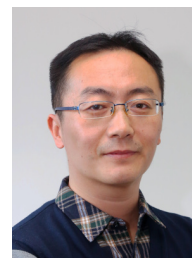


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Post and Contact

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Research Interests

Physics- and AI-based computational biology focusing on membrane proteins, in particular:

- Development of computational methods in biophysics and bioinformatics
- Molecular mechanisms of membrane proteins and peptides
- Prediction and Design of membrane proteins and peptides

Education

- Shandong University, China
 - Sep 2002 – Jun 2007, Condensed Matter Physics, Ph.D.
 - Sep 1998 – Jun 2002, Physics, B.Sc.

Professional Experience

- Peking University, Beijing, China
 - Since Aug 2023, Associate Professor with Tenure
 - Apr 2016 – Jul 2023, Tenure Track Assistant Professor
- University of Oxford (Sansom Group), Oxford, United Kingdom
 - Jan 2014 – Dec 2015, Marie Curie Research Fellow
 - Jan 2013 – Dec 2013, Newton International Postdoc Fellow
- Max Planck Institute for Biophysical Chemistry (de Groot Group), Göttingen, Germany
 - Feb 2012 – Dec 2012, Max-Planck Postdoc Fellow

- Dec 2009 – Jan 2012, Alexander von Humboldt Postdoc Fellow
- University of Western Australia (Corry Group), Perth, Australia
- Jul 2007 – Jul 2009, Postdoc Research Associate

Publications

Peer-reviewed Publications since Joining Peking University

1. Zhu, Z.; **Song, C.*** FoldDoF: Utilizing the Primary Degrees of Freedom of Protein Backbone for Geometric Modeling and Generation. *J. Chem. Inf. Model.* 2026, <https://doi.org/10.1021/acs.jcim.6c00617>.
2. Dong, R.; Awang, T.; Cao, Q.; Kang, K.; Wang, L.; Zhu, Z.; **Song, C.*** PepMCP: A Graph-Based Membrane Contact Probability Predictor for Membrane-Lytic Antimicrobial Peptides. *Bioinformatics* 2026, btag453.
3. Song, C.[†]; Ma, L.[†]; Xue, L.; Xu, Y.; Zhang, Q.; Liu, Y.; **Song, C.**; Lin, Y.* Navigating High-Order Protein Fitness Landscapes via Deep Learning on Directed Evolution Trajectories. *Proc. Natl. Acad. Sci. U.S.A.* 2026, 123, e2520561123.
4. Yan, L.[†]; Xu, Z.[†]; Yao, Y.[†]; Awang, T.[†]; Wang, X.; Wang, Y.; Ma, C.; Li, N.; **Song, C.***; Chen, X.*; Gao, N.* The Erlin1/2 Complex Is A Dynamic Scaffold for Membrane Microdomain Assembly on the Endoplasmic Reticulum. *Mol. Cell* 2026, 86, 1362-1376.
5. Han, Z.; Wang, L.; **Song, C.*** Improved Anisotropic Network Models for Membrane Protein Dynamics and Mechanosensitive Ion Channels. *PRX Life* 2026, 4, 013025.
6. Wang, L.[†]; Kang, K.[†]; **Song, C.*** ProtRAP-LM: Efficient Protein Relative Accessibility Prediction and Proteome-Wide Membrane Protein Screening. *Genom. Proteom. Bioinform.* 2026, qzag013.
7. Li, J.; Guo, H.; **Song, C.*** MemConverter: An Iterative Pipeline for Reprogramming Protein Localization in Membrane or Aqueous Solution. *J. Chem. Theory Comput.* 2026, 22, 2028–2042.
8. Fan, X.[†]; Chen, J.[†]; Xue, L.[†]; Wang, H.; Wu, T.; Huang, X.; Lu, F.; Jin, X.*; **Song, C.***; Huang, J.*; Yan, N.* Open-State Structure of Veratridine-Activated Human Nav1.7 Reveals the Molecular Choreography of Fast Inactivation. *Vita* 2026, <https://doi.org/10.15302/vita.2026.01.0003>.
9. Liu, C.; Han, Z.; Ma, R.*; **Song, C.*** Lipid Bilayer Membranes with Asymmetrically Distributed LPC and DAG. *Phys. Chem. Chem. Phys.* 2026, 28, 3550-3561.
10. Zhou, D.[†]; Zhang, Y.[†]; Chen, N.[†]; Huang, S.; **Song, C.***; Zhang, Z.* Structural Basis of G6P/Pi Transport and Inhibition in SLC37A4. *Nat. Struct. Mol. Biol.* 2026, 33, 123-133.
11. Li, J.[†]; Yang, C.[†]; Dong, R.; Juarez, J.; Wang, L.; Wettstein, M.; Wang, D.; Cao, C.; Lu, Y.*; **Song, C.*** Mechanism-Driven Screening of Membrane-Targeting and Pore-Forming Antimicrobial Peptides. *Adv. Sci.* 2026, 13, e16470.
12. Dong, R.; Cao, Q.; **Song, C.*** Painting Peptides With Antimicrobial Potency Through Deep Reinforcement Learning. *Adv. Sci.* 2025, e06332.

