Xingcheng Lin

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Position and Scientific Appointments

- **Assistant Professor** Aug. 2023−Present
  Department of Physics, Bioinformatics Research Center, North Carolina State University
- **Postdoctoral Associate** Dec. 2018−Aug. 2023
  Department of Chemistry, Massachusetts Institute of Technology
- **Postdoctoral Research Fellow** May. 2018−Dec. 2018
  Center for Theoretical Biological Physics, Rice University
- **Graduate Research Assistant** Jun. 2012−May. 2018
  Center for Theoretical Biological Physics, Rice University

Education

- **Rice University, Houston, TX, USA** Aug. 2011−May. 2018
  Ph.D. in Biological Physics
  Dissertation Title: Uncovering the Molecular Mechanism Underpinning the Function of Influenza Hemagglutinin
  Dissertation Committee: José N. Onuchic, Herbert Levine, and Cecilia Clementi
- **Xiamen University, Xiamen, Fujian, China** Sept. 2007−June 2011
  B.S. in Physics wth minor in LED engineering
  Research Advisors: Jiao Wang (2010-2011), Xiwei Yao (2009-2010), Jianwei Shuai (2009)
  Thesis Title: Investigation of Jarzynski Equality Using One Dimensional Ideal Gas Model

List of Publications

selected publications with summary

† shared authorship

⋆ corresponding author

33. Yunrui Qiu, Shuming Liu, **Xingcheng Lin**, Ilona Christy Unarta, Xuhui Huang⋆, Bin Zhang⋆ "Nucleosome condensate and linker DNA alter chromatin folding pathways and rates", *Biophys. J.*, (2025). DOI
32. Qin Zhou, Jose Alberto de la Paz, Alexander D Stanowick, **Xingcheng Lin**, Faruck Morcos⋆ "Characterizing DNA recognition preferences of transcription factors using global couplings and high-throughput sequencing", *Nucleic Acids Res.*, (2025). DOI

31. Yafan Zhang, Irene Silvernail, Zhuyang Lin, **Xingcheng Lin**⋆ "Interpretable Protein-DNA Interactions Captured by Structure-Sequence Optimization", *eLife*, (2025). DOI
This study introduces a predictive biophysical model, "IDEA," which integrates structural and sequence data of protein-DNA complexes into an optimized energy model. The model can quantitatively predict genomic binding sites and binding affinities for DNA-binding proteins. Additionally, the model is incorporated into a simulation framework, facilitating mechanistic studies of protein-DNA interactions. Previous models used machine learning trained on large protein and DNA sequence datasets and cannot be applied to cases with limited data. We have overcome this limitation by incorporating structural information into our model training, achieving state-of-the-art predictive accuracy using only a few protein-DNA complex structures and sequences.

30. Rina Li, **Xingcheng Lin**⋆ "Connected Chromatin Amplifies Acetylation-Modulated Nucleosome Interactions", *Biochem.*, 64, 1222-1232, (2025). DOI
This study investigates the acetylation of histone 4 lysine 16 (H4K16ac), a key gene-activating modification known to destabilize chromatin. Using an explicit-ion chromatin model combined with enhanced-sampling simulations, we quantitatively characterized the interaction landscape of both wild-type and acetylated nucleosomes across multiple structural levels. Our results reveal that H4K16ac weakens inter-nucleosome interactions, an effect further amplified when nucleosomes are connected within higher-order chromatin structure. This leads to nucleosome destacking and increased exposure of nucleosomal DNA, thereby facilitating the transcription process. Our findings are consistent with observations from sedimentation and cryogenic electron tomography experiments.

29. Ailun Wang, **Xingcheng Lin**⋆, Kevin Ng Chau, José N. Onuchic, Herbert Levine, and Jason T George⋆ "RACER-m Leverages Structural Features for Sparse T Cell Specificity Prediction", *Sci. Adv.*, 10, 20, May 15, (2024). DOI
This study introduces RACER-m, a multi-template computational protocol designed for reliable prediction of T cell recognition specificity towards antigenic peptides. By incorporating the structural details of target TCR-pMHC complexes, we demonstrate RACER-m's transferability in predicting binding specificities across different TCRs and their associated peptides. Additionally, RACER-m can predict TCR binding specificities to point-mutated variants of antigen peptides.

