

Haoran Sun

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Education

Chinese University of Hong Kong, Shenzhen (CUHK-Shenzhen)

B.Sc., Bioinformacis; cumulative GPA: 3.716/4.000, rank 1/38; major GPA: 3.831/4.000, rank 1/38

Shenzhen, China

Sept. 2019–Present

University of California, Berkeley

Summer visiting program; GPA: 4.000/4.000

Berkeley, CA

June 2022–Aug. 2022

Courses: MATH104 Introduction to Real Analysis, MATH128A Numerical Analysis, CS61C Machine Structure.

Research Experience

Prof. Hajime Hirao's group, CUHK-Shenzhen

Research assistant

Shenzhen, China

Apr. 2022–Aug. 2022

Project: Study the Bonding Nature of Fe-CO Complexes in heme Proteins, **accepted**

- Wrote an example Lewis configuration of P450 Cpd I for natural bonding orbital (NBO) input.
- Fixed Q-Chem SCF convergence problems by disabling DIIS algorithm when the error is small.

Prof. Hajime Hirao's group, CUHK-Shenzhen

Research assistant

Shenzhen, China

Aug. 2021–Dec. 2021

Project: Reaction Pathway Analysis of P450 C-S Bond Formation by TleB (PDB ID: 6J83)

- Built a truncated model and performed DFT calculations along the proposed reaction pathway to identify electronic configurations under different spin states.
- Performed molecular dynamics simulation of the initial reaction complex to determine the preferable starting structure of the reaction.
- Utilized quantum mechanics and molecular mechanics (QM/MM) hybrid method to investigate the protein-substrate interaction, revealing an electron transfer pattern of the initial reaction complex.

Prof. Hajime Hirao's group, CUHK-Shenzhen

Research internship

Shenzhen, China

Apr. 2021–June 2021

Training: Theoretical Studying of Quantum Chemistry by Modern Quantum Chemistry

- Implemented SCF algorithm for RHF 6-31G H_2 and UHF 6-31G H_2^- by Fortran.
- Fixed problems in the original DIIS algorithm, which are used for accelerating SCF algorithm.

Prof. Hsien-da Huang's group, CUHK-Shenzhen

Research assistant

Shenzhen, China

Sept. 2020–Dec. 2020

Project: Effects of Traditional Chinese Medicine on Gene Regulation

- Utilized PCA and t-SNE for dimensionality reduction of gene expression profile.
- Arranged a group tutorial about using Connectivity Map to identify differentially expressed genes (DEGs) perturbed by traditional medicines and interpreted statistics.

Publications

Liu, Shuyang, Songyan Xia, Dongxiao Yue, **Haoran Sun**, and Hajime Hirao. "The Bonding Nature of Fe-CO Complexes in Heme Proteins". *Inorganic Chemistry* (2022). Accepted.

Zhang, Luoqiang, Daoyong Zhu, Jingyao Hu, **Haoran Sun**, Hajime Hirao, Yonggui Robin Chi, and Jianrong Steve Zhou. "Pursuing High Efficiency in Photocatalytic Oxidative Couplings of Heteroarenes and Aliphatic C-H bonds". *Organic Chemistry Frontiers* (2022). Submitted (QO-RES-10-2022-001558).

Teaching Experience

CUHK-Shenzhen

Undergraduate student teaching fellow of BIM2005 Computational Biology

Shenzhen, China

Sept. 2021–Dec. 2021

Tutorials: docking tool Autodock-Vina; Hatree determinants; mathematical background and Numpy implementation of PCA algorithm.

CUHK-Shenzhen

Undergraduate student teaching fellow of BIM3013 Organic Chemistry

Shenzhen, China

Jan. 2022–May 2022

Tutorials: basic concepts of stereochemistry; mechanisms of condensation reactions.

Honors and Awards

- **Bowen Scholarship**, 30,000 RMB/year, in total 120,000 RMB, CUHK-Shenzhen
- **Dean's List Award**, CUHK-Shenzhen
- **Contemporary Undergraduate Mathematical Contest in Modeling**, The Second prize
- **Chinese Chemistry Olympiad**, The First prize

Sept. 2019–June 2023.

Sept. 2020–Sept 2022.

Sept. 2021.

Sept. 2018.

Skills

- Coding languages: Python, Fortran, C, CUDA C++ and CUDA Fortran, OpenMP, MPI, MATLAB, \LaTeX
- Tools: Linux (system configuration, multi-user management, software installation), WSL, Git
- Compt. bio./chem. tools: Amber, Gromacs, Q-Chem, Gaussian, VMD, Autodock Tools