[†]: co-first authorship; *: (co-)corresponding authorship.

13. Yang, Y.[†]; Wang, S.[†]; Wang, G.[†]; Lian, Y.[†]; Xue, L.; Jiang, W.; Guo, Q.; **Song, C.***; Li, L.* Dynamic TOM–TIM23 Supercomplex Directs Mitochondrial Protein Translocation and Sorting. *Nat. Struct. Mol. Biol.* 2025, 32 (11), 2231–2241.
14. Duan, J.; **Song, C.*** Twist Is the Key to the Gating of Mechanosensitive Ion Channel NOMPC. *eLife* 2025, 13, RP102941.
15. Xue, L.; Yan, N.; **Song, C.*** Deciphering Ca²⁺ Permeation and Valence Selectivity in Cav1: Molecular Dynamics Simulations Reveal the Three-Ion Knock-On Mechanism. *Proc. Natl. Acad. Sci. U.S.A.* 2025, 122, e2424694122.
16. Yang, S.; **Song, C.*** Multiple-Basin Gō–Martini for Investigating Conformational Transitions and Environmental Interactions of Proteins. *J. Chem. Theory Comput.* 2025, 21, 5304–5321.
17. Hu, Q.[†]; You, H.[†]; Li, K.; Lai, L.*; **Song, C.*** GPx4 is Bound to Peroxidized Membranes by a Hydrophobic Anchor. *J. Mol. Biol.* 2025, 437, 169122.
18. Zhou, D.; Chen, N.; Huang, S.; **Song, C.**; Zhang, Z.* Mechanistic Insights into the Acetyl-CoA Recognition by SLC33A1. *Cell Discov.* 2025, 11, 36.
19. Song, Z.; Xue, L.; Ouyang, Q.; **Song, C.*** Impact of a Terahertz Electromagnetic Field on the Ion Permeation of Potassium and Sodium Channels. *Commun. Chem.* 2025, 8, 101.
20. Xue, L.; Song, Z.; Ouyang, Q.; **Song, C.*** Protocol for Simulating the Effect of THz Electromagnetic Field on Ion Channels. *Quant. Biol.* 2025, 13, e94.
21. Xu, H.[†]; Zhou, S.[†]; Zhu, Z.; Vitelli, V.*; Chen, L.*; Dai, Z.*; Yang, N.*; Lai, L.*; Yang, S.*; Ovchinnikov, S.*; Qiao, Z.*; Liu, S.*; **Song, C.***; Pei, J.*; Wen, H.*; Feng, J.*; Zhang, Y.*; Xie, Z.*; Liu, Y.*; Li, Z.*; Jin, F.*; Li, H.*; Lotfollahi, M.*; Zhang, X.*; Yang, G.*; Zhang, S.*; Gao, G.*; Li, P.*; Liu, Q.*; Han, J.* Biomedical data and AI. *Sci. China Life Sci.* 2025.
22. Ou, X.[†]; Ma, C.[†]; Sun, D.[†]; Xu, J.[†]; Wang, Y.[†]; Wu, X.; Wang, D.; Yang, S.; Gao, N.*; **Song, C.***; Li, L.* SecY Translocon Chaperones Protein Folding During Membrane Protein Insertion. *Cell* 2025, 188, 1912–1924.
23. Liu, C.; Zhong, Q.; Kang, K.; Ma, R.*; **Song, C.*** Asymmetrical Calcium Ions Induced Stress and Remodeling in Lipid Bilayer Membranes. *Phys. Chem. Chem. Phys.* 2025, 27, 740–753.
24. Zhang, K.[†]; Duan, J.[†]; Li, C.*; **Song, C.**; Chen, Z.* How Do DNA Molecular Springs Modulate Protein–Protein Interactions: Experimental and Theoretical Results. *Biochemistry* 2024, 63, 3369–3380.
25. Zhang, Y.[†]; Dai, F.[†]; Chen, N.[†]; Zhou, D.; Lee, C.-H.*; **Song, C.***; Zhang, Y.*; Zhang, Z.* Structural Insights into VACHT Neurotransmitter Recognition and Inhibition. *Cell Res* 2024, 34, 665–668.
26. Yue, W.[†]; Li, X.[†]; Zhan, X.[†]; Wang, L.; Ma, J.; Bi, M.; Wang, Q.; Gu, X.; Xie, B.; Liu, T.; Guo, H.; Zhu, X.; **Song, C.**; Qiao, J.; Li, M.* PARP inhibitors suppress tumours via centrosome error-induced senescence independent of DNA damage response. *EBioMedicine* 2024, 103, 105129.
27. Dang, Y.[†]; Zhang, T.[†]; Pidathala, S.[†]; Wang, G.[†]; Wang, Y.[†]; Chen, N.[†]; **Song, C.**; Lee, C.-H.*; Zhang, Z.* Substrate and Drug Recognition Mechanisms of SLC19A3. *Cell Res.* 2024, 34, 458–461.