28. Mayu Shibata, **Xingcheng Lin**, José N. Onuchic, Kei Yura, and Ryan R. Cheng⋆ "Residue coevolution and mutational landscape for OmpR and NarL response regulator subfamilies", *Biophys. J.*, 123, 1–12, March 19 (2024). DOI

27. **Xingcheng Lin** and Bin Zhang⋆ "Explicit Ion Modeling Predicts Physicochemical Interactions for Chromatin Organization", *eLife*, Jan 30 (2024). DOI
In this study, we introduced an explicit-ion treatment in a coarse-grained chromatin model to quantitatively characterize the physicochemical interactions of nucleosomes under various ionic conditions. The model has demonstrated quantitative accuracy in reproducing experimental measurements of nucleosome stability, inter-nucleosome interactions, and chromatin higher-order structure across a wide range of salt concentrations. In addition, our simulations revealed compelling evidence for the critical contribution of intrinsic physicochemical interactions in driving chromatin compartmentalization in vivo, as well as the compensatory role of linker histones in mediating inter-nucleosome interactions.

26. Kevin Ng Chau, Jason T George, José N. Onuchic, **Xingcheng Lin** and Herbert Levine⋆ "Contact map dependence of a T-cell receptor binding repertoire", *Phys. Rev. E*, 106, 014406 (2022). DOI

25. Shuming Liu†, **Xingcheng Lin**†, Bin Zhang⋆ "Chromatin fiber breaks into clutches under tension and crowding", *Nucleic Acids Res.*, 50, 17, pp 9738-9747, (2022). DOI
This computational study applied coarse-grained and machine-learning models to study the impact of tension and crowding on chromatin organization. Our study shows that the chromatin breaks into

nucleosome clutches under tension, facilitating the formation of a highly stable interdigitated configuration by two chromatin chains. Our study suggests a viable mechanism for the sol-gel transition of chromatin.

24. Shwetha Srinivasan†, Raju Regmi†, **Xingcheng Lin**, Steven D. Quinn, Wei He, Kermit L. Carraway, III, Matthew A. Coleman, Bin Zhang*, Gabriela S. Schlau-Cohen* "Ligand-induced transmembrane conformational coupling in monomeric EGFR", *Nat. Commun.*, 13:3709, (2022). DOI
This work studies a ligand-binding induced conformational change of monomeric EGFRs and reveals the molecular mechanism underlying the EGFR signaling cascade across a cellular membrane.

23. **Xingcheng Lin**†, Yifeng Qi†, Andrew Latham, Bin Zhang* "Multiscale Modeling of Genome Organization with Maximum Entropy Optimization", *J. Chem. Phys.* 155, 010901, (2021). DOI
Featured as Cover Article.
In this comprehensive review, we describe the details of maximum entropy optimization algorithm and its applications in creating new computational models to study genome organization.

22. **Xingcheng Lin**, Rachel Leicher, Shixin Liu, Bin Zhang* "Cooperative DNA Looping by PRC2 Complexes via Allosteric Communication", *Nucleic Acids Res.*, 49, 11, pp 6238-6248, (2021). DOI
This computational study combines homology modeling, all-atom simulation, and coarse-grained simulation to model multiple oligomeric structures of Polycomb Repressive Complex 2 (PRC2). The study discovers that multiple PRC2 complexes cooperatively loop DNA into a hairpin structure, compacting chromatin via an allosteric communication mechanism. Importantly, our study predicts that the exposure of the C2 domain of PRC2 serves as an additional DNA binding motif, which is blocked when PRC2 is associated with the AEBP2 subunit. This prediction is further supported by single-molecule experiments. Our work establishes the molecular basis of PRC2 function, which can be used to guide future therapeutic applications.

