

## Haiqing Zhao

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- **Computational biophysicist and systems biologist in molecular modeling, free energy calculations, structural bioinformatics, ML/AI model developments**
- **Research interests: Protein-Protein Interactions, Omics data, Protein dynamics, Drug discovery**
- **Biology interests: Host-Pathogen Interactions; Epigenetics/Cancer**

### Employment

Assistant Professor, Dept. of Biochemistry & Molecular Biology; Core Faculty Member, Sealy Center for Structural Biology and Molecular Biophysics, University of Texas Medical Branch (09/2024 -now)

Adjunct Research Scientist, Columbia University (09/2024 – now)

Associate Research Scientist, Dept. of Systems Biology, Columbia University (08/2022 – 08/2024)

Visiting Assistant Professor, Duke University (06/2020 – 12/2020)

### Education & Training

Postdoc, Systems Biology, Columbia University (08/2018 – 07/2022, PI: Barry Honig)

Ph.D., Biophysics Program, IPST, University of Maryland at College Park (09/2012 – 07/2018, advisor: Garegin Papoian; Yamini Dalal, NCI/NIH)

M.S., Physics, Michigan Technological University (09/2010 – 07/2012, advisor: Ulrich Hansmann)

B.S., Physics (minor in Computer Science), Northeast Normal University (09/2006 – 07/2010, advisor: Taiyu Zheng; Yanting Wang, Institute of Theoretical Physics, Chinese Academy of Sciences)

### Research Support

2025-2028     UT System STAR Award (Rising STAR), \$250,000 (PI)

### Institutional Services

Keck Faculty, Gulf Coast Consortia (Quantitative Biomedical Science), Texas Medical Center (2024-)

UTMB BCMB Graduate Admission Committee (2024-2025);

Qualifying Exam Committee: Justin T. Nguyen (UTMB); Justin Zhu (UTMB)

## Research

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|---|-----------------------------------|
| <p>University of Texas Medical Branch (Galveston, TX)</p> <p>(a). <i>Developing Computational Methods for Cell-specific Protein-Protein Interactions</i></p> <p>(b). <i>Developing Computational Methods for Protein-Protein Binding affinity</i></p> <p>(c). <i>Applying ML/DL methods on biological applications such as aaRS, Reelin, suPAR, dynamin, PROTAC, Henipavirus Polymerase, antibody design etc.</i></p> <ul style="list-style-type: none"> <li>• Collaborators include Minkuo Luo (Sloan Kettering), Heather Stevenson-Lerner (UTMB), etc.</li> </ul> | <p>09/2024–now</p>                |
| <p>Columbia University Irving Medical Center (Honig Lab, Systems Biology):</p> <p>(a). <i>Developing Computational Methods for Predicting Protein-Protein Interactions Using Structure-based Modeling, Information Theory and Machine Learning</i></p> <p>(b). <i>Developing Genome-wide Databases of Protein-Protein Interactions</i></p> <ul style="list-style-type: none"> <li>• Collaborating with Haiyuan Yu (Cornell University), Jeffrey Skolnick (Georgia Tech)</li> </ul>  | <p>08/2018–08/2024</p>            |
| <p>University of Maryland at College Park (Papoian Group, Computational Chemistry):</p> <p>(a). <i>Computational Study of Chromatin Structure and Dynamics</i></p> <ul style="list-style-type: none"> <li>• Collaborated with Yamini Dalal at NCI/NIH; David Fushman at UMD</li> </ul> <p>(b). <i>Finding Minimum Free Energy Path in Protein Folding and Binding Energy Landscapes.</i></p> <p>(c). <i>Development of Coarse-grained Force Field for Simulating IDP.</i></p>   | <p>03/2013–07/2018</p>            |
| <p>Universität Düsseldorf &amp; Jülich Supercomputing Centre, Germany</p> <p>(a). <i>Developing steered MD Method for FRET-based Structure Modeling</i></p> <ul style="list-style-type: none"> <li>• Worked with Clauz Seidel and Holger Gohlke</li> </ul>  | <p>2012 summer</p>                |
| <p>Institute of Theoretical Physics, Chinese Academy of Science, China</p> <p>(a). <i>Investigating the Nanophenomenon of Tail Aggregation of Ionic Liquid</i></p> <ul style="list-style-type: none"> <li>• Worked with Yanting Wang</li> </ul>   | <p>06-09/2009,<br/>01-05/2010</p> |

