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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 H_2 molecule
  - UHF 6-31G H_2^- molecule
- SCF acceleration by DIIS algorithm
  - Fixed problematic DIIS algorithm in original group 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 α or β 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

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 (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

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

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, bioinformacis, computational genomics and proteomics, machine learning in computational biology, design and analysis of bioinformacis algorithms
Biology	Biochemistry, cell and molecular biology, genetics

Language Skills

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