Weiren Zhao

August 26, 1999
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ZWR0
Current Lab

Core Competencies

- **AI for Science**
- **Cheminformatics**
- **Bioinformatics**
- **Data Analysis**
- **Deep Learning**

Education

Kyoto University
2025 – Present
Ph.D. Student | Informatics
Machine Learning & Metabolic Modeling

Dalian Univ. of Technology
2022 – 2025
M.Eng. | Chemical Engineering
GPA: 3.29 / 4.0

Qingdao Univ. of Sci. & Tech.
2018 – 2022
B.S. | Applied Chemistry
GPA: 3.10 / 4.0

Languages

Chinese ●●●●
English ●●●○
Japanese ●●○○

Professional Profile

Dedicated to building bridges at the intersection of machine learning, chemistry, and biological data. Leveraging a strong chemical background and solid experience in deep learning development, I specialize in utilizing PyTorch, GNNs, and custom Attention models to solve complex modeling problems in biochemical systems.

Research Experience

Integration of Machine Learning and Metabolic Models 2025 – Present
Ph.D. Research | Kyoto University (Lab: Tatsuya Akutsu)

- **InterKcat Model Development:** Optimized advanced neural network architectures using PyTorch to achieve high-precision predictions of enzyme catalytic activity.
- **High-Performance Computing:** Trained protein language models using CUDA-based GPU parallel acceleration to efficiently handle large-scale biochemical training datasets.
- **Interdisciplinary Decoding:** Applied linear algebra and statistical tools to parse complex biological data and construct robust predictive systems.

ML-Based Catalyst Design & Reaction Prediction 2022 – 2025
Master's Research | Dalian Univ. of Technology (Supervisor: Yang Li)

- **Computational Chemistry:** Investigated transition metal catalytic mechanisms and characterized novel aromatic systems using quantum chemistry approaches.
- **Solvent Screening System:** Developed a clustering algorithm based on physicochemical descriptors for precise solvent candidate identification, earning high recognition from academic peers.
- **Automated Data Mining:** Wrote Python scripts to automatically crawl and analyze thousands of academic papers in the field of perovskite solar cells.

Publications

[1] Y. Wang, **W. Zhao**, J. Wang, et al. "Beyond Rapid Nucleation: Unveiling the Role of Solvent-Precursor Interactions in Antisolvent-Free Perovskite Fabrication." *Energy Environ. Sci.*, 2026, DOI: 10.1039/D6EE00170J.

[2] **W. R. Zhao**, S. Wang, Y. Li. "Designing BuchwaldHartwig Reaction Graph for Yield Prediction." *The Journal of Organic Chemistry*, 90(37), 12975-12983.

[3] S. Wang, **W. R. Zhao**, M. Zhou, et al. "Machine Learning for Stability Enhancement in Perovskite Solar Cells: A Pathway to Commercial Viability." *Progress in Photovoltaics: Research and Applications*.

[4] S. Wang, **W. R. Zhao**, Y. Liu, et al. "Multi-modal Homogeneous Chemical Reaction Performance Prediction with Graph and Chemical Language Information." *Chinese Journal of Chemistry*, 43(11), 1230-1238.

[5] S. Wang, Y. Liu, **W. R. Zhao**, et al. "Optimizing Model Learning Performance on a Challenging Heck Reaction Yield Data Set." *The Journal of Organic Chemistry*, 90(36), 12768-12777.

[6] **W. R. Zhao**, Y. Li. "Predicting the Yield of Pd-Catalyzed BuchwaldHartwig Amination Using Machine Learning with Extended Molecular Fingerprints and Selected Physical Parameters." *ChemistrySelect*, 9(33), e202402529.

Technical Skills

Programming & Tools
- Python ●●●●
- Linux ●●●●
- R ●●●○

Domain Knowledge
- Deep Learning ●●●●
- Statistical Data Analysis ●●●●
- Protein Language Models ●●●○