Curriculum Vitae

Name	Honghui Zhang	**Nation**	Shenzhen, Guangdong, China
Tel	+86 15889455816	**E-mail**	221059040@link.cuhk.edu.cn

★ Motivation

The intricate and complex nature of biological systems has always puzzled me, sparking my curiosity. The fusion of biology and computer science in Computational Biology offers a pathway to probe these perplexities. My desire to decode these mysteries, coupled with my passion for both fields, motivates me to pursue a Ph. D. in Computational Biology. So that is why I am applying for Ph.D.: curiosity and confusion are the motive force.

★ Research Interests

1) Computational Biology
2) Biomacromolecules and Molecular Machines
3) Enzyme Catalysis
4) Viral Protein Mechanisms in Disease

★ Educational Background

2021.09-2025.08	The Chinese University of Hong Kong, Shenzhen	**Biological Science**	PH. D.
2016.09-2019.06	Wuhan Textile University	**Textile Science and Engineering**	Master
2011.09-2015.06	Wuhan Textile University	**Fashion Design and Engineering**	B. E.

★ Working Experience

2025.06-present	Warshel Institute for Computational Biology, CUHKSZ	**Research Assistant**
2021.01-2021.08	Warshel Institute for Computational Biology, CUHKSZ	**Research Assistant**
2020.06-2020.12	Institute for Advanced Study, Shenzhen University	**Research Assistant**
2019.06-2020.05	Shanxi University of Science and Technology	**Research Assistant**

★ Research projects

1) Computational Studies of Regio- and Enantioselective Oxidation of Free Fatty Acids by human P450s (2024-now)
2) Exploring the Phospholipid Transport Mechanism of ATP8A1-CDC50 (2021-2023).
3) Predicting Mutational Effects on Receptor Binding of the Spike Protein of SARS-CoV-2 Variants (2021).
4) Comparative Study of DNA-binding Mechanisms of Human and Mouse cGAS (2020).
5) Effects of High Hydrostatic Pressure on Amylose Conformation (2019).
6) Weak Interaction Mechanisms of Crystalline Cellulose Iα (2016-2018).

(I performed the model construction, and data analysis and drafted the manuscript for projects 1, 2, 5 and 6. And I performedthe part of the simulation for projects 3 and 4)

★ Research findings

1) **Zhang, H.**, Hirao, H., Mechanism of Regio- and Enantioselective Hydroxylation of Arachidonic Acid Catalyzed by Human CYP2E1: A Combined Molecular Dynamics and Quantum Mechanics/Molecular Mechanics Study[J]. *Journal of Chemical Information and Modeling,* 65(4), 2080-2092 (2025). https://doi.org/10.1021/acs.jcim.5c00115
2) Hirao, H., Yue D., Xia S., Zhang E., **Zhang H.**, Yan J., Xiao Z. Computational Studies on Human Cytochrome P450: Advancing Insights into Drug Metabolism. *Trends in Chemistry*. 7(7), 358-371 2025. https://doi.org/10.1016/j.trechm.2025.05.002
3) Shi, D., Zhu, X., **Zhang, H.**, Yan, J., Bai, C. Catalytic Mechanism Study of ATP-citrate Lyase during Citryl-CoA Synthesis Process[J]. *iScience*, 27(9), 110605 (2024). https://doi.org/10.1016/j.isci.2024.110605
4) An K., Yang X., Luo M., Yan J., Xu P., **Zhang H.**, Li Y. et al. Mechanistic study of the transmission pattern of the SARS-CoV-2 omicron variant[J]. *Proteins: Structure, Function, and Bioinformatics*, 92(6), 705-719 (2024).

5) **Zhang, H.**, Zhang, Y., Xu, P. et al. Exploring the Phospholipid Transport Mechanism of ATP8A1-CDC50[J]. *Biomedicines*, 11(2), 546 (2023). https://doi.org/10.3390/biomedicines11020546

6) Shi D.,† An K.,† **Zhang H.†** et al. Application of Coarse-Grained (CG) Models to Explore Conformational Pathway of Large-Scale Protein Machines[J]. *Entropy*, 24(5), 620 (2022). https://doi.org/10.3390/e24050620

7) Zhang Y., Zhu X., **Zhang H.** et al. Mechanism Study of Proteins under Membrane Environment[J]. *Membranes*,12(7), 694 (2022). https://doi.org/10.3390/membranes12070694

8) Bai C., Wang J., Chen G., **Zhang H.** et al. Predicting Mutational Effects on Receptor Binding of the Spike Protein of SARS-CoV-2 Variants[J]. *Journal of the American Chemical Society*, 143(42): 17646-17654 (2021). https://doi.org/10.1021/jacs.1c07965

9) Chen Z.**†**, **Zhang H.†** Wade K. et al. The analysis of the effects of high hydrostatic pressure (HHP) on amylose molecular conformation at atomic level based on molecular dynamics simulation[J]. *Food Chemistry,* 327: 127047 (2020). https://doi.org/10.1016/j.foodchem.2020.127047

10) Wang X., **Zhang H**., Li W. DNA-binding mechanisms of human and mouse cGAS: a comparative MD and MM/GBSA study[J]. *Physical Chemistry Chemical Physics*, 22(45): 26390-26401 (2020). https://doi.org/10.1039/D0CP04162A

11) **Zhang H**., Jiang X. Revealing the Weak Interaction Mechanism of Crystalline Cellulose Iα by Molecular Dynamics Simulations[J]. *Journal of Fiber Bioengineering and Informatics* 12(4): 167-178 (2019). https://doi.org/10.3993/jfbim00324.

12) **Zhang H.**, Jiang X., Zhao S. Research on the Influence of discount rate on the sales of fast fashion men's wear[J]. *Fasion Guide*, 7(01):38-43 (2018).

13) Jiang X., **Zhang H.**, Zhong A. Revealing the Interaction Mechanism Stabilizing Crystalline Cellulose Iβ by Molecular Dynamics Simulations[J]. *Journal of Fiber Bioengineering and Informatics*, 10(3): 141-154 (2017). https://doi.org/10.3993/jfbim00267.

14) Bai C., Shi D., An K., Zhang Y., Zhu X., **Zhang H.**, Yan J., Xu P. A method for constructing chemical space of targeted drug molecules devices, computer equipment and readable storage media. (Patent 2021)

★ Skills

1) IELTS 6.5 point, possessing a good ability for literacy, can quick browsing of English professional literature and books, speaking ability is not good, but can communicate normally. Own good communication skills. Have the good ability to work with different people.
2) Always in Linux, Python and R; used SPSS, MATLAB, in master study; Proficient in research software such as Amber, GROMACS, Gaussian, VMD and Pymol; Using GitHub or Visual Studio Code.

★ Award/Honors

1) Outstanding graduate student award (2025) 2) Gang Hong scholarship for PH. D. student (2021-2025)
3) First-grade scholarship for master's degree (2018) 4) First-grade scholarship for master's degree (2017)
5) 3rd place in Wuhan Textile University Research Forum (2017)
6) Outstanding Thesis" of the 10th Textile Bioengineering and Informatics Symposium (2017)
7) 3rd place in Wuhan Textile University Research Forum (2016)
8) 1st place in Creative Artistic Expression in Wuhan Textile University Research Forum (2016)