## Publications

(Co-first author #; Co-corresponding author \*)

1. **H. Zhao**, S. Rui, and Y. Wang. "Nanoscale tail aggregation in ionic liquids: Roles of electrostatic and van der waals interactions." *Communications in Theoretical Physics* 56, no. 3 (2011): 499.
2. D. Winogradoff, **H. Zhao**, Y. Dalal, and G. A. Papoian. "Shearing of the CENP-A dimerization interface mediates plasticity in the octameric centromeric nucleosome." *Scientific Reports* 5 (2015): 17038.

3. D. P. Melters, J. Nye, **H. Zhao**, and Y. Dalal. "Chromatin dynamics in vivo: a game of musical chairs." *Genes* 6, no. 3 (2015): 751-776.
4. **H. Zhao**, D. Winogradoff, M. Bui, Y. Dalal, and G. A. Papoian. "Promiscuous histone mis-assembly is actively prevented by chaperones." *Journal of the American Chemical Society* 138, no. 40 (2016): 13207-13218. (Highlighted on the cover)
5. **H. Zhao**, D. Winogradoff, Y. Dalal, G. Papoian. "The Oligomerization Landscape of Histones." *Biophysical Journal*, 116, no. 10: (2019) 1845-1855. (Highlighted on journal website)
6. **H. Zhao**\*, H. Wu, D. Abeykoon, A. Guseman, C. Camara, Y. Dalal, D. Fushman, and G. A. Papoian. "The Role of Cryptic Ancestral Symmetry in Histone Folding Mechanisms Across Eukarya and Archaea", *PLOS Computational Biology* 20.1 (2024): e1011721.
7. **H. Zhao**<sup>#</sup>, D. Winogradoff<sup>#</sup>, Y. Dalal, G. Papoian. "Computational Modeling of Histone Complexes, Nucleosomes and Their Modifications", *Accounts of Chemical Research*, (invited review, to be submitted)
8. **H. Zhao**\*, "Self-assembled nucleoid proteins scaffold bacterial DNA", *Biophysical Journal* 120 (5), 754, (2021)
9. Z. Sheng, J. Bimela, P. Katsamba, S. Patel, Y. Guo, **H. Zhao**, Y. Guo, P. Kwong, and L. Shapiro. "Structural basis of antibody conformation and stability modulation by framework somatic hypermutation." *Frontiers in immunology* (2022): 5573.
10. Z. Su, N. Kon, J. Yi, **H. Zhao**, W. Zhang, Q. Tang, H. Li, Z. Li, S. Duan, Y. Liu, Z. Zhang, B. Honig, J.J. Manfredi, A.K. Rustgi, W. Gui. "Specific regulation of BACH1 by the hot-spot mutant p53R175H reveals a distinct gain of function mechanism", *Nature Cancer*, 2023: 1-18
11. D. Petrey<sup>#</sup>, **H. Zhao**<sup>#</sup>, S. Trudeau, D. Murray and B. Honig, "PrePPI: A Structure-Informed Proteome-Wide Database of Protein-Protein Interactions", *Journal of Molecular Biology*, 2023: 168052
12. **H. Zhao**, D. Petrey, D. Murray, and B. Honig, "ZEPPI: proteome-scale sequence-based evaluation of protein-protein interaction models", *Proceedings of the National Academy of Sciences* 121.21 (2024): e2400260121.
13. S. Farmer, A. Solbach, S. Xu, B. Rios, X. Ye, A. Gao, D. Covarrubias, Y. Yu, L. Ye, V. Chuong, E. Stimming, **H. Zhao**, S. Zhang, "Structural-functional analyses of the Huntingtin/HAP40 complex in *Drosophila* and Humans", *Journal of Biomolecular Structure and Dynamics*, accepted (2025)
14. **H. Zhao**, A. Saha, C. Velez, A. Naravane, D. Petrey, J. Skolnick, D. Murray, and B. Honig, "Combining structural modeling and deep learning to calculate the *E. coli* protein interactome and functional networks", *Nature Communications* (under revision), 2025
15. N. Aniket, C. Velez, **H. Zhao**, D. Murray, D. Petrey, and B. Honig, "PrePPI-yeast: a comprehensive yeast database of structure-based protein-protein and protein-metabolite interactions", in preparation, 2025

