Haoran SUN

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Education

2019.9–Present **B.Sc.**, Bioinformacis, Chinese University of Hong Kong, Shenzhen (CUHK-Shenzhen).
GPA, cumulative 3.716/4.000 **rank** 1/37
GPA, major 3.831/4.000 **rank** 1/37
Courses: Computational Biology, Design and Analysis of Bioinformacis Algorithms, Machine Learning in Computational Biology, Biophysical Chemistry, Biophysics, Molecular Simulation and Modeling I, Ordinary Differential Equations, Advanced Linear Algebra, Parallel Programming, Partial Differential Equations, Advanced Quantum Mechanics, etc.

2022.6–2022.8 **Summer visiting program**, University of California, Berkeley (UCB).
GPA 4.000/4.000
Courses: MATH104 introduction to real analysis, MATH128A numerical analysis, CS61C machine structure

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Research Experiences

2022.4–2022.8 **Research assistant**, Hajime Hirao's group, CUHK-Shenzhen.
Project: energy decomposition analysis (EDA) and natural bonding orbital (NBO) analysis of the nature of protein-drug interaction at the heme iron center in cytochrome P450 inhibition
- Write an example Lewis configuration for NBO input
- Performed energy decomposition analysis (EDA) using Q-Chem.
- Fixed SCF convergence problems by disabling DIIS algorithm when the error is small.
- ***Accepted*** Journal: Inorganic Chemistry. Manuscript ID: ic-2022-02387h.R2

2021.8–2021.12 **Research assistant**, Hajime Hirao's group, CUHK-Shenzhen.
Project: reaction pathway analysis–P450 C-S bond formation by TleB (PDB ID: 6J83)
- Build truncated model to perform 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.

2021.4–2021.6 **Research assistant**, Hajime Hirao's group, CUHK-Shenzhen.
Training project: 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.

2020.1–2020.12 **Research assistant**, Hsien-da Huang's group, CUHK-Shenzhen.
Project: effects of traditional Chinese medicine in gene regulation: identify DEGs using statistical methods
- Utilized PCA and t-SNE for dimensionality reduction and visualization of gene expression profile.
- Arranged tutorial about using Connectivity Map to identify differentially expressed genes (DEGs) perturbed by traditional medicines and interpreted statistics.
- Performed gene set enrichment analysis (GSEA)

Teaching Experiences

2021.9–2021.12 **Undergraduate student teaching fellow**, computational biology, CUHK-Shenzhen.
- Tutorial sessions: how to simplify the Schrödinger equation of hydrogen atom using atomic units; molecular docking tool Autodock-Vina; review basic principles of quantum mechanics and quantum chemistry; mathematical background and hands-on Python implementation of principal component decomposition (PCA) algorithm ↗

2022.1–2022.5	**Undergraduate student teaching fellow**, organic chemistry, CUHK-Shenzhen.
	○ Tutorial sessions: basic concepts and exercises of stereochemistry; detailed mechanism of keto-enol tautomerism, aldol reaction, and Claisen condensation reaction, and related exercises

Skills

Coding langs	Python, Fortran, C, CUDA C++, MATLAB, LaTeX
Computer skills	Linux (including system configuration, multi-user management, software compliation and installation), WSL, Git
Coding tools	Vim, VSCode, Jupyter Lab, Windows Terminal
Scientific softs	Amber, Gromacs, Q-Chem, Gaussian, VMD, Autodock Tools

Achievements and Honors

2022.9	**Dean's List Award**, School of Life and Health Sciences, CUHK-Shenzhen.
2020.9	**Dean's List Award**, School of Science and Engineering, CUHK-Shenzhen.
2021.9	**Dean's List Award**, School of Life and Health Sciences, CUHK-Shenzhen.
2021.9	**The Second prize**, Contemporary Undergraduate Mathematical Contest in Modeling, provincial level.
2019.9–2023.6	**Bowen Scholarship**, 30,000 RMB/year, in total 120,000 RMB, CUHK-Shenzhen.
2018.9	**The First prize**, Chinese Chemistry Olympiad.

Language Skills

Chinese: native
English: TOEFL 107/120, with reading 30, listing 29, speaking 23, writing 25