

# Haiqing Zhao

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- **Computational biophysicist and systems biologist with expertise in molecular modeling, free energy calculations, structural bioinformatics, and ML/AI-based method developments.**
- **Research interests: Protein Dynamics, Protein-Protein Interactions (PPIs), Mutation and Post-Translational Modification effects, Drug Discovery**
- **Particularly interested biology questions: Pathogen-Host Interaction and Epigenetics**

## Employment

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

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 Research Scientist, Dept. of Systems Biology, Columbia University (08/2018 – 07/2022, PI: Barry Honig)

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

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

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

## Research

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

(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 Mohammed AlQuraishi and Haiyuan Yu at Cornell University

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 Free Energy Path in Protein Folding and Binding Energy Landscapes.*

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

Universität Düsseldorf & Jülich Supercomputing Centre, Germany

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

- Worked with Clauz Seidel and Holger Gohlke

Düsseldorf,

Germany

2012 summer

Institute of Theoretical Physics, Chinese Academy of Science, China

(a). *Investigating the Nanophenomenon of Tail Aggregation of Ionic Liquid*

- Worked with Yanting Wang

Beijing, China

06-09/2009

01-05/2010

## 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<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. Murray, D. Petrey, 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. **H. Zhao**, D. Murray, D. Petrey, and B. Honig, “PrePPI-DL: a language model enhanced protein-protein interaction prediction method”, in preparation, 2024
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, 2024

## Teaching

- Introduction to Biophysics, Duke University (designed & instructed; PHYS303) Fall 2020
- Introduction to Brain Biophysics, Zuckerman Institute, Columbia University Spring 2019  
(designed & instructed; to selected senior 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
- Beijing 2014 Biophysics summer school, University of Chinese Academy of Science 2014  
(invited instructor)
- College Physics: Mechanics; Electricity & Magnetism (PHYS161 & 260, TA @UMD) 2015, 2018
- Quantum Physics II (PHYS402, TA @UMD) 2012
- Mathematical Methods in Physics (PHYS274, TA @UMD) 2016
- 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
- Supervised graduate students: Hao Wu (2014 - 2017), Mary Pitman (2015 - 2017)
- Supervised undergraduate students: Aniket Naravane (2023 - now), Jeffrey Wang (2015 - 2016), Michelle Thomas (2013 fall), Robert Liu (2015 summer), Gulcan Kose (2017 summer)
- Supervised high school students: Victor Robila (2023 summer), Bruce Yang (2016 - 2018), Boxuan Zhang (2018)

## 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 Communication, 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> (0.1%, worldwide)
2018	<b>Dean's Outstanding Teaching Award</b> (award one in College of Computer,
2017	Mathematical, and Natural Sciences)
2016	<b>Ann G. Wylie Dissertation Fellowship</b>
2016	Education Committee Travel Award, American Biophysical Society
2013-2015	Ralph Myers & Friends Physics Award (excellence in teaching physics)
2013, 2015	<b>NCI-UMD Partnership Fellow</b>
2013	Jacob K. Goldhaber Travel Grant
2007-2009	International Conference Student Support Award, Research Grant from National Students' Scientific Innovation Program, Chinese Ministry of Education
2008	2nd prize in Jilin province, China Undergraduate Mathematical Contest in Modeling, Chinese Ministry of Education
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

### 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      |