

Haiqing Zhao

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- **Computational biophysicist and systems biologist in molecular modeling, structural bioinformatics, ML/AI model developments on biological systems**

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)

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)

Funding Support

2026-2029 Welch Research Grant (PI)

2025-2028 UT System Rising STARS Award (PI)

2024-2027 University of Texas Medical Branch Startup Fund (PI)

2026-2031 Maximizing Investigators' Research Award (MIRA ESI), NIGMS (PI, pending)

2026-2029 R61/R33 grant, NCCIH/NIH, (co-I, pending)

2026-2031 R01 grant, NIAID/NIH, (co-I, pending)

2026-2031 R01 grant, NIGMS/NIH, (co-I, pending)

2026-2031 R01 grant, NIDDK/NIH, (co-I, pending)

2026-2031 R01 grant, NIA/NIH, (co-I, pending)

Institutional Services

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

Graduate Admission Committee: BCMB program (2024, 2025);

Qualifying Exam Committee: Justin T. Nguyen; Justin Zhu; Maria C. Do Nascimento Garcia Leal; Eduardo Aguirre; Lauren Gansereit

Dissertation Committee: Dario Villacreses

Faculty Search Committee: BMB (2025)

Research

University of Texas Medical Branch (Galveston, TX) 09/2024–now

(a). *Developing Computational Methods for Cell-specific Protein-Protein Interactions*

(b). *Developing Computational Methods for Protein-Protein Binding Affinity*

(c). *Applying ML/DL methods on biological applications such as aaRS, Reelin, suPAR, dynamin, PROTAC, Henipavirus Polymerase, antibody design etc.*

- Collaborators include Minkuo Luo (Sloan Kettering), Heather Stevenson-Lerner (UTMB), Bingning Dong (Baylor), etc.

Columbia University Irving Medical Center (Honig Lab, Systems Biology): 08/2018–08/2024

(a). *Developing Computational Methods for Predicting Protein-Protein Interactions Using Structure-based Modeling, Information Theory and Machine Learning*

(b). *Developing Genome-wide Databases of Protein-Protein Interactions*

- Collaborating with Haiyuan Yu (Cornell University), Jeffrey Skolnick (Georgia Tech)

University of Maryland at College Park (Papoian Group, Computational Chemistry): 03/2013–07/2018

(a). *Computational Study of Chromatin Structure and Dynamics*

- Collaborated with Yamini Dalal at NCI/NIH; David Fushman at UMD

(b). *Finding Minimum FE Path in Protein Folding and Binding Energy Landscapes.*

(c). *Development of Coarse-grained Force Field for Simulating IDP.*

Universität Düsseldorf & Jülich Supercomputing Centre, Germany 2012 summer

(a). *Developing steered MD Method for FRET-based Structure Modeling*

- Worked with Clauz Seidel and Holger Gohlke

Institute of Theoretical Physics, Chinese Academy of Science, China 06-09/2009,

(a). *Investigating the Nanophenomenon of Tail Aggregation of Ionic Liquid* 01-05/2010

- Worked with Yanting Wang

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#**, D. Winogradoff#, 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#, **H. Zhao#**, 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*, (2025): 1-16.
14. 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
15. 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)
16. **H. Zhao**, C. Velez, A. Saha, 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*, 2026

17. C. Hou, **H. Zhao**, Y. Shen, “Protein language models trained on biophysical dynamics inform mutation effects”, *Proceedings of the National Academy of Sciences*, 123.4 (2026): e2530466123
18. R. Wong, Z. Song, Y. Zheng, **H. Zhao***, D. Bai*, “Quantifying Electrostatic Control of Docking and Binding Energetics in Functional Cx36 Gap Junctions”, *Communication Biology* (2026)

Mentoring & Teaching

- Current trainees at UTMB: Zhiyuan Song (postdoc); Surendra Negi (research scientist); Rui Tang (MS student researcher, New York University, Biostatistics); Raymond Li Wang (undergraduate researcher, UC Berkeley, EE/CS); Darren Pai (undergraduate researcher, Rice University); Roger Zhen (high school intern, Clear Lake High School)
- Mentored trainees at UTMB: Ziyu Shi (research associate); Hao Wang (undergraduate intern, Washington University in St. Louis, Math/CS); Vincent Thai (undergraduate intern, University of Houston, Chemistry); Gary Sun (undergraduate intern, UC Berkeley, EE/CS)
- Mentored trainees at Columbia University: Aniket Naravane (2023 – 2024, Columbia), Victor Robila (2023 summer, Columbia), Emily Ward (2024 summer, Wesley College)
- Introduction to Biophysics, Duke University (designed & instructed; PHYS303) Fall 2020
- Introduction to Brain Biophysics, Zuckerman Institute, Columbia University Spring 2019
(independently designed course for selected high-school students)
- 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, Journal of Chemical Information and Modeling

Fellowships, Honors and Awards

2020	Duke University Global Fellow
2019	Chinese Government Award for Outstanding Students Studying Abroad
2018	Dean's Outstanding Teaching Award (one in College of Computer, Mathematical, and
2017	Natural Sciences)
2016	Ann G. Wylie Dissertation Fellowship
2016	Education Committee Travel Award, Biophysical Society
2013-2015	Ralph Myers & Friends Physics Award (excellence in teaching)
2013, 2015	NCI-UMD Partnership Fellow
2013	Jacob K. Goldhaber Travel Grant
2007-2009	International Conference Student Support Award, Research Grant from National
2008	Students' Scientific Innovation Program, Chinese Ministry of Education
2008	2nd prize in Jilin province, China Undergraduate Mathematical Contest in Modeling
2006-2010	Outstanding Citizen Honor (for volunteering service), Changchun City Government 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, 67th 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
- “Zooming in and out of Protein-Protein Interactions with Graph-based Models”, **keynote speaker**, 35th SCSB annual symposium, 2026
- “Protein-Protein Interactions from Molecular Biology to Systems Biology”, **featured speaker**, 30th SCBA-TX annual symposium, 2026

Others

- 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, 2nd Place (Columbia Chinese Soccer Team) 2019