

YUERU ZHANG

Incoming M.Sc. Student in Chemical Engineering, Nanyang Technological University

Email: YUERU002@e.ntu.edu.sg | Phone: +86 182 0872 7610

ORCID: [0009-0000-3912-3882](https://orcid.org/0009-0000-3912-3882)

EDUCATION

Nanyang Technological University | M.Sc. in Chemical Engineering (Incoming)

Aug. 2026

Singapore; expected enrollment in August 2026

Hohai University | B.Eng. in Environmental Engineering; average: 82.14/100; degree GPA: 3.68/5.00

Sep. 2022 - Jun. 2026

Nanjing, China; undergraduate thesis rated Excellent

RESEARCH INTERESTS

Molecular machine learning; low-data learning; transfer learning; electrochemical and energy-material property prediction; reliable AI for chemistry and chemical engineering; physics-informed and hybrid mechanistic/data-driven modelling; AI-driven scientific discovery.

RESEARCH PROFILE

Incoming NTU Chemical Engineering M.Sc. student with research experience in supervised molecular pretraining, adaptive multi-source transfer, rigorous QSPR benchmarking, and pruning-based transfer analysis. Developed end-to-end Python/PyTorch workflows spanning molecular data processing, graph neural networks, model development, controlled multi-seed evaluation, and negative-transfer analysis. Interested in extending data-efficient and reliable machine-learning methods toward electrochemical systems, energy and functional materials, process and multiscale modelling, and hybrid mechanistic/data-driven scientific discovery.

SELECTED RESEARCH OUTPUTS

- **Yueru Zhang**, Minghua Zhu*. *Adaptive Source-Task Expert Routing for Supervised Molecular Pretraining in Low-Data Electrochemical Property Prediction*. ChemRxiv, 2026. DOI: [10.26434/chemrxiv.15004913/v2](https://doi.org/10.26434/chemrxiv.15004913/v2).
- **Yueru Zhang**, Jianxin Guo, Wenyu Zhai, Yong Guo*. *A Molecule-Level QSPR Benchmark of RDKit Descriptors, Morgan Fingerprints, and Graph Neural Networks for Oxidation-Potential Prediction under Low-Data and Scaffold-Split Settings*. ChemRxiv, 2026. DOI: [10.26434/chemrxiv.15003831/v1](https://doi.org/10.26434/chemrxiv.15003831/v1). Manuscript prepared for resubmission.

* Corresponding author.

RESEARCH EXPERIENCE

Independent Research Project: Supervised Molecular Pretraining and Adaptive Source-Task Transfer

2026 - Present

Hohai University; independent research; ChemRxiv preprint available

- Developed an end-to-end molecular machine-learning pipeline using supervised QM9 source tasks and OxPot/RedDB downstream tasks, with consistent RDKit preprocessing across SMILES and SDF inputs.
- Implemented GIN/GINE encoders and transfer-learning workflows in PyTorch and PyTorch Geometric for low-data electrochemical molecular property prediction.
- Developed an adaptive source-task expert-routing model with learnable gating for multi-source transfer; compared learned routing with equal-weight fusion and evaluated robustness to weak or irrelevant source tasks.
- Designed matched, multi-seed comparisons across random and scaffold splits, training budgets, source tasks, and downstream endpoints; analyzed source-task alignment and negative-transfer behavior.

Independent Research Project: Molecular Representation Benchmark for Oxidation-Potential Prediction

2026 - Present

Hohai University; manuscript prepared for resubmission

- Benchmarked RDKit descriptors, Morgan fingerprints, multilayer perceptrons, tree-based models, and GINE under leakage-controlled random and scaffold splits.
- Conducted five-seed evaluations across multiple low-data budgets and analyzed how representation choice, sample size, and molecular distribution shift affect predictive performance.

Independent Ongoing Research Project: Pruning-Derived Feature-Usage Signatures for Selective Transfer and

2026 - Present

Negative-Transfer Risk Control

Self-initiated and primarily self-directed

- Investigating whether magnitude-pruning-derived feature-usage signatures can provide an interpretable view of task relationships and transfer behavior.
- Combining controlled synthetic experiments with molecular settings involving QM9, OxPot, and RedDB to evaluate selective-transfer and risk-constrained strategies for reducing negative-transfer exposure.

RESEARCH EXPERIENCE (CONTINUED)

- Research Intern: Adsorption and Desorption of Chromium(VI) in Soil in a Flow-Stirred Reactor

Institute of Soil Science, Chinese Academy of Sciences; Supervisor: Prof. Jing Song

Designed and optimized a flow-stirred reactor model using CAD and Revit; conducted Cr(VI) adsorption/desorption experiments and Python-based data analysis.
- Collaborative Research Project: Environmental Functional Materials and Flocculant Development

Hohai University; collaborative manuscript in preparation

Contributed to experimental design, material preparation, performance evaluation, data analysis, figure organization, and manuscript preparation.
- Provincial Undergraduate Innovation Project: Land-Use Change and Water Quality in the Yangtze and Yellow River Basins

Project Leader

Led data collection and analysis using land-use transfer matrices, regression, ridge regression, random forests, GIS, and remote-sensing tools; coordinated documentation and presentation.
-

TECHNICAL SKILLS

Programming & Machine Learning: Python, PyTorch, PyTorch Geometric, scikit-learn, XGBoost, pandas, NumPy, Matplotlib
Molecular Machine Learning: RDKit, SMILES/SDF processing, molecular descriptors and fingerprints, molecular graph construction, GIN/GINE, supervised pretraining, transfer learning, pruning
Evaluation & Research Methods: low-data evaluation, random and scaffold splits, multi-seed benchmarking, paired comparisons, negative-transfer analysis, controlled experimental design
Additional Tools: ArcGIS, QGIS, CAD, Revit, Origin, MATLAB, SPSS

ADDITIONAL EXPERIENCE

- R&D Intern

Yunnan Geological Big Data Center; geographic information software testing and data-output validation

Jan. 2025 - Feb. 2025
- Data Processor

Kunming Hairuo Information Technology Co., Ltd.; GIS, remote-sensing data processing, and thematic mapping

Dec. 2022 - Mar. 2023

HONORS, AWARDS, AND LEADERSHIP

- Second Prize (National Level), 16th National College Students' Innovation Competition of Advanced Drawing and Product Information Modeling, Aug. 2023.
- Second Prize (Jiangsu Provincial Level), 16th National College Students' Innovation Competition of Advanced Drawing and Product Information Modeling, 2023.
- Project Leader, Provincial Undergraduate Innovation and Entrepreneurship Training Program, Apr. 2024 - Jun. 2025.