21. Xinqiang Ding†, **Xingcheng Lin**†, Bin Zhang* "Stability and Folding Pathways of Tetra-nucleosome from Six-dimensional Free Energy Surface", *Nat. Commun.*, 12:1091, (2021). DOI
In this paper, we used enhanced sampling and deep learning techniques to quantitatively characterize the high-dimensional free-energy landscape of a tetranucleosome. We find multiple tetranucleosome conformations that are as stable as the reported crystal structure, offering an explanation for the prevalence of irregular chromatin in *in vivo* experiments

20. **Xingcheng Lin**†, Jason T. George†, Nicholas P. Schafer, Kevin Ng Chau, Cecilia Clementi, José N. Onuchic*, Herbert Levine*, "Rapid Assessment of T-Cell Receptor Specificity of the Immune Repertoire", *Nat. Comput. Sci.*, 1, 362-373, (2021). DOI
This work applied supervised machine learning to optimize a molecular energy model for accurate and rapid prediction of T-cell recognition specificity of antigens at the repertoire level. It also presents direct evidence of highly differentiated recognition of tumor-associated neoantigens compared to self-peptides, providing a quantitative argument for the effectiveness of immunotherapy, which targets point-mutated neoantigens.

19. Antonio B. Oliveira Junior, **Xingcheng Lin**, Prakash Kulkarni, José N. Onuchic, Susmita Roy* and Vitor B P. Leite* "Exploring Energy Landscapes of Intrinsically Disordered Proteins: Insights into Functional Mechanisms" *J. Chem. Theory Comput.*, 17, 5, 3178–3187, (2021). DOI

18. Rachel Leicher, Eva J. Ge†, **Xingcheng Lin**†, Matthew J. Reynolds†, Thomas Walz, Bin Zhang*, Tom W. Muir, Shixin Liu* "Single-molecule and in Silico Dissection of the Interaction between Polycomb Repressive Complex 2 and Chromatin" *Proc. Natl. Acad. Sci. USA*, 117, pp 30465-30475, (2020). DOI
This collaborative single-molecule experiment and computational work shows that PRC2 bridges predominantly non-adjacent nucleosomes for enzymatic activities and broadens our understanding about how PRC2 spreads epigenetic modifications and compact chromatin.

17. Shikai Jin, Mitchell D. Miller, Mingchen Chen, Nicholas P. Schafer, **Xingcheng Lin**, Xun Chen, George N. Phillips Jr, Peter G. Wolynes* "Molecular-replacement Phasing Using Predicted Protein Structures from AWSEM-Suite", *IUCrJ*, 7, 6, pp 1168-1178, (2020). DOI

16. Wen-Hao Guo, Xiaoli Qi, Xin Yu, Yang Liu, Chan-I Chung, Fang Bai, **Xingcheng Lin**, Dong Lu, Lingfei Wang, Jianwei Chen, Lynn Hsiao Su, Krystle J Nomie, Feng Li, Meng C Wang, Xiaokun Shu, José N. Onuchic, Jennifer A. Woyach, Michael L. Wang, Jin Wang* "Enhancing Intracellular Accumulation and Target Engagement of PROTACs with Reversible Covalent Chemistry", *Nat. Commun.*, 11, 4268, (2020). DOI

15. Shikai Jin, Mingchen Chen, Xun Chen, Carlos Bueno, Wei Lu, Nicholas P. Schafer, **Xingcheng Lin**, José N. Onuchic, Peter G. Wolynes* "Protein Structure Prediction in CASP13 Using AWSEM-Suite", *J. Chem. Theory Comput.*, 16, 6, pp 3977-3988, (2020). DOI

14. Mingchen Chen, Xun Chen, Shikai Jin, Wei Lu, **Xingcheng Lin**, Peter G. Wolynes* "Protein Structure Refinement Guided by Atomic Packing Frustration Analysis", *J. Phys. Chem. B*, 124, 48, 10889–10898, (2020). DOI

