

Rui-Xi (Ray) Wang

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RESEARCH INTERESTS

AI for Science, AI for Health

EDUCATION

Massachusetts Institute of Technology, Cambridge, MA 09/2022 — 05/2025 (expected)
Bachelor of Science in Computer Science and Engineering and Mathematics (double major) Cumulative GPA: 5.0/5.0

National Taiwan University, Taipei, Taiwan 09/2021 — 06/2022
Bachelor of Engineering in Electrical Engineering (incomplete) Cumulative GPA: 4.06/4.3

RESEARCH EXPERIENCE

Connor Coley's Lab, MIT Cambridge, MA
Advisor: prof. Connor Coley 05/2024 — Present

- Developing GNN and Transformer-based Mass Spectrum Prediction model with Retrieval Augmented Generation (RAG) and graph matching algorithm

Camera Culture Group, MIT Media Lab Cambridge, MA
Advisor: prof. Ramesh Raskar 11/2024 — Present

- Developing Decentralized AI system for healthcare with methylation data

Learning Matter Lab, MIT Cambridge, MA
Advisor: prof. Rafael Gómez-Bombarelli 01/2023 — 05/2024

- Organizing and Bench-marking the performance of various models on NIR and UV-VIS spectrum datasets

PUBLICATIONS

(* denotes Equal Contribution)

Journal paper

Conference Paper

- Wang, R.*; **Wang, R.-X.***; Manjrekar, M.; Coley, C. Neural Graph Matching Improves Retrieval Augmented Generation in Molecular Machine Learning. In International Conference on Machine Learning, **ICML 2025**
- Greenman, K. P.; **Wang, R.-X.**; Joung, J. F.; Han, M.; Green, W. H. Toward Accurate Prediction of Near-Infrared Absorption: Physics-Based Calculations, Machine Learning, and the Crucial Role of Data. Submitted to **2025 AIChE Annual Meeting** (under review)

AWARDS

Gold Medal Osaka, Japan (remote)
International Chemistry Olympiad 08/2021

Fu Bell Scholarship(top freshman student) Taipei, Taiwan
National Taiwan University 09/2021

WORK EXPERIENCES

Microsoft Redmond, WA
Software Engineering Intern 06/2025 — 08/2025 (expected)

Delta Biosciences Vilnius, Lithuania
Research Intern 06/2023 — 08/2023

SKILLS

- **Programming Languages:** Python, C++, C, Go, SQL, RISC-V

- **Libraries:** Numpy, Pandas, Matplotlib, PyTorch, Tensorflow, scikit-learn
- **Tools:** Linux, Git