16. Q. Yang, X. Fan, J. Bian, **H. Zhao**, R. Yin, “SEHI-PPI: An End-to-End Sampling-Enhanced Human-Influenza Protein-Protein Interaction Prediction Framework with Double-View Learning”, submitted (2025)
17. C. Hou, **H. Zhao**, Y. Shen, “Learning Biophysical Dynamics with Protein Language Models”, Proceedings of the National Academy of Sciences (under revision) (2025)

## Mentoring & Teaching

- Current trainees at UTMB: Zhiyuan Song (postdoc); Ziyu Shi (research associate); Surendra Negi (research scientist); Lauren Gansen (co-mentored PhD student); Hao Wang (undergraduate researcher, Washington University in St. Louis, Math/CS); Vincent Thai (undergraduate researcher, University of Houston, Chemistry); Rui Tang (MS student researcher, New York University, Biostatistics); Raymond Li Wang (undergraduate researcher, UC Berkeley, EE/CS); Gary Sun (undergraduate researcher, UC Berkeley, EE/CS) 2024–now
- Mentored trainees at Columbia University: Aniket Naravane (2023 – 2024, Columbia), Victor Robila (2023 summer, Columbia), Emily Ward (2024 summer, Wesley College) 2022–2024
- Introduction to Biophysics, Duke University (designed & instructed; PHYS303) Fall 2020
- Introduction to Brain Biophysics, Zuckerman Institute, Columbia University (independently designed course for selected high-school students) Spring 2019
- Evidence-based Teaching and Learning Seminar at Teacher’s College, Columbia University (semester-long pedagogy workshops for how to design an advanced STEM course) Fall 2018
- Mathematical Methods in Physics (PHYS274, TA @UMD) 2016
- College Physics: Mechanics; Electricity & Magnetism (PHYS161 & 260, TA @UMD) 2015, 2018
- Quantum Physics II (PHYS402, TA @UMD) 2012
- College Chemistry Laboratory (CHEM132, TA @UMD) 2013
- Physics Laboratory: Electricity and Magnetism (PHYS276, TA @UMD) 2012
- Physics Laboratory: Mechanics (PH1111/1141, TA @Michigan Tech) 2010–2011
- Co-trained students at UMD: Jeffrey Wang (2015 - 2017), Robert Liu (2015 summer), Gulcan Kose (2017 summer), Bruce Yang (2016 - 2018), Boxuan Zhang (2018) 2015–2017

## Professional Services:

### Editorial Board:

2020 – present: Review Editor on the Editorial Board of Computational Physiology and Medicine (specialty sections: Frontiers in Bioengineering and Biotechnology; Frontiers in Physiology)

### Ad-hoc Journal Reviewer:

Nature Communications, Proceedings of the National Academy of Sciences, PRX-Life, IEEE Journal of Biomedical and Health Informatics, Biophysical Journal, Journal of Molecular Biology, PLOS Computational Biology, PLOS One, Protein Science, Proteins, Physical Chemistry Chemical Physics, Journal of Biomolecular Structure & Dynamics, Bioscience Reports, Journal of Molecular Modeling, Frontier in Physiology, BMC Bioinformatics