13. **Xingcheng Lin**, Nicholas P. Schafer, Wei Lu, Shikai Jin, Xun Chen, Mingchen Chen, José N. Onuchic and Peter G. Wolynes*, "Forging Tools for Refining Predicted Protein Structures", *Proc. Natl. Acad. Sci. USA*, 116, pp 9400-9409, (2019). DOI
Featured by Rice University in a Press Release. Re-featured by Phys.org, ScienceDaily, EurekAlert!, Nanowerk, etc.
This work develops a simulation-based method to refine intermediate resolution protein structures. Our comprehensive test of this principal component-guided refinement scheme on targets from a recent CASP competition shows that the method achieves state-of-the-art performance and can refine some targets to within experimental accuracy but use only very modest computational resources.

12. Supriyo Bhattacharya* and **Xingcheng Lin**, "Recent Advances in Computational Protocols Addressing Intrinsically Disordered Proteins", *Biomolecules*, 9, pp 146-167, (2019). DOI

11. **Xingcheng Lin**, Prakash Kulkarni*, Federico Bocci, Mohit K. Jolly, Nicholas P. Schafer, Susmita Roy, Min-Yeh Tsai, Yanan He, Yihong Chen, Krithika Rajagopalan, Steven M. Mooney, Yu Zeng, Keith Weninger, Alex Grishaev, Federico Bocci, José N. Onuchic*, Herbert Levine, Peter G. Wolynes, Ravi Salgia, Govindan Rangarajan, Vladimir Uversky, John Orban* and Mohit Kumar Jolly*, "Structural and Dynamical Order of a Disordered Protein: Molecular Insights into Conformational Switching of PAGE4 at the Systems Level", *Biomolecules*, 9, pp 77-94, (2019). DOI

10. Mingchen Chen†, **Xingcheng Lin**†, Wei Lu†, Nick P. Schafer, José N. Onuchic and Peter G. Wolynes*, "Template-Guided Structure Prediction and Refinement Using Optimized Folding Landscape Force Fields" *J. Chem. Theory Comput.*, 14, 11, pp 6102-6116, (2018). DOI

9. **Xingcheng Lin**, Jeffrey K. Noel, Qinghua Wang, Jianpeng Ma and José N. Onuchic*, "Atomistic Simulations Indicate the Functional Loop-to-coiled-coil Transition in Influenza Hemagglutinin is not Downhill", *Proc. Natl. Acad. Sci. USA*, 115, pp E7905-E7913, (2018). DOI
Featured by Rice University in a Press Release. Re-featured by ScienceDaily, EurekAlert!, Futurity, Primeur Magazine, Bionity, etc.
This work finds the critical B-loop transition of group 2 influenza hemagglutinin is not strongly downhill. A conserved threonine residue pauses the B-loop transition, leading to the formation of an asymmetric kinetic intermediate that can serve as a possible target for therapeutics.

8. **Xingcheng Lin**, Susmita Roy, Mohit K. Jolly, Federico Bocci, Nick P. Schafer, Min-Yeh Tsai, Yihong Chen, Yanan He, Alexander Grishaev, Keith Weninger, John Orban, Prakash Kulkarni, Govindan Rangarajan, Herbert Levine and José N. Onuchic*, "PAGE4 and Conformational Switching: Insights from Molecular Dynamics Simulations and Implications for Prostate Cancer", *J. Mol. Biol.*, 430, pp 2422-2438, (2018). DOI

This work applied a multiscale model and revealed a phosphorylation-induced fly-casting mechanism of Prostate-associated gene 4 (PAGE4), an intrinsically disordered protein causally related to prostate cancer.

