

Haoran SUN

Education

Sep. 2019–Present **B.Sc.**, Bioinformacis, Chinese University of Hong Kong, Shenzhen (CUHK-Shenzhen).
Cumulative GPA 3.671/4.000 rank 3/38
Major GPA 3.800/4.000 rank 1/38

Research Experiences

- Apr. 2021–Present **Research assistant**, Hajime Hirao's group, CUHK-Shenzhen.
- Apr. 2021–June 2021 **Training:** theoretical learning of quantum chemistry
- Learning *Modern Quantum Chemistry*
 - SCF algorithm coding by Fortran
 - RHF 6-31G H₂ molecule
 - UHF 6-31G H₂⁺ molecule
 - SCF acceleration by DIIS algorithm
 - Fixed problematic DIIS algorithm in original group Fortran code
- June 2021–July 2021 **Training:** reaction pathway analysis–hydroxylation reaction between P450 Cpd I and propane
- Scan along the reaction path
 - Geometry optimization of intermediates
 - Calculation under different spin states
 - Writing scripts to extract information and generate report efficiently
- Aug. 2021–Dec. 2021 **Project:** reaction pathway analysis–P450 C-S bond formation by TleB (PDB ID: 6J83)
- Design the whole research plan
 - DFT calculation
 - Build truncated model
 - DFT calculations along the proposed reaction pathway
 - Identify electronic configurations under different spin states
 - Swap electrons in π or σ orbitals to get stable configuration
 - Molecular dynamics simulation of initial reaction complex
 - Calculate MM parameters, correct protonated state, setup model
 - Perform MD simulations, check non-bonding interactions, check clusters in trajectory by statistical algorithms
 - MMPBSA free energy approximation to compare population between states
 - QM/MM
 - 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:** EDA and NBO analysis of the nature of coordinate bond at the heme iron center in cytochrome P450 inhibition
- Write an example Lewis configuration for NBO input
 - EDA analysis using Q-Chem
 - Fix convergence problem by shutdown DIIS when error is small

- 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
 - 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

Skills

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| Coding langs | Python, Fortran, 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 |
| Compt. chem. tools | Amber, Gromacs, Q-Chem, Gaussian, VMD, Autodock Tools |

Teaching Experiences

- Sep. 2021–Dec. 2021 **Undergraduate student teaching fellow (USTF)**, Computational Biology (BIM2005), CUHK-Shenzhen.
- Create a slide about how to simplify the Schrödinger equation of hydrogen atom using atomic units
 - Tutorial session: molecular docking tool Autodock-Vina
 - Tutorial session: review basic principles of quantum mechanics and quantum chemistry
 - Tutorial session: 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 (USTF)**, Organic Chemistry (BIO2003), CUHK-Shenzhen.
- Tutorial session: basic concepts and exercises of stereochemistry
 - Tutorial session: detailed mechanism of keto-enol tautomerism, aldol reaction, and Claisen condensation reaction, related exercises
 - Hold office hours, homework grading, exam invigilation

Achievements and Honors

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| Sep. 2018 | The First prize , Chinese Chemistry Olympiad, provincial level. |
| Sep. 2019–June 2023
(expected) | Bowen Scholarship , 30,000 RMB/year (total 120,000 RMB), CUHK-Shenzhen. |
| Sep. 2020 | Academic Year 2019-20 Dean's List Award , School of Science and Engineering, CUHK-Shenzhen. |
| Sep. 2021 | Academic Year 2020-21 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. |

Courses Taken

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| Math & stat | Calculus I and II, ordinary differential equations, linear algebra, advanced linear algebra, probability and statistics I |
| Chem & physics | Mechanics, organic chemistry, physical chemistry I, computational (structural) biology, computational biology laboratory, biophysics, molecular simulation & modeling I (including statistical mechanics theories, monte carlo, MD simulation algorithms) |

- Informatics Introduction to computer science: programming methodology, computational laboratory, bioinformatics, computational genomics and proteomics, machine learning in computational biology, design and analysis of bioinformatics algorithms
- Biology Biochemistry, cell and molecular biology, genetics

Language Skills

Chinese (native)

English (GRE Q155)

Japanese (elementary, only able to read)