimum pH Prediction[J]. *Journal of Chemical Information and Modeling* (in press)
- A creatinase mutant applied to creatinine detection, along with its mutation site selection, purification, and detection methods + CN117448306A (First Inventor)
- A creatinase mutant with enhanced thermal stability and its applications + CN116694608A (Second Inventor)
- A T7 RNA polymerase mutant with high thermal stability and its applications + CN117070493A (First Inventor)

Conference Reports

- International Conference on Neutron Scattering (ICNS) 2022----Poster
- 5th International Workshop on Dynamics in Confinement (Confit 2022 in ILL) ---- Oral
- 9th International Discussion Meeting on Relaxations in Complex Systems(9IDMRCS) 2023----Poster

Other Activities

9th China International "Internet+" Innovation and Entrepreneurship Competition (Shanghai Gold Prize)
 2025 Data Element X Competition (First Prize in the Technology Innovation Track)