28. Yang, S.; **Song, C.*** Switching Gō-Martini for Investigating Protein Conformational Transitions and Associated Protein–Lipid Interactions. *J. Chem. Theory Comput.* 2024, 20, 2618–2629.
29. Li, J.; Wang, L.; Zhu, Z.; **Song, C.*** Exploring the Alternative Conformation of a Known Protein Structure Based on Contact Map Prediction. *J. Chem. Inf. Model.* 2024, 64, 301–315.
30. Tian, Y.[†]; Song, Y.[†]; Xia, Y.[†]; Hong, J.[†]; Huang, Y.; Ma, R.; You, S.; Guan, D.; Cao, D.; Zhao, M.; Chen, J.; **Song, C.**; Liu, K.; Xu, L.-M.*; Gao, Y. Q.*; Wang, E.-G.*; Jiang, Y.* Nanoscale One-Dimensional Close Packing of Interfacial Alkali Ions Driven by Water-Mediated Attraction. *Nat. Nanotechnol.* 2024, 19, 479–484.
31. Wang, D.[†]; Li, J.[†]; Wang, L.; Cao, Y.; Kang, B.; Meng, X.; Li, S.*; **Song, C.*** Toward Atomistic Models of Intact Severe Acute Respiratory Syndrome Coronavirus 2 via Martini Coarse-Grained Molecular Dynamics Simulations. *Quant. Biol.* 2023, 11 (4), 421–433.
32. Gao, S.[†]*; Yao, X.[†]; Chen, J.[†]; Huang, G.; Fan, X.; Xue, L.; Li, Z.; Wu, T.; Zheng, Y.; Huang, J.; Jin, X.; Wang, Y.; Wang, Z.; Yu, Y.; Liu, L.; Pan, X.; **Song, C.***; Yan, N.* Structural Basis for Human Cav1.2 Inhibition by Multiple Drugs and the Neurotoxin Calciseptine. *Cell* 2023, 186 (24), 5363–5374.
33. Liu, C.; Xue, L.; **Song, C.*** Calcium Binding and Permeation in TRPV Channels: Insights from Molecular Dynamics Simulations. *J. Gen. Physiol.* 2023, 155 (12), e202213261.
34. He, R.; Zhang, J.; Shao, Y.; Gu, S.; **Song, C.**; Qian, L.; Yin, W.-B.*; Li, Z.* Knowledge-Guided Data Mining on the Standardized Architecture of NRPS: Subtypes, Novel Motifs, and Sequence Entanglements. *PLoS Comput. Biol.* 2023, 19, e1011100.
35. Schackert, F. K.[†]; Biedermann, J.[†]; Abdolvand, S.; Minniberger, S.; **Song, C.**; Plested, A. J. R.; Carloni, P.*; Sun, H.* Mechanism of Calcium Permeation in a Glutamate Receptor Ion Channel. *J. Chem. Inf. Model.* 2023, 63, 1293–1300.
36. Kang, K.[†]; Wang, L.[†]; **Song, C.*** ProtRAP: Predicting Lipid Accessibility Together with Solvent Accessibility of Proteins in One Run. *J. Chem. Inf. Model.* 2023, 63, 1058–1065.
37. Dong, L.; Yang, S.; Chen, J.; Wu, X.; Sun, D.; **Song, C.***; Li, L.* Structural Basis of SecA-Mediated Protein Translocation. *Proc. Natl. Acad. Sci. U.S.A.* 2023, 120, e2208070120.
38. Wang, L.; Zhang, J.; Wang, D.; **Song, C.*** Membrane Contact Probability: An Essential and Predictive Character for the Structural and Functional Studies of Membrane Proteins. *PLoS Comput. Biol.* 2022, 18, e1009972.
39. Wang, Y.[†]; Guo, Y.[†]; Li, G.; Liu, C.; Wang, L.; Zhang, A.; Yan, Z.*; **Song, C.*** The Push-to-Open Mechanism of the Tethered Mechanosensitive Ion Channel NOMPC. *eLife* 2021, 10, e58388.
40. Liu, C.; Zhang, A.; Yan, N.; **Song, C.*** Atomistic Details of Charge/Space Competition in the Ca²⁺ Selectivity of Ryanodine Receptors. *J. Phys. Chem. Lett.* 2021, 12, 4286.
41. Liu, Y.; Ke, P.; Kuo, Y.-C.; Wang, Y.; Zhang, X.*; **Song, C.***; Shan, Y.* A Putative Structural Mechanism Underlying the Antithetic Effect of Homologous RND1 and RhoD GTPases in Mammalian Plexin Regulation. *eLife* 2021, 10, e64304.
42. Li, W.[†]; Gu, X.[†]; Liu, C.; Shi, Y.; Wang, P.; Zhang, N.; Wu, R.; Leng, L.; Xie, B.; **Song, C.**; Li, M.* A Synergetic Effect of BARD1 Mutations on Tumorigenesis. *Nat. Commun.* 2021, 12, 1243.

