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Haoran SUN

Education

Sept. 2019–June 2023 (expected) **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

Skills

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

Computer skills: Linux (including system configuration, multi-user management, software compliation and installation), WSL, Git, LaTeX

Programming tools: Vim, VSCode, Jupyter Lab, Windows Terminal

Compt. chem. tools: Amber, Gromacs, Q-Chem, Gaussian, VMD, Autodock Tools

Teaching Experiences

Sept. 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 about how to use molecular docking tool Autodock-vina
- Tutorial session to help the student review basic principles of quantum mechanics and quantum chemistry
- Tutorial session about the mathematical background and hands-on Python implementation of principal component decomposition (PCA) algorithm
- Hold office hours, homework grading, exam investigation

Jan. 2022–May 2022 (expected) **Undergraduate student teaching fellow (USTF)**, Organic Chemistry (BIO2003), CUHK-Shenzhen.

- Tutorial session about basic concepts and exercises of stereochemistry
- Tutorial session about detailed mechanism of keto-enol tautomerism, aldol reaction, and Claisen condensation reaction, related exercises
- Hold office hours, homework grading, exam investigation

Research Experiences

Jan. 2020–Apr. 2021 **Research assistant**, Hsien-da Huang's research group, Warshel Institute for Computational Biology, CUHK-Shenzhen .

Project: exploring how traditional Chinese medicine affects gene regulation: identify DEGs using statistical methods

- Performed visualization of gene expression profile using dimensionality reduction algorithms: a linear scheme using PCA and a non-linear scheme using t-SNE
- Delivered a group tutorial about how to use Connectivity Map: exploring databases, submitting a query, and understanding the statistics in output heatmap
- Performed gene set enrichment analysis (GSEA) for traditional Chinese medicines perturbed gene expression profile to identify differentially expressed genes (DEGs)

Apr. 2021–Present **Research assistant**, Hajime Hirao's research group, Warshel Institute for Computational Biology, CUHK-Shenzhen.

Project: theoretical learning of quantum chemistry
- Learning quantum chemistry using *Modern Quantum Chemistry* by Attilia Szabo and Neil S.Outlund motivated of Prof. Hirao
- Coding implementation of SCF algorithm using Fortran: RHF 6-31G H_2 molecule and UHF 6-31G H_2^- molecule
- Accelerating SCF algorithm by DIIS algorithm
  - Fixed problematic DIIS algorithm in original group code

Project: reaction pathway analysis of hydroxylation reaction between P450 Cpd I and propane
- Performed scan along the reaction path and geometry optimization of intermediates
- Performed calculation under different spin states
- Writing python and shell script to extract information and generate instant report in high-efficient way

Project: reaction pathway analysis of P450 C-S bond formation by TleB (PDB ID: 6J83)
- Extracted Heme center and substrate, constructed a simplified model, and performed pure DFT calculations along the proposed reaction mechanism to get the first insight of the reaction
- Constructed QM/MM models, fit substrate MM parameters, performed ONIOM calculations
- Performed molecular dynamics simulation to explore non-bonding interactions; compared the free energy differences under different binding pose of substrate using MMPBSA method

Project: EDA and NBO analysis of the nature of coordination bonding at the heme iron center in cytochrome P450 inhibition
- Determine the Lewis structures of P450 Fe^{2+} and Fe^{3+} species
- Help to perform a part of EDA analysis

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.

Language Skills

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