Hongrui (Sam) Sheng

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EDUCATION

Fudan University, Shanghai, China Expected 06/2027
Bachelor of Science in Chemistry
· GPA: 3.84/4.00 | Rank: 10/94
· **Key Coursework**: Quantum Chemistry (H): A+; Organic Chemistry II (H): A; Physical Chemistry II (H): A

Stanford University, California, USA 06/2025 - 08/2025
International Honors Program Participant
· STATS117 Introduction to Probability Theory: A+; CS106B Programming Abstractions: A

PUBLICATION

1. C. Lei, Y. Meng, **Sheng, Hongrui**, X. Liu, Z. Deng, and M. Gong*, "Heterogeneous or homogeneous: The interplay of ions and surfaces during deposition/dissolution equilibrium for neutral-pH electrocatalytic biomass valorization," *Unpublished manuscript*, 2025, Submitted.

RESEARCH EXPERIENCE

Research Program Leader, Wangdao Research Program | Professor Ming Gong Since 05/2025
AI-aided tailoring electrocatalysts for the selective valorization of glycerol
· Implementing machine learning methods to accelerate the discovery of novel electrocatalysts.
- Curate data from journal articles and utilize SISSO/LASSO to identify key physicochemical factors.
- Propose novel electrocatalysts via genetic algorithm screening of Materials Project and Catalysis Hub databases.
- Validate results via DFT calculations and wet-lab experiments.

Trainee researcher | Professor Ming Gong 03/2024 - 04/2025
Biomass Valorization via Electrocatalysis
· Executed multi-step protocols for catalyst fabrication, post-synthesis bleaching, and electrochemical testing.

SELECTED PROJECTS

Automated Computational Workflow for S_N2 Mechanisms | Codes on GitHub 11/2025 - 12/2025
Computational Chemistry Course Project, AI-assisted
· Engineered an end-to-end **Python** pipeline to automate **Gaussian** workflows for amine methylation.
· Implemented **SISSO-inspired** multivariate regression ($R^2 > 0.95$) to predict activation energies using electronic (Q_N) and topological (κ_3) descriptors.
· Integrated **RDKit** for automated complex assembly and feature extraction, revealing the interplay between steric hindrance and nucleophilicity.

AWARDS

Outstanding Student of Fudan University 2025
Second Prize, Syensqo Scholarship, Syensqo (formerly Solvay) 2025
Second Prize, Scholarship for Outstanding Students, Fudan University 2024, 2025

SKILLS, LANGUAGES, AND INTERESTS

Skills Programming: Python, LaTeX, C++; Computational Chemistry: Psi4, Gaussian, ASE, MACE
Languages Chinese (Native), English (TOEFL iBT 107/120), Japanese (JLPT N1)
Interests Hobby Aquarist, Rock and Classical Music, Traditional Chinese Medicine

LEADERSHIP & SERVICE

Founding President, Fudan Integrative Medicine Association 11/2024 - 09/2025
Established the first student organization promoting interdisciplinary medicine at Fudan.

Executive President, Fudan Traditional Chinese Medicine Club 03/2024 - 09/2025
*Revitalized the club; **automated outreach workflows using Python** to recruit 100+ members.*