

Haoran SUN

Education

- Sep. 2019–Present **B.Sc.**, Bioinformacis, Chinese University of Hong Kong, Shenzhen (CUHK-Shenzhen).
Cumulative GPA 3.716/4.000 rank 1/39
Major GPA 3.831/4.000 rank 1/39
- June 2022–Aug. 2022 **Summer visiting program**, University of California, Berkeley (UCB).
Courses taken: MATH104 introduction to real analysis, MATH128A numerical analysis, CS61C machine structure
GPA 4.000/4.000

Skills

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

Teaching Experiences

- Sep. 2021–Dec. 2021 **Undergraduate student teaching fellow**, computational biology, CUHK-Shenzhen.
- Create a slide about how to simplify the Schrödinger equation of hydrogen atom using atomic units
 - Tutorial sessions: 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 ↗
 - Hold office hours, homework grading, exam invigilation
- Jan. 2022–May 2022 **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, related exercises
 - Hold office hours, homework grading, exam invigilation

Achievements and Honors

- Sep. 2018 **The First prize**, Chinese Chemistry Olympiad.
- Sep. 2019–June 2023 **Bowen Scholarship**, 30,000 RMB/year, in total 120,000 RMB, CUHK-Shenzhen.
- Sep. 2020 **Dean's List Award**, School of Science and Engineering, CUHK-Shenzhen.
- Sep. 2021 **Dean's List Award**, School of Life and Health Sciences, CUHK-Shenzhen.
- Sep. 2021 **The Second prize**, Contemporary Undergraduate Mathematical Contest in Modeling, provincial level.

Research Experiences

- Apr. 2021–Present **Research assistant**, Hajime Hirao's group, CUHK-Shenzhen.

- Apr. 2021–June 2021 **Training:** theoretical studying of quantum chemistry by *Modern Quantum Chemistry*
- SCF algorithm coding by Fortran, including RHF 6-31G H₂ molecule and UHF 6-31G H₂⁻ molecule
 - Fixed problematic DIIS algorithm in original group Fortran code which used for acceleration
- Aug. 2021–Dec. 2021 **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
 - Molecular dynamics simulation of initial reaction complex to determine the starting path of the reaction
 - Deriving MM parameters, setup system, perform MD simulations, check non-bonding interactions, check clusters in trajectory by statistical algorithms, found minor sub-states by clustering algorithm
 - MMPBSA free energy approximation to compare population between states, in order to find which binding pose is more favorable for protein
 - Using quantum mechanics + molecular mechanics (QM/MM) hybrid method to investigate into the protein-substrate interaction
 - Determine QM region of the system, use MM parameters to build up QM/MM model
 - Use small basis set when performing optimization, then use large basis set and electronic embedding scheme to investigate electronic configurations and effect of protein
- Apr. 2022–Present **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 batch EDA analysis using Q-Chem, fix convergence problem by shutdown DIIS when error is small
 - The research could provide insight into inhibition drug design for P450
 - Under review
- Jan. 2020–Dec. 2020 **Research assistant,** Hsien-da Huang's group, CUHK-Shenzhen.
- Project:** effects of traditional Chinese medicine in gene regulation: identify DEGs using statistical methods
- Visualization of gene expression profile using PCA and t-SNE to get a first sight of data's distribution
 - Group tutorial about how to use Connectivity Map
 - Exploring databases, submitting a query, interpreting statistics and heatmap
 - Gene set enrichment analysis (GSEA) for traditional Chinese medicines perturbed gene expression profile to identify differentially expressed gene sets

Language Skills

Chinese (native)

English (GRE V155)

Japanese (elementary, only able to read)