

# Qinan Huang

CHEMISTRY · UNDERGRADUATE STUDENT

Hunan University, Changsha, Hunan, 410082, P.R.China

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## Education

### Hunan University

B.S. IN CHEMISTRY

Changsha Hunan, China

Sep. 2020 - July. 2024

### University of California, Berkeley

CHEMISTRY VISITING STUDENT PROGRAM

Berkeley CA, United States

Jan. 2023 - May. 2023

## 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.\* A Non-Canonical Ullmann Coupling Mechanism Occurring Through Copper(II). *Science* **2023**, *381*, 1079-1085. DOI: [10.1126/science.adi9226](https://doi.org/10.1126/science.adi9226)
- Tang, L.; **Huang, Q.-N.**; Wu, F.; Xiao, Y.; Zhou, J.-L.; Xu, T.-T.; Wu, W.-B.\*; Qu, S.\*; Feng, J.-J.\* C(sp<sup>2</sup>)-H Cyclobutylation of Hydroxyarenes Enabled by Silver- $\pi$ -Acid Catalysis: Diastereocontrolled Synthesis of 1,3-Difunctionalized Cyclobutanes. *Chem. Sci.* **2023**, *14*, 9696-9703. DOI: [10.1039/D3SC03258B](https://doi.org/10.1039/D3SC03258B)
- 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* (38), 8015-8024. DOI: [10.1021/acs.jpca.3c04558](https://doi.org/10.1021/acs.jpca.3c04558)

\* Corresponding author

## Skills

|                              |   |
|------------------------------|---|
| <b>Computational Skills</b>  | Using software such as Gaussian, ORCA, Amber, GROMACS                                     |
| <b>Instrumental Analysis</b> | Familiar with techniques such as infrared spectroscopy (IR), and X-ray diffraction (XRD). |
| <b>Office Automation</b>     | Latex, Pack Office (Word, Excel, PowerPoint)  |

## Experience

### Gino Dilabio Group - The University of British Columbia

Kelowna BC, Canada (Hybrid)

ACCURATE POTENTIAL ENERGY SURFACES USING ATOM-CENTERED POTENTIALS AND MINIMAL HIGH-LEVEL DATA

Jun 2023 - Sep 2023

- Created a new formula to describe the vibration characteristics of molecules.
- Conducted extensive computational simulations on small molecules to verify the accuracy of the formula.

### John Hartwig Group - University of California, Berkeley

Berkeley CA, United States (On-site)

CROSS-COUPLING BY A NONCANONICAL MECHANISM INVOLVING THE ADDITION OF ARYL HALIDE TO Cu(II)

Jan. 2023 - May. 2023

- Assisted in research on a copper-based chemical reaction, discovering a new reaction pathway that differs from traditional theory.
- Used software to analyze this chemical systems, helping to better understand the reaction.

### Shuanglin Qu Group - Hunan University

Changsha, China (On-site)

C(SP<sup>2</sup>)-H CYCLOBUTYLATION OF HYDROXYARENES ENABLED BY SILVER- $\pi$ -ACID CATALYSIS

Apr. 2022 - Dec. 2022

- Used software to calculate the binding energies between silver ions and small organic molecules.
- Revealed a new Ag ion activation mode in BCB esters, where Ag ion binds directly to the bridgehead carbon, activating the BCB bridge bond, rather than binding to the ester oxygen.
- Developed a new theoretical framework for understanding how silver ions react with organic molecules.