

Qian Ouyang

Machine learning for materials and molecular simulation.

qouyang@nd.edu | cv.qianoy.uk

github.com/Owen-Ou-Yang

Education

Xi'an Jiaotong University

Fourth-year undergraduate | Artificial Intelligence

Artificial Intelligence Experimental Class

2023 - 2027 (expected)

Academic experience

Research Assistant

October 2025 - Present

University of Notre Dame

Prof. Tengfei Luo's group | Department of Aerospace and Mechanical Engineering

Summer Research Participant (iSURE)

July - September 2026

University of Notre Dame

International Summer Undergraduate Research Experience (iSURE).

Visiting Student

August - December 2025

University of Notre Dame

Research interests

AI for Materials; Molecular Dynamics & Machine Learning Potentials; HPC Optimization of ML Interatomic Potentials; Coarse-Grained Molecular Modeling; Representation Learning / JEPA; Polymer Property Prediction.

Technical skills

Molecular simulation & MLIPs: Experience with UMA/FAIR-Chem and MACE for molecular simulation.

High-performance computing: Experience using Notre Dame's Center for Research Computing (CRC) for research computing.

Systems & networking: Independent setup and configuration of a VPN.

Programming languages: C++, Python