Haoran SUN

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Education

Sep. 2019–Present	**B.Sc.**, Bioinformacis, Chinese University of Hong Kong, Shenzhen (CUHK-Shenzhen).
	Cumulative GPA 3.706/4.000 rank 1/38
	Major GPA 3.817/4.000 rank 1/38
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, 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
Compt. chem. tools	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, provincial level.
Sep. 2019–June 2023	**Bowen Scholarship**, 30,000 RMB/year (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.

Courses Taken

Math & stat	Calculus I & II, introduction to real analysis, numerical analysis, ordinary differential equations, linear algebra, advanced linear algebra, probability and statistics I
Chem & physics	Mechanics, general chemistry, 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, bioinformacis, computational genomics and proteomics, machine learning in computational biology, design and analysis of bioinformacis algorithms
Biology	General biology, biochemistry, cell and molecular biology, genetics

Research Experiences

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

Apr. 2021–June 2021   **Training:** theoretical learning 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
- <u>Fixed problematic DIIS algorithm</u> 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)
- <u>Design the whole research plan</u>
- Build truncated model to perform DFT calculations along the proposed reaction pathway, identify electronic configurations under different spin states
- Molecular dynamics simulation of initial reaction complex
  - 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, find one mode energetically more stable
- 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:** energy decomposition analysis (EDA) and natural bonding orbital (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
- Performed batch 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

Language Skills

Chinese (native)
English (GRE V155)
Japanese (elementary, only able to read)