QINAN HUANG

Undergraduate Student | Chemistry

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♥ Hunan University, Changsha, China

Computational Chemistry / Machine Learning / Organometallic Chemistry / Quantum Chemistry / Analytical Chemistry / Nanotechnology / Molecular Dynamics / Synthetic Biology / Molecular Cloning /



EDUCATION

2020 - 2024 BSc in Chemistry, Hunan University

> **GPA:** 3.72/4;

> Ranking: 2/111;

> TOEFL: Total: 103/120 (Reading: 29 Listening: 29 Speaking: 23 Writing: 22), June 2023

2023.1 - 2023.5 Visiting Student, University of California, Berkeley

> **GPA:** 3.77/4;

- > CHEM121, Introduction to Computational Chemistry: Grade: A
- > CHEM142, Machine Learning, Statistical Models, and Optimization for Molecular Problems: Grade:
- > Graduate Courses: CHEM220B Statistical Mechanics, CHEM262 Metals in Organic Synthesis, CHEM263B Synthetic Design II



EXPERIENCE

Present May 2023

Undergraduate Researcher, University of California, Los Angeles, United States

Houk Group:

> Studied mechanism of enzyme-catalyzed reactions using quantum mechanics and molecule dyna-

DFT Quantum Mechanics | Molecule Dynamics | Computational Biology

May 2023

Undergraduate Researcher, University of California, Berkeley, United States

February 2023

Hartwig Group:

> DFT calculation for Copper catalyst with significant multi-reference characters.

DFT Organometallic Chemistry

Present

Undergraduate Researcher, THE UNIVERSITY OF BRITISH COLUMBIA, Canada

December 2022 **Dilabio** Group:

- > Developed system specific ACPs(Atom-Centered Potentials) for quantum dynamics and vibrational spectroscopy;
- > Applied database to delta machine learning.

DFT Caculation Database Machine Learning

December 2022

Undergraduate Researcher, Hunan University, China

April 2022 Qu and Duan Group:

- > Study on mechanism and control methods of metal-organic catalytic reactions;
- > Computational design of privileged chiral catalyst.

DFT Calculation | Catalyst Design | Organometallic Chemistry | Quantum Mechanics

Octobor 2022

IGEM Team Member, HUNAN UNIVERSITY, China

March 2022

IGEM (International Genetically Engineered Machine)

Team HNU China:

- > Developed. coli engineered to absorb phosphates in water;
- > Designed of temperature-sensitive biological switches.

Synthetic Biology | Molecular Cloning | Biological Mathematical Modeling

Nov 2022

Undergraduate Researcher, Hunan University, China

May 2021

Song Group:

- > Design of ratiometric fluorescent probes based on Prussian blue;
- > In vivo molecular imaging: acoustic imaging, long afterglow imaging, chemiluminescence, nuclear magnetic imaging;
- > Early diagnosis, treatment and efficacy testing of cancer.

MRI Acoustic Imaging (PA) Chemical Probes Photodynamic therapy (PDT)

July 2021 June 2021

Internship, HUNAN UNIVERSITY, China

Luo Group:

> Measurement and Correlation for Solubilities of Adipic Acid, Glutaric Acid, and Succinic Acid in Different Alcohol Solvents.

June 2021

Research Assistant, Hunan University, China

December 2020 He Group:

> Developed bacterium sensor based on 16S rRNA and "DNA-RNA switch".

Microbial and Virus Sensors

COMPETENCE

Wet Lab Skills Molecular cloning technology(PCR,WB, restriction enzyme digestion .etc),Organic synthesis.

Dry Lab Skills DFT caculation, Mathematical modeling, Gaussian, ORCA.

Scientific Drawing Origin, Adobe Illustrator

Instrumental Analysis MRI,PA,UVIS,XRD

Office Automation MTFX, Pack Office(Word, Excel, PowerPoint).



Publications

- Delaney, C. P., Lin, E., Huang, Q., Yu, I. F., Rao, G., Tao, L., Jed, A., Fantasia, S. M., Püntener, K. A., Britt, R. D., & Hartwig, J. F. (2023). A non-canonical Ullmann coupling mechanism occurring through copper(II). Submitted to Science.
- 2022 Huang, Y., Zhang, L., Yan, M., Huang, Q., Zhang, Y., Ren, Y., & Luo, W. (2022). Measurement and Correlation for Solubilities of Adipic Acid, Glutaric Acid, and Succinic Acid in Different Alcohol Solvents, Journal of Chemical & Engineering Data 67 (1), 245-256

AWARDS

- 2022 International Genetically Engineered Machine (iGEM) competition 2022, Silver Medal
- 2022 Mathematical Contest in Modeling (MCM), Meritorious Winner (7%)
- National Scholarship, Ministry of Education of the People's Republic of China 2021