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# 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: introduction to real analysis, numerical analysis, machine structure

## Skills

Coding langs: Python, Fortran, C, CUDA C++ and CUDA Fortran (elementary), MATLAB, LaTeX

Computer skills: Linux (including system configuration, multi-user management, software compliation 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 $H_2$ molecule and UHF 6-31G $H_2^-$ 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)