Kai **Zhu**

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"Unveiling nature through atomistic simulation and machine learning."

Summary

I am a Ph.D. student in Pharmaceutics at Zhejiang University, advised by Prof. Hou Tingjun. I am also a visiting student at the Italian Institute of Technology, working with Luigi Bonati and Prof. Michele Parrinello. My research focuses on developing machine learning–based enhanced sampling methods and their applications to atomic systems.

Education

Atomistic Simulations Group, Italian Institute of Technology — *Genova, Italy*

Joint Ph.D. Student — *Dec. 2025 – Dec. 2027*

College of Pharmaceutical Sciences, Zhejiang University — *Hangzhou, China*

Ph.D. in Pharmaceutics — *Sep. 2023 – Jun. 2028*

College of Pharmaceutical Sciences, Wenzhou Medical University — *Wenzhou, China*

B.S. in Pharmaceutics — *Sep. 2019 – Jun. 2023*

Research Experience

Italian Institute of Technology — *Genova, Italy*

RESEARCH INTERN, ADVISED BY **PHD. LUIGI BONATI** AND **PROF. MICHELE PARRINELLO** — *Dec. 2025 – Dec. 2027*

Research Topics: machine learning, enhanced sampling, atomic simulation

Zhejiang University — *Hangzhou, China*

PHD STUDENT, ADVISED BY **PROF. TINGJUN HOU** AND **PROF. DAN LI** — *Jun. 2023 – Jun. 2025*

Research Topics: machine learning, enhanced sampling, intrinsically disordered proteins

Honors & Awards

Domestic

2025 **Qiu Shi Flying Eagle Scholarship**, Zhejiang University — *Hangzhou, China*

Publication

† Co-first author; * Corresponding author;

2025 **Enhanced Sampling in the Age of Machine Learning: Algorithms and Applications** [5]
K. Zhu†, E. Trizio†, J. Zhang, R. Hu, L. Jiang, T. Hou*, L. Bonati*. **Chemical Reviews**

2025 **A Scalable and Quantum-Accurate Foundation Model for Biomolecular Force Field via Linearly Tensorized Quadrangle Attention** [4]
Q. Su†, **K. Zhu†**, Q. Gou†, ..., J. Wang*, C. Hsieh*, T. Hou*. **ARXIV PREPRINT** 2507.00884.

2025 **Self-Supervised Evolution Operator Learning for High-Dimensional Dynamical Systems** [3]
G. Turri, L. Bonati, **K. Zhu**, M. Pontil, P. Novelli* **ARXIV PREPRINT** 2505.1867.

2025 **Revisiting Protein–Protein Docking: A Systematic Evaluation Framework.** [2]
L. Jiang†, K. Zhang†, **K. Zhu**, Y. Wang, Y. Kang*, T. Hou*. **Journal of Chemical Information and Modeling** 65(19), 10573–10587.

2025 **From Traditional Methods to Deep Learning Approaches: Advances in Protein–Protein Docking.** [1]
L. Jiang, K. Zhang, **K. Zhu**, H. Zhang, C. Shen*, Tingjun Hou*. **Wiley Interdisciplinary Reviews: Computational Molecular Science** 15(2), e70016.

Skills

Programming	Python, C++, C, LaTeX, Linux
Frameworks	PyTorch, TensorFlow, NumPy, Git, Anaconda
Atomic simulation	GROMACS, PLUMED, AMBER, OpenMM, ASE, LAMMPS, CP2K