# QINAN **HUANG**

## Undergraduate Student | Chemistry

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Hunan University,Changsha,China

## Education

2020 - 2024 **BSc in Chemistry , Hunan University**

- **Thesis Advisor :** Shuanglin Qu
- **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**

- **Advisor :** John Hartwig
- **GPA :** 3.77/4;
- **CHEM121, Introduction to Computational Chemistry :** Grade : A
- **CHEM142, Machine Learning, Statistical Models, and Optimization for Molecular Problems :** Grade : A
- **Graduate Courses : CHEM220B** Statistical Mechanics, **CHEM262** Metals in Organic Synthesis, **CHEM263B** Synthetic Design II

2023.5 - 2023.7 **Visiting Student , University of California, Log Angeles**

- **Advisor :** Ken Houk

2023.7 - 2023.9 **Mitacs Global Research Internship, University of California, Log Angeles**

- **Advisor :** Gino Dilabio

## Publications

2023 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.*, A non-canonical Ullmann coupling mechanism occurring through copper(II), **Science**, 2023, 14, 9696-9703, **381**, 1079-1085.**DOI :** 10.1126/science.adi9226

2023 Tang, L†., **Huang, Q.-N.**†, Wu, F., Xiao, Y., Zhou, J.-L., Xu, T.-T., Wu, W.-B.*, Qu, S.*, Feng, J.-J.* , C(sp2)−H Cyclobutylation of Hydroxyarenes Enabled by Silver-π-Acid Catalysis : Diastereocontrolled Synthesis of 1,3-Difunctionalized Cyclobutanes, **Chem. Sci.**, 2023, **14**, 9696-9703. **DOI :** 10.1039/D3SC03258B

2023 Ashani, M. N., **Huang, Q.**, Flowers, A. M., Brown, A., Aerts, A.*, Otero-de-la-Roza, A.*, & DiLabio, G. A.*, Accurate Potential Energy Surfaces using Atom-Centered Potentials and Minimal High-Level Data, **J. Phys. Chem. A** , 2023, **127**, 8015–8024. **DOI :**10.1021/acs.jpca.3c04558

2022 Huang, Y., Zhang, L., Yan, M., **Huang, Q.**, Zhang, Y., Ren, Y., & Luo, W.*, Measurement and Correlation for Solubilities of Adipic Acid, Glutaric Acid, and Succinic Acid in Different Alcohol Solvents, **J. Chem. Eng. Data** , 2023, **67**, 245-256. **DOI :** 10.1021/acs.jced.1c00699

†These authors contributed equally
* Corresponding author

## Experience

Present
January 2023

**Undergraduate Researcher , University of California, Los Angeles, United States**
**Kendall Houk** Group :
**Mechanistic Studies of Enzymatic Retro [2 + 2] Cycloaddition**

- Optimized the transition state structures without enzyme catalysis using DFT (Density Functional Theory), and investigated the potential energy surface of the non-enzymatic reactions.
- Docked transition states into the enzyme active sites, and studied the interactions between different transition states and enzymes.
- Conducted molecular dynamics simulations of enzyme-ligand complexes using Amber to investigate the binding scenarios of transition states with enzymes.

DFT | Quantum Mechanics | Molecule Dynamics | Docking | Computational Biology

May 2023
February 2023

**Undergraduate Researcher , University of California, Berkeley, United States**
**John Hartwig** Group :
**Cross-coupling by a noncanonical mechanism involving the addition of aryl halide to Cu(II)**

- Demonstrated the existence of Cu(II) resting state through EPR.
- Proven through kinetic experiments that the concerted oxidative addition to Cu(II) state is a rate-determining step.
- Investigated the multi-reference state characteristics of the system and analyzed the source of stability in high-valent copper intermediates.
- Conducted computational analyses which revealed that the radical character on the oxalamide ligand compensates for what would be an abnormally high valence at copper observed in a typical oxidative addition scenario

DFT | Organometallic Chemistry

Present
December 2022

**Undergraduate Researcher , The University of British Columbia, Canada**
**Gino Dilabio** Group :
**Accurate Potential Energy Surfaces using atom-Centered Potentials and Minimal High-Level Data**

- Prepared reference energies for the potential energy surface at the CCSD(T)-F12/cc-pVTZ-F12 level.
- Recorded the discrepancies between calculation results at the B3LYP/def2-TZVPP level and reference energies, as well as molecular structure information, into a database for machine learning purposes.
- Utilized LASSO (Least Absolute Shrinkage and Selection Operator) to derive ACPs (atom-centered potentials), enabling low-accuracy methods to achieve results similar to high-accuracy methods.

DFT | Database | Machine Learning | Theoretical Chemistry

December 2022
April 2022

**Undergraduate Researcher , Hunan University, China**
**Shuanglin Qu and A'bing Duan** Group :
**C(sp2)−H Cyclobutylation of Hydroxyarenes Enabled by Silver-π-Acid Catalysis**

- Utilized DFT (Density Functional Theory) calculations to uncover a new mode of Ag ion activation in BCB esters, where the Ag ion directly binds to the bridgehead carbon of BCB, instead of the ester oxygen, thereby activating the BCB bridge bond.
- nvestigated the origins of regioselectivity and enantioselectivity in the Ag-ion catalyzed synthesis of 1,3-difunctionalized cyclobutanes.
- Employed second-order perturbation methods to analyze the contributions of hydrogen bonding and orbital overlap in selectivity.

DFT | Catalyst Design | Organometallic Chemistry | Quantum Mechanics

## Competence

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| **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** | LaTeX, Pack Office(Word, Excel, PowerPoint). |

## Awards

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