Yuxuan Ren

Curriculum Vitae

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EDUCATION

Bachelor of Technology in Chemistry
Year of completion: 2024
University of Science and Technology of China
School of Chemistry and Materials Science

- Overall GPA: 3.45/4.3 Rank: 27/134

EMPLOYMENT

Research Intern
Year-Year: 2023-2024
Microsoft Research AI for Science
Worked on developing the SFM system, a foundational model designed for multitask learning in the chemical domain.
Mentor: Chang Liu
Contributed to the AI2BMD system, a method aimed at facilitating large protein simulation dynamics.
Mentor: Wang Tong

Research Intern
Year-Year: 2024-2025
Beijing Academy of Artificial Intelligence, Health computing
Worked on OpenCryo, focusing on solving the inverse problem in the Cryo-ET domain.

Research Scientist
Year-Year: 2025-present
Beijing Academy of Artificial Intelligence, Health computing
I worked on OpenCryo and multimodal Protein–protein-language representation and generation.
Mentor: Qiwei Ye,

RESEARCH EXPERIENCE

Scientific Foundation Model & Physical Consistency in Molecular Science Multi-Task Learning
Advisors: Dr. Chang Liu & Dr. Bin Shao Dec. 2023 - Jun. 2024
Microsoft Research AI for Science

- Investigated multi-task learning approaches and current molecular datasets in molecular science.
- Implemented diffusion processes and energy prediction terms for foundational models.
- Enhanced model performance by leveraging scientific laws across tasks, connecting diffusion generation to the energy landscape based on Boltzmann distribution equations and the principle of minimum energy for DFT optimized structures.

AI2BMD & Neural P3M
Advisors: Dr. Tong Wang & Dr. Bin Shao Aug. 2023 - Jan. 2024
Microsoft Research AI for Science

- Help developed the AI2BMD system for protein dynamics using a dipeptide-based algorithm, eliminating the need for retraining at different atomic scales.
- Constructed an active learning dataset to stabilize the force dynamics process.
- Investigated long-range force calculation methods for classical molecular dynamics (MD), including Ewald summation and P3M.
- Designed a heterogeneous graph-based machine learning force field for large and periodic molecules, utilizing the P3M method.

OpenCryo
Advisors: Dr. Kai Chen July. 2024 - Present
Beijing Academy of Artificial Intelligence, Health computing

- Investigated deep learning-based inverse problem solutions and Cryo-ET data processing pipelines.
- Introduced an energy-based framework for inverse problems, applying it to solve the missing wedge and low signal-to-noise ratio issues in Cryo-ET.

PUBLICATIONS

Conference Proceedings

Physical Consistency Bridges Heterogeneous Data in Molecular Multi-Task Learning
Yuxuan Ren*, Dihan Zheng*, Chang Liu, Peiran Jin, Yu Shi, Lin Huang, Jiyan He, Shengjie Luo, Tao Qin, Tie-Yan Liu, 38th Conference on Neural Information Processing Systems (NeurIPS 2024).

Neural P3M: A Long-Range Interaction Modeling Enhancer for Geometric GNNs
Yusong Wang*, Chaoran Cheng*, Shaoning Li*, **Yuxuan Ren**, Bin Shao, Ge Liu, Pheng-Ann Heng, Nanning Zheng, 38th Conference on Neural Information Processing Systems (NeurIPS 2024).

CryoGEN: Cryogenic Electron Tomography Reconstruction via Generative Energy Nets
Yunfei Teng*, **Yuxuan Ren***, Kai Chen, Xi Chen, Zhaoming Chen, Qiwei Ye, 13th International Conference on Learning Representations (ICLR 2025).

SELECTED COURSES

Stochastic Process (A+)
Probability Theory (A)
Machine Learning Methods (A-)
Operating System (A)
Data Intelligence and Material Science (A)
Algorithm Basics (A-)
Calculus (A+)
Organic Chemistry (A+)
Statistical Mechanics (A)
Quantum Chemistry (A)