ZHOUYI HE

+86 13647460321 ◇ zhouyi.he@connect.ust.hk ◇ Personal Page
Rm 4207, Theoretical Chemistry Lab, Academic Building, HKUST, Hong Kong, China

EDUCATION

Hong Kong University of Science and Technology (HKUST) *08/2019 - 06/2022*
Master of Philosophy in Chemistry (Chemical Physics) GPA: 3.33/4.3

Main courses: Advanced Inorganic Chemistry (B+), Statistical Mechanics(A).

MPhil Thesis: Statistical Methods for Protein Function and Evolution Analysis

University of Science and Technology of China (USTC) *08/2015 - 06/2019*
Bachelor of Science in Chemistry (Chemical Physics) GPA: 3.23/4.3 (Major GPA: 3.44/4.3)

Main courses: Mechanics (A-), Calculus (B+), Linear Algebra (B+), Computer Programming (A-), Electromagnetism & Electrodynamics (A-), Computational Methods (A), Molecular Spectroscopy (A), Applied Quantum Chemistry (A-), Chemical Kinetics and Dynamics(A).

BSc Thesis: Discussion on the Unit Cell Consistency of Maximally Localized Wannier Function

TOEFL:107 (Reading:30, Listening:30, Speaking: 22, Writing: 25) *09/2022*

PUBLICATIONS AND CONFERENCES

Xiaolong Yang, Zhouyi He, and Xiao Zheng. "Unit cell consistency of maximally localized Wannier functions." Electronic Structure 2.1 (2020): 014001.

Zhouyi He, et al. "Dynamic Expedition of Leading Mutations in SARS-CoV-2 Spike Glycoproteins." bioRxiv (2021). (Preprint, under review)

Impact of mutations in CRISPR Cas9, presented in The 1st International Symposium on Marine Science and Engineering for Young Scientists and Postgraduates

RESEARCH EXPERIENCE

Sequence-dependent Target searching and binding dynamics of CRISPR Cas9 M.Phil
Prof. Haibin Su's research group, department of chemistry, HKUST *01/2021 - now*

· PAM searching dynamics of CRISPR Cas9, is modelled by stochastic equations with the frame work of facilitated diffusion, namely the combination of 3D diffusion and 1D sliding. This work fills the gap of Cas9 target search dynamics and could be combined with sequence-dependent models to further understand the binding free energy landscape of other DNA-targeting proteins.

· Combined with protein sequence analysis, a conformation-dependent model is constructed to link the off-target effect and kinetic changes and to explain the sequence discrimination in target binding. This work provides a comprehensive understading of Cas binding dynamics thus sheds lights on Cas9 variants design and off-target rate minimization. *Presented in Symposium*

Dynamic Expedition of Leading Mutations in SARS-CoV-2 Spike Glycoproteins M.Phil
Prof. Haibin Su's research group, department of chemistry, HKUST *05/2021 - 01/2022*

· A time-resolved statistical method, dynamic expedition of leading mutations (deLemus), to analyze the evolution dynamics of the spike protein. Together with analysis on single amino-acid polymorphism, we quantified the mutation strength of each amino acid to unravel mutation pattern of spike glycoprotein and effectively detect the potential signal of emergent variants thus facilitate the design of spike-targeting vaccine. *Preprint under review, 1st Author*

Evolution of CRISPR Cas9 systems in Streptococcus Genus M.Phil
Prof. Haibin Su's research group, department of chemistry, HKUST *06/2020 - 05/2021*

· Statistical coupling analysis is applied to retrieve sectors, which are the evolutionary units of 3-D structure that could reflect their evolutionary histories. Interaction of bacteria and virus species through the CRISPR system, as well as the Horizontal Gene Transfer, is also investigated, which suggests the trade-off in benefits of HGT and defensive level of bacteria. *Presented in Symposium*

Unit Cell Consistency of Maximally Localized Wannier Functions Undergraduate Thesis
Prof. Xiao Zheng's research group, department of chemical physics, USTC *09/2018 - 07/2019*

· Wannier functions are the localized molecular orbitals of crystalline systems, which are maximally localized when spread function is minimized. In this project, I was responsible for the theoretical derivation of equations for higher dimensionality and computational validation of our theoretical prediction using VASP and wannier90 starting from unit cell and super cell. *Published, 2nd Author*

Physicochemical and Aggregation Properties of Alpha-synuclein Research Assistant
Prof. Jinqing Huang's research group, department of chemistry, HKUST *07/2018 - 08/2018*

· Structural characterization and physicochemical properties of single-molecule alpha-synuclein using Optical Tweezers and Ramon Spectroscopy.

Design of Single-Atom Catalyst with Atomic Layer Deposition Research Assistant
Prof. Junling Lu's research group, department of chemical physics, USTC *03/2017 - 06/2018*

· Synthesis of catalysts with Pt atomic layer deposition on $g - C_3N_4$; optimization of their performance in catalyzing hydrogen-releasing reactions by testing reaction activity and stability.

PROFESSION

Discipline	Chemical Physics, Theoretical Biophysics, Statistical Physics, Computational Chemistry, Material Science and Biology, etc.
Software/Coding	Python, MATLAB, C, Bioinformatics tools, MS Office, etc.

ACADEMIC ACHIEVEMENTS

Postgraduate Studentship @HKUST	*2019 - 2022*
National Endeavor Scholarship @USTC	*2016, 2018*
Second Prize in 28th China High School Chemistry Olympic Competition	*2014*
Third Prize in Hunan High School Mathematics Olympic Competition	*2014*
Outstanding student Scholarship @USTC	*2016, 2018*
Valedictorian of Changsha Experimental High School	*2015*
Teaching Assistant of *Physical Chemistry II* @HKUST	*2022*
Teaching Assistant of *Mathematical Methods for Physical Chemistry* @HKUST	*2020, 2021*
Teaching Assistant of *Physical Chemistry* @USTC	*2018*

EXTRA-CURRICULAR ACTIVITIES PARTICIPATION

Leader of teaching volunteers of aid education @Western Hunan, China	*2015*
Church Youth Fellowship @Clearwater Bay International Baptism Church	*2019 - 2022*
Leader of university hiking team @HKUST	*2021*
Leader of the university student union and basketball association @USTC	*2015 - 2019*
Championship in university basketball competition @USTC	*2017*
Volunteer of in 30th China High School Chemistry Olympic Competition @USTC	*2015*

HOBBIES

Photography, Literature, Music, Movie, Hiking, Traveling, Basketball, etc.