## Fellowships, Honors and Awards

2020	<b>Duke University Global Fellow</b>
2019	<b>Chinese Government Award for Outstanding Students Studying Abroad</b>
2018	<b>Dean's Outstanding Teaching Award</b> (one in College of Computer, Mathematical, and Natural Sciences)
2017	<b>Ann G. Wylie Dissertation Fellowship</b>
2016	Education Committee Travel Award, Biophysical Society
2016	Ralph Myers & Friends Physics Award (excellence in teaching)
2013–2015	<b>NCI-UMD Partnership Fellow</b>
2013, 2015	Jacob K. Goldhaber Travel Grant
2013	International Conference Student Support Award, Research Grant from National
2007–2009	Students' Scientific Innovation Program, Chinese Ministry of Education
2008	2nd prize in Jilin province, China Undergraduate Mathematical Contest in Modeling
2008	Outstanding Citizen Honor (for volunteering service), Changchun City Government
2006–2010	University scholarships for four years, Northeast Normal University

## Conferences & Talks

- “Use Associated memory, Water mediated, Structure and Energy Model to Study Protein Folding and Binding Problems”, **Invited Instructor** at Beijing 2014 Biophysics summer school, University of Chinese Academy of Science, 2014
- “THE ASSOCIATION LANDSCAPE OF UBIQUITIN DIMERIZATION”, poster, BPS annual meeting, Baltimore, 2015
- “Free Energy Calculation of Di-ubiquitin Shows the Closed Conformation is the Energy Minimum Binding State”, Physics of Living Systems 2015 Annual Meeting, Arlington, VA, 2015

- “CENP-A/H4 Has a Tougher Dimerization Process Than H3/H4”, **Contributed Talk** at "From Computational Biophysics to Systems Biology (CBSB2015)" workshop, University of Oklahoma, 2015
- “Dual-resolution modeling demonstrates greater conformational heterogeneity of CENP-A dimer than that of H3 dimer”, talk, APS March Meeting, Baltimore, 2016
- “Revealing the asymmetrical role in the histone dimer dynamics”, poster, Gordon Research Conference, West Dover, VT, 2016
- “Promiscuous Histone Mis-assembly is Actively Prevented by Chaperones”, poster, BPS annual meeting, New Orleans, 2017
- “The Biophysical Features of Histone Oligomerization”, poster, Conference of modeling protein-protein interactions, Lawrence, Kansas, 2018
- “Protein-protein interaction: from its molecular biophysics to co-evolution-based interface prediction”, **Invited talk**, NCI 50th Anniversary/CCR 20th Anniversary Seminar, NCI (online), 2021
- “Combining Structural and Evolutionary Information to Predict Protein-Protein Interactions”, talk, Department of Systems Biology, Columbia University, 2022
- “Combining Structural and Evolutionary Information to Predict Protein-Protein Interactions”, talk, Columbia-wide Biophysics & Biochemistry Mixer, Columbia University, 2023
- “Z-interface: A New Evaluation Method for Predict Protein-Protein Interactions”, poster, 67<sup>th</sup> Biophysical Society Annual Meeting, San Diego, 2023
- “Proteome-scale Predictions of Protein-Protein Interactions”, poster 2024 International Conference on Intelligent Biology and Medicine, Houston, 2024
- “Predicting Protein-Protein Interactions on the Genome-wide Scale”, **invited talk**, SCBA-Texas | Baylor Medical School, Houston, 2024
- “Predicting Protein-Protein Interactions using Structure-based ML/AI Modeling”, **invited talk**, International Conference on Intelligent Biology and Medicine, Columbus, Ohio, 2025
- “Genome-wide Protein-Protein Interaction Predictions Using Structure-based ML/AI Modeling”, **invited talk**, Department of Integrative Biology & Pharmacology, UT Health, 2025
- “Predicting Protein Bindings with Structure-based and Chemistry-Enhanced ML/DL Modeling”, **invited talk**, Pacificchem, 2025

## Others

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| • Co-captain of UMD-CSSA soccer team (University Intramural Champion)            | 2013–2015 |
| • Volunteer for Biophysical Society (Maryland Day and 2014 BPS Meeting)          | 2012–2014 |
| • NE Cup Soccer Tournament, 2 <sup>nd</sup> Place (Columbia Chinese Soccer Team) | 2019      |