7. Xi-Wei Yao, Hengyan Wang, Zeyang Liao, Ming-Cheng Chen, Jian Pan, Jun Li, Kechao Zhang, **Xingcheng Lin**, Zhehui Wang, Zhihuang Luo, Wenqiang Zheng, Jianzhong Li, Meisheng Zhao, Xinhua Peng, and Dieter Suter, "Quantum Image Processing and Its Application to Edge Detection: Theory and Experiment", *Phys. Rev. X*, 7, pp 031041(14) (2017). DOI
6. Mingchen Chen†, **Xingcheng Lin**†, Wei Lu, José N. Onuchic and Peter G. Wolynes⋆, "Protein Folding and Structure Prediction from the Ground Up II: AAWSEM for α/β Proteins", *J. Phys. Chem. B*, 121, pp 3473-3482, (2016). DOI
5. **Xingcheng Lin**†, Jeffrey K. Noel†, Qinghua Wang, Jianpeng Ma and José N. Onuchic⋆, "Lowered pH Leads to Fusion Peptide Release and a Highly-dynamic Intermediate of Influenza hemagglutinin", *J. Phys. Chem. B*, 120, pp 9654-9660, (2016). DOI
   This work used detailed atomistic simulations and systematically investigated the pH trigger of the structural rearrangement of influenza hemagglutinin under a lowered pH environment. The simulation reveals a long-lived asymmetric structural intermediate that suggests a cooperative mechanism for multiple hemagglutinins to induce membrane hemifusion.
4. Mingchen Chen, **Xingcheng Lin**, Weihua Zheng, José N. Onuchic and Peter G. Wolynes⋆, "Protein Folding and Structure Prediction from the Ground Up: The Atomistic Associative Memory, Water Mediated, Structure and Energy Model (AAWSEM)", *J. Phys. Chem. B*, 120, pp 8557-8565, (2016). DOI
3. **Xingcheng Lin**†, Nathan R. Eddy†, Jeffrey K. Noel, Qinghua Wang, Jianpeng Ma and José N. Onuchic⋆, "Order and Disorder Control the Functional Rearrangement of Influenza Hemagglutinin", *Proc. Natl. Acad. Sci. USA*, 111, pp 12049-12054, (2014). DOI
   Featured by Rice University in a Press Release. Re-featured by ScienceDaily, EurekAlert!, etc.
   This work simulated the entire structural transition of influenza hemagglutinin and reveals two functional pathways utilized by hemagglutinin to induce membrane hemifusion for viral entry.
2. Xiwei Yao, Birong Zeng, Qin Liu, Xiaoyang Mu, **Xingcheng Lin**, Chun Yang, Jian Pan and Zhong Chen, "Subspace Quantum Process Tomography via Nuclear Magnetic Resonance", *Acta Physica Sinica*, 59, pp 6837-6841 (2010). DOI
1. Xiwei Yao, Ziwei Chen, Xiaoyang Mu, Jian Pan, Chun Yang, **Xingcheng Lin**, Jianhui Lian and Xinwei Wang, "Measurement Method of Logical Gate in Bulk Spin Quantum Computer", *Journal of Wuhan University of Technology*, 32, pp 142-145 (2010). DOI

Manuscripts Under Review

† shared authorship

⋆ corresponding author

1. Shwetha Srinivasan, **Xingcheng Lin**, Xuyan Chen, Raju Regmi, Wei He, Kermit L. Carraway, III, Matthew A. Coleman, Bin Zhang, Gabriela S. Schlau-Cohen⋆ "Active regulation of the epidermal growth factor receptor by the membrane bilayer", bioRxiv (2025, August 18) DOI
2. Jiajia Guo, Xuyan Chen, Premashis Manna, **Xingcheng Lin**, Madelyn N. Scott, Wei Jia Chen, Mikaila Hoffman, Bin Zhang, Gabriela S. Schlau-Cohen, "Single-molecule acceptor rise time (smART) FRET for nanoscale distance sensitivity". bioRxiv, (2023, March 16) DOI
3. Zahra S Ghoreyshi, Noah Tubo, Luca Zammataro, Xizeng Mao, Ho Ngai, Duncheng Wang, Yibin Chen, Qiuming He, Eduardo Cisneros, Shoudan Liang, Priya J Koppikar, **Xingcheng Lin**⋆, Jeffrey J Molldrem⋆, Jason T George⋆, (2025, May 28). "Biophysical modeling for accurate T cell specificity prediction of viral and tumor antigens". DOI