43. Zhang, X.[†]; Yu, H.^{†*}; Liu, X.; **Song, C.*** The Impact of Mutation L138F/L210F on the Orai Channel: A Molecular Dynamics Simulation Study. *Front. Mol. Biosci.* 2021, 8, 755247.
44. Zhang, A.; Yu, H.; Liu, C.; **Song, C.*** The Ca²⁺ Permeation Mechanism of the Ryanodine Receptor Revealed by a Multi-Site Ion Model. *Nat. Commun.* 2020, 11, 922.
45. Zhao, X.[†]; Tian, J.[†]; Yu, H.[†]; Bryksa, B. C.; Dupuis, J. H.; Ou, X.; Qian, Z.; **Song, C.***; Wang, S.*; Yada, R. Y.* Insights into the Mechanism of Membrane Fusion Induced by the Plant Defense Element, Plant-Specific Insert. *J. Biol. Chem.* 2020, 295, 14548. (Editor's Picks & Cover Story)
46. Wang, D.; Liu, X.; Liu, J.; **Song, C.*** Phosphorylation-Dependent Conformational Changes of Arrestin in the Rhodopsin-Arrestin Complex. *Phys. Chem. Chem. Phys.* 2020, 22, 9330.
47. Dupuis, J. H.; Wang, S.; **Song, C.**; Yada, R. Y.* The Role of Disulfide Bonds in a Solanum Tuberosum Saposin-like Protein Investigated Using Molecular Dynamics. *PLoS One* 2020, 15, e0237884.
48. **Song, C.***; de Groot, B. L.; Sansom, M. S. P. Lipid Bilayer Composition Influences the Activity of the Antimicrobial Peptide Dermcidin Channel. *Biophys. J.* 2019, 116, 1658.
49. Xu, Y.; Lin, K.; Wang, S.; Wang, L.; Cai, C.; **Song, C.**; Lai, L.; Pei, J.* Deep Learning for Molecular Generation. *Future Med. Chem.* 2019, 11, 567–597.
50. Vestergaard, M.; Berglund, N. A.; Hsu, P.-C.; **Song, C.**; Koldsø, H.; Schiøtt, B.*; Sansom, M. S. P.* Structure and Dynamics of Cinnamycin–Lipid Complexes: Mechanisms of Selectivity for Phosphatidylethanolamine Lipids. *ACS Omega*, 2019, 4, 18889–18899.
51. Zhang, M.; Wang, D.; Kang, Y.; Wu, J.-X.; Yao, F.; Pan, C.; Yan, Z.*; **Song, C.***; Chen, L.* Structure of the Mechanosensitive OSCA Channels. *Nat. Struct. Mol. Biol.* 2018, 25, 850.
52. Dupuis, J. H.; Yu, H.; Habibi, M.; Peng, X.; Plotkin, S. S.; Wang, S.; **Song, C.**; Yada, R. Y.* pH Dependent Membrane Binding of the Solanum Tuberosum Plant Specific Insert: An in Silico Study. *Biochim. Biophys. Acta - Biomembr.* 2018, 1860, 2608–2618.
53. Wang, D.; Yu, H.; Liu, X.; Liu, J.; **Song, C.*** The Orientation and Stability of the GPCR-Arrestin Complex in a Lipid Bilayer. *Sci. Rep.* 2017, 7, 16985.
54. Trick, J. L.; **Song, C.**; Wallace, E. J.; Sansom, M. S. P.* Voltage Gating of a Biomimetic Nanopore: Electrowetting of a Hydrophobic Barrier. *ACS Nano* 2017, 11 (2), 1840–1847.
55. Kutzner, C.; Köpfer, D. A.; Machtens, J.-P.; de Groot, B. L.; **Song, C.**; Zachariae, U.* Insights into the Function of Ion Channels by Computational Electrophysiology Simulations. *Biochim. Biophys. Acta BBA – Biomembr.* 2016, 1858 (7, Part B), 1741–1752.

