Haoran Sun

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Education

Chinese University of Hong Kong, Shenzhen (CUHK-Shenzhen) **Shenzhen, China**
B.Sc., Bioinformacis; cumulative GPA: 3.716/4.000, rank 1/37; major GPA: 3.831/4.000, rank 1/37 *Sept. 2019–Present*

University of California, Berkeley **Berkeley, CA**
Summer visiting program; GPA: 4.000/4.000 *June 2022–Aug. 2022*
Courses: MATH104 Introduction to Real Analysis, MATH128A Numerical Analysis, CS61C Machine Structure.

Research Experiences

Prof. Hajime Hirao's group, CUHK-Shenzhen **Shenzhen, China**
Research assistant *Apr. 2022–Aug. 2022*
Project: Study the Bonding Nature of Fe-CO Complexes in heme Proteins, **published**
- 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 **Shenzhen, China**
Research assistant *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 **Shenzhen, China**
Research internship *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 is used for accelerating SCF algorithm.

Prof. Hsien-da Huang's group, CUHK-Shenzhen **Shenzhen, China**
Research assistant *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).

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 Experiences

CUHK-Shenzhen **Shenzhen, China**
Undergraduate student teaching fellow, BIM2005 Computational Biology *Sept. 2021–Dec. 2021*
Tutorials: docking tool Autodock-Vina; Hatree determinants; mathematical background and Numpy implementation of PCA algorithm.

CUHK-Shenzhen **Shenzhen, China**
Undergraduate student teaching fellow, BIM3013 Organic Chemistry *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. *Sept. 2019–June 2023*
- ***Dean's List Award***, CUHK-Shenzhen. *Sept. 2020–Sept. 2022*
- ***Contemporary Undergraduate Mathematical Contest in Modeling***, The Second prize. *Sept. 2021*
- ***Chinese Chemistry Olympiad***, The First prize. *Sept. 2018*

Skills

- Coding languages: Python, Fortran, C, 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