4. Eduardo Cisneros de la Rosa, Yafan Zhang, **Xingcheng Lin**⋆ "IRIS Integrates Sparse Sequence, Experimental, and AI-Predicted Structures for Protein-RNA Affinity Prediction and Motif Discovery", (2025, September 16) DOI

5. Yafan Zhang, Rina Li, Junhao Zhong, **Xingcheng Lin**⋆ "mIDEA: An Interpretable Structure-Sequence Model for Methylation-Dependent Protein-DNA Binding Sensitivity", (2025, November 16) DOI

6. Thomas Thornton and **Xingcheng Lin**⋆ "Efficient RNA Folding Simulation via a Structure-Based Single-Site-Per-Nucleotide Model", (2025, December 14) DOI

Honors and Awards

- **Invited Platform Co-Chair** Biophysical Society 70th Annual Meeting 2026
- **Amazon Research Awards (ARA)** (Selected recipient - Think Big category; Declined due to institutional policy) 2025
- **MIT Infinite Expansion Award** 2022
- **Invited Platform Co-Chair** Biophysical Society 66th Annual Meeting 2022
- **Biophysical Society Travel Award** 2020
- **Rice Physics Bonner Book Awards** for outstanding graduate students 2012

Teaching Experiences

- **PY208, NC State University** 2023-Present
  PHY 208 Physics for Engineers and Scientists II

Selected Professional Services

- NWO Dutch Research Council mail-in reviewer 2025
- NSF NCEMS mail-in reviewer 2025
- NSF Graduate Research Fellowships Program (GRFP) panel 2025
- Reviewer for the NC State Genetics and Genomics Academy seed grant applications 2024-Present
- Graduate admission and recruiting committees of NC State Physics department 2023-Present
- Biophysical Society Multiscale Genome Organization (MGO) subgroup postdoctoral organizer 2022-2023
- Reviewer for over 20 scientific journals 2019-Present

Invited Presentations

9. "Integrating Sequence and Structure to Enhance Predictive Protein-Nucleic Acid Interactions", ERBL Seminar Series, National Institute of Environmental Health Sciences, September 2025
8. "Fusing structure and sequence to learn physicochemical rules governing protein-nucleic acid interactions", Southeastern Regional Meeting of the American Chemical Society (SERMACS), Atlanta, Georgia, October 2024
7. "Integrating Structure and Dynamics to Enhance Data-Driven Modeling of Molecular Biophysics", Molecular and Structural Biochemistry Symposium, North Carolina State University, April 2024
6. "Genome Organization from the Ground Up – Deciphering Molecular Mechanisms for Chromatin Organization", Wilson College of Textiles, North Carolina State University, February 2024

5. "Genome Organization from the Ground Up – Deciphering Molecular Mechanisms for Chromatin Organization", Biomathematics Seminar Series, North Carolina State University, September 2023
4. "Genome Organization from the Ground Up – Deciphering Molecular Mechanisms for Chromatin Organization", Department of Chemistry, Duke University, September 2023
3. "Genome Organization from the Ground Up – Deciphering Molecular Mechanisms for Chromatin Organization", Physical Chemistry seminar, Boston University, June 2023
2. "Deciphering the Mechanisms of Epigenetic Regulation via a Near-atomistic Resolution Chromatin Model", Biophysical Society Multiscale Genome Organization Webinar, Virtual, April 2022
1. "Near-atomistic Modeling of Chromatin – Leveraging Computational Advances to Uncover Mechanistic Insights", Lennard-Jones Centre, University of Cambridge, February 2022
   Presentation Link