Selected Publications prior to Joining Peking University

1. Köpfer, D. A.[†]; **Song, C.^{†*}**; Gruene, T.; Sheldrick, G. M.; Zachariae, U.*; de Groot, B. L.* Ion Permeation in K⁺ Channels Occurs by Direct Coulomb Knock-On. *Science* 2014, 346, 352–355.
2. **Song, C.**; Weichbrodt, C.; Salnikov, E. S.; Dynowski, M.; Forsberg, B. O.; Bechinger, B.; Steinem, C.; de Groot, B. L.; Zachariae, U.*; Zeth, K.* Crystal Structure and Functional Mechanism of a Human Antimicrobial Membrane Channel. *Proc. Natl. Acad. Sci. U. S. A.* 2013, 110, 4586.

3. **Song, C.**; Corry, B.* Testing the Applicability of Nernst-Planck Theory in Ion Channels: Comparisons with Brownian Dynamics Simulations. *PLoS One* 2011, 6, e21204.
4. **Song, C.**; Corry, B.* Ion Conduction in Ligand-Gated Ion Channels: Brownian Dynamics Studies of Four Recent Crystal Structures. *Biophys. J.* 2010, 98, 404–411.
5. **Song, C.**; Corry, B.* Intrinsic Ion Selectivity of Narrow Hydrophobic Pores. *J. Phys. Chem. B* 2009, 113, 7642–7649.
6. **Song, C.***; Xia, Y.; Zhao, M.; Liu, X.; Li, F.; Ji, Y.; Huang, B.; Yin, Y. The Effect of Salt Concentration on DNA Conformation Transition: A Molecular Dynamics Study. *J. Mol. Model.* 2006, 12, 249–254.

For a complete publication list including preprints, please visit [my google scholar](#).

Oral Presentations

International Talks

1. Oral Presentation: Membrane Contact Probability Prediction and Proteome-Wide Membrane Protein Screening, BPS2026 Annual Meeting, San Francisco, USA, Feb 22, 2026.
2. Invited Talk: Ca^{2+} permeation and selectivity of ryanodine receptors and voltage-gated calcium channels, Pacificchem 2025, Hawaii, USA, Dec 19, 2025.
3. Invited Talk: Multiscale simulations of the binding of GPx4 to membranes, SMART Symposium: 2025 Frontier in Computational Chemistry, Biophysics, and Biological Sciences, Shenzhen, China, Oct 26, 2025.
4. Invited Talk: Molecular Mechanisms of Valence Selectivity in Ca^{2+} Channels: A Computational Study, The 10th iHuman Forum, Shanghai, China, Nov 1, 2025.
5. Invited Talk: Improved Anisotropic Network Models for Membrane Protein Dynamics and Mechanosensitive Ion Channels, 2025 Hong Kong Symposium on Molecular Modeling and Simulation, Hong Kong, China, May 24, 2025.
6. Invited Presentation: Showcase of AI-assisted class in computational biology, Global MOOC and Online Education Conference 2024, London, UK, Dec 12, 2024.
7. Invited Talk: CTGoMartini: Simulating Protein Conformational Transitions with $\text{G}\bar{\text{O}}$ -Martini Models, 2024 Frontier Symposium in Computational Chemistry, Biophysics, and Biological Sciences, Seoul, Korea, Nov 8, 2024.
8. Invited Talk: Gating mechanism of the mechanosensitive ion channel NOMPC: new insights from molecular dynamics simulations. The CHARMM-GUI/GENESIS MD Workshop, Kobe, Japan, Jul 1, 2024.
9. Invited Talk: Modeling multi-state structures of proteins and simulating their conformational transitions. The 21st International Union for Pure and Applied Biophysics Congress, Kyoto, Japan, Jun 28, 2024.
10. Invited Talk: Molecular dynamics simulations of Ca^{2+} ion channels. The Molecular Modelling Conference 2023, Wollongong, Australia, Dec 8, 2023.

11. Invited Talk: Molecular dynamics simulations of Ca^{2+} ion channels with a multisite Ca^{2+} model. The 10th Federation of the Asian and Oceanian Physiological Societies Congress, Daegu, Korea, Nov 1, 2023.
12. Invited Talk: From K^+ to Ca^{2+} : Continuing computational studies of ion channels. The 20th Anniversary Symposium at the Department of Theoretical and Computational Biophysics, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany, Oct 13, 2023.
13. Invited Talk: Prediction and simulation of protein conformation transitions. RIKEN Seminar, Wakō, Japan, Sep 15, 2023.
14. Invited Talk: Exploring the alternative conformation of a known protein structure based on deep learning predictions. Frontier of Dynamic Structural Biology, Japan (virtual), Oct 18, 2022.
15. Invited Talk: Push to open: the gating mechanism of the mechanosensitive ion channel NOMPC. The 15th World Congress on Computational Mechanics, Japan (virtual), Aug 2, 2022.
16. Invited Talk: Prediction of lipid contacting residues based on the simulation data of membrane proteins, The HECBioSim Seminar, UK (virtual), April 26, 2021.
17. Oral Presentation: Molecular Dynamics Simulations on the Mechanosensitive Ion Channel NOMPC, The 20th Hünfeld Workshop of Computer Simulation and Theory of Macromolecules, Germany (virtual), April 24, 2021.
18. Invited Talk: Combining Physics-based and Knowledge-based Computational Methods for the Study of Membrane Proteins, The 65th Annual Meeting of the Biophysical Society, *The Future of Biophysics Symposium*, USA (virtual), Feb 24, 2021.
19. Invited Talk: Multiscale molecular dynamics simulations for antimicrobial peptides study, Multiscale Modeling for Biotherapeutics Symposium (virtual), Schrödinger, Inc., Nov 19, 2020.
20. Invited Talk: The Ca^{2+} permeation mechanism of the open-state ryanodine receptor 1, University of California, Irvine, Feb 5, 2020.
21. Invited Talk: Computational Studies of Ca^{2+} -permeable channels, Riken, Japan, Aug 27, 2019.
22. Invited Talk: How Do Calcium Ions Permeate through the Ryanodine Receptor 1, The 1st KIAS-Beijing Workshop on Biological Sciences, Seoul, Korea, July 3-5, 2019.
23. Invited Talk: Activation of the mechanosensitive ion channel OSCA. Victor Chang Cardiac Research Institute, Sydney, Australia, Feb 15, 2019.
24. Invited Talk: To understand, predict and design membrane proteins. Australian National University, Canberra, Australia, Feb 6, 2019.
