Erh-Wei (Winnie) Sheng

ewinnie@gapp.nthu.edu.tw princesswinnie1122.github.io
Taipei, Taiwan · +886 905-783-100

Education

National Tsing Hua University Hsinchu, Taiwan
B.S. in Chemical Engineering & Computer Science *Sep 2022 - Dec 2026*
(Interdisciplinary Program of Engineering)

Selected coursework: Physical Chemistry I&II, Quantum Mechanics I, Statistical Thermodynamics, Mathematical Methods for Physicists, Linear Algebra, Design and Analysis of Algorithms, Computational Chemistry, Computational Condensed Matter Physics

Research Interests

My interests revolve around representation learning that respects the symmetries of nature. Recently, I've been particularly drawn to neural quantum states and variational modeling of quantum many-body systems beyond the practical reach of conventional ab initio methods, such as strongly correlated systems.

Research Experience

SU(2)-Equivariant Spinor Message Passing for Molecular Magnetism

Undergraduate Research Fellow, Caltech *Feb 2026 - present*

- Anima AI+Science Lab; Advised by Prof. Anima Anandkumar
- Proposed eSpinor, an SU(2)-equivariant graph neural network that propagates spinor features to predict molecular magnetic anisotropy arising from spin–orbit coupling.
- Manuscript (first author): Submitted to the NeurIPS 2026 SIMBIOCHEM workshop; preparing for submission to PRX Intelligence.

Equivariant GNNs for Vibrational Circular Dichroism (VCD)

Undergraduate Research Fellow, NTHU *Dec 2025 - present*

- Lab for Material and Molecular Design; Advised by Prof. Kun-Han Lin
- Developing an equivariant GNN to predict VCD spectra of organic crystals. The goal is to assign absolute configurations in larger periodic systems using limited AIMD data.

GPU Acceleration of the OrbitAll Foundation Model

Undergraduate Research Fellow, Caltech *Jul 2025 - Nov 2025*

- Anima AI+Science Lab; Advised by Prof. Anima Anandkumar
- Migrated OrbitAll's equivariant tensor-product backend to NVIDIA cuEquivariance, improving GPU efficiency and scalability for quantum-chemistry training.
- Code release: To be released as open source upon publication of OrbitAll.

AutoFF: Automated Force-Field Parameterization

Undergraduate Researcher, NTHU *Jun 2024 - Dec 2024*

- Lab for Material and Molecular Design; Advised by Prof. Kun-Han Lin
- Developed an automated OPLS-AA parameterization toolkit to streamline molecular-dynamics simulations of organic semiconductors.
- Presentation: Honorable Mention, oral presentation, 2024 TwIChE National Conference.

Research Experience

High-Entropy Alloys for the Hydrogen Evolution Reaction
Undergraduate Researcher, NTHU *Nov 2023 - Oct 2024*

- Lab for Material and Molecular Design; Advised by Prof. Kun-Han Lin
- Used density functional theory to optimize hydrogen adsorption in high-entropy alloys by combining metals with different hydrogen affinities.
- Manuscript: Under review at JACS.
- Presentation: Poster, 2024 TwIChE National Conference.

LLM Reasoning and Evaluation in Low-Resource Languages
LLM Research Intern (Part-time), National Center for High-Performance Computing (NCHC) *Oct 2024 - June 2026*

- Building culturally grounded corpora to evaluate and align LLM reasoning, with a focus on gender bias in low-resource languages.
- Co-developed a platform for LLM evaluation, annotation, and fine-tuning data preparation.

Selected Honors & Fellowships

Summer Undergraduate Research Fellowship (SURF), Caltech *2025, 2026*

2nd place worldwide, ISC Student Cluster Competition (on-site, Hamburg) *2025*
Represented Taiwan; qualified by winning the 2024 APAC HPC-AI Competition.

1st of 21 teams, APAC HPC-AI Competition (Asia) *2024*

2nd of 9 teams, High Performance Application Competition (Taiwan) *2024*

Grand Finalist (top 6), UAiTED Innovation Competition *2023*
Selected from 300 participants across 16 partner universities in Asia.

2nd place in Chemistry, Taiwan International Science Fair *2021*
Selected to represent Taiwan at MOSTRATEC.

3rd place in Chemistry, MOSTRATEC International Science Fair *2021*
International Highlights distinction.

Skills

Programming: Python, C/C++, Julia, MATLAB, Fortran.

ML & HPC: Linux, PyTorch, CUDA, parallel programming (OpenMP, MPI), GPU performance profiling (NVIDIA Nsight), containers (Docker, Singularity), cluster management

Scientific software & libraries: VASP, AMS, GROMACS, LAMMPS, ASE, RDKit

Languages: English (full professional proficiency), Chinese (native)

Others: Git, LaTeX, web & app development (HTML, CSS, JavaScript, Flutter)

Leadership & Service

Captain, NTHU Student Cluster Competition Team
Led NTHU teams at national, Asia-Pacific, and international competitions.

Teaching Assistant

- Fundamental & Advanced High-Performance Computing Cluster Practice
- 2025 HPC × AI Winter Camp (Co-organized by NCHC & NTHU)

Conference Service

- Selected Student Volunteer, SC25 Conference
- Staff, QRACON (2024) and Chemistry National Meeting of Taiwan (2023)

Student Activities: protein simulations and data analysis for the NTHU iGEM team, marketing and visual design for the NYCU Niche team (STEM talks for girls)