Conference Presentations

19. "Predicting physicochemical interactions of chromatin via explicit ion modeling", BPS Annual Meeting, Philadelphia, PA, February 2024
18. "Near-atomistic Modeling Reconciles Difference between Irregular and Regular Chromatin", BPS Annual Meeting, San Francisco, CA, February 2022
    Co-chair of the platform session
17. "Near-atomistic modeling reconciles difference between irregular and regular chromatin", Gordon Research Conference: Protein Folding Dynamics, Oxnard, CA, January 2022
    Discussion leader of Gordon Research Seminar
16. "Coarse-Grained Modeling of PRC2-Mediated Inter-Nucleosomal Interactions",BPS Annual Meeting, San Diego, CA, February 2020
15. "Atomistic Simulations Indicate the Functional Loop-to-coiled-coil Transition in Influenza Hemagglutinin is not Downhill", Gordon Research Conference: Protein Folding Dynamics, Galveston, TX, January 2018.
14. "High-resolution Prediction and Refinement of Protein Structures", Q-bio Conference, Houston, TX, June 2018
13. "Atomistic Simulations Reveal a Hindered Transition of the B-Loop Domain of Influenza Hemagglutinin",BPS Annual Meeting, San Francisco, CA, February 2018
12. "PAGE4 and Conformational Switch: Simulating an 'Intrinsically' Disordered Protein", International physics of living systems (iPoLS) Annual Meeting, Rice University, Houston, TX, June 2018
11. "Quantify the Energy Landscape of Influenza Hemagglutinin Structural Rearrangement: Symmetry Breaking and B-loop Transition", Sealy Center for Structural Biology and Molecular Biophysics Annual Symposium, Galveston, TX, May 2017
10. "Investigation of the pH Induced Structural Transition of Influenza Hemagglutinin", NSF Committee Review, Center for Theoretical Biological Physics, Rice University, Houston, TX, February 2017
9. "Seeking Out the Functional Mechanism of Influenza Hemagglutinin (HA)", Smalley-Curl Institute Transdisciplinary Symposium, Rice University, Houston, TX, February 2017
   2017 Symposium Winners
8. "Quantify the Energy Landscape of Influenza Hemagglutinin Structural Rearrangement: Symmetry Breaking and B-loop Transition", International physics of living systems (iPoLS) Annual Meeting, Harvard University, Boston, MA, July 2016.
7. "Investigation of pH induced change of influenza hemagglutinin: Fusion peptide release and symmetry-breaking", Sealy Center for Structural Biology and Molecular Biophysics Annual Symposium, Galveston, TX, May 2016.

6. “Exploring the Low pH Induced Switch of Influenza Hemagglutinin”, Gordon Research Conference: Protein Folding Dynamics, Galveston, TX, January 2016.
5. “Investigation of the pH induced conformational rearrangement of influenza hemagglutinin”, BPS Annual Meeting, Los Angeles, CA, February 2016
4. “Exploring the Low pH Induced Switch of Influenza Hemagglutinin in Explicit Solvent Simulation”, Sealy Center for Structural Biology and Molecular Biophysics Annual Symposium, Galveston, TX, May 2015.
3. “Getting Thermodynamics from Conformational Change of Influenza Hemagglutinin”, Sealy Center for Structural Biology and Molecular Biophysics Annual Symposium, Galveston, TX, April 2014.
2. “Multiple Routes for the Conformational Transition of influenza Hemagglutinin”, Gordon Research Conference: Protein Folding Dynamics, Galveston, TX, January 2014.
1. “Order-disorder Transition During the Conformational Change of Influenza Hemagglutinin”, APS March Meeting, Denver, CO, March 2014.

Editorial and Referee Experience

- Nature Communications
- Nucleic Acids Research
- Proceedings of the National Academy of Sciences of the United States of America
- Elife
- PLOS Computational Biology
- Biophysical Journal
- PROTEINS: Structure, Function, and Bioinformatics
- The Journal of Chemical Physics
- JACS Au
- The Journal of Physical Chemistry Letters
- The Journal of Physical Chemistry B
- Journal of Chemical Theory and Computation
- Journal of Chemical Information and Modeling
- Journal of Molecular Biology
- Physical Chemistry Chemical Physics
- Briefings in Bioinformatics
- Frontiers in Molecular Biosciences
- Frontiers in Physics
- Communications Biology
- Chromosoma
- Macromolecular Rapid Communications