25. Invited Talk: Ion permeation and gating mechanism of the mechanosensitive ion channel OSCA revealed by molecular dynamics simulations. The 18th KIAS Conference on Protein Structure and Function, Seoul, Korea, November 15-17, 2018.
26. Invited Talk: "Multiscale MD simulations on PSI and ion channel X", The 101st Canadian Chemistry Conference and Exhibition, Edmonton, Canada, May 27-31, 2018.

27. Invited Talk: "Exploring permeation pathways of ion channels by multi-scale molecular dynamics simulations", The CECAM Workshop: Multiscale modelling in electrophysiology: from atoms to organs, Lugano, Switzerland, Mar 26-28, 2018.
28. Invited Talk: "Is Plant-specific insert a membrane fusion protein?", The CECAM Workshop: Frontiers in Computational Biophysics: understanding conformational dynamics of complex lipid mixtures relevant to biology, Lugano, Switzerland, Jan 10, 2018.
29. Oral Presentation: Dermcidin oligomer in action, presented at the Workshop on Computer Simulation and Theory of Macromolecules, Hünfeld, Germany, Apr 21, 2012.

Domestic Talks

1. Invited Talk: Computational Design of Membrane Peptides and Proteins, The 4th Conference on Protein Design, Applications, and Interdisciplinary Life Sciences, Tianjin, June 13, 2026.
2. Invited Talk: CTGoMartini: Development and Implementation of G $\bar{o}$ -Martini Models, The 35th Chinese Chemical Society (CCS) Congress, Chongqing, April 14, 2026.
3. Invited Talk: Membrane contact probability and its applications in computational biology, 2026 Frontier Symposium on Structure Prediction and Simulation of Biomolecules, Nanjing University, March 29, 2026.
4. Invited Talk: Ca²⁺ permeation and selectivity mechanisms of voltage-gated ion channel Ca_v, The 8th National Conference on Statistical Physics and Complex Systems, Ningbo, Jul 30, 2025.
5. Invited Talk: Multiscale Simulations of Membrane Proteins, The 3rd National Conference on Biomolecular Structure Prediction and Simulation, Changchun, Jun 15, 2025.
6. Invited Talk: Virtual Directed Evolution of Antimicrobial Peptides through Deep Reinforcement Learning, The 18th Chinese Chemical Society National Conference on Computer Chemistry of China, Xi'an, Apr 27, 2025.
7. Invited Talk: Mechanism-driven screening of antimicrobial peptides, The 7th National Conference of Protein & Peptide Chemical Biology, Qingdao, Apr 19, 2025.
8. Invited Talk: Biophysical chemistry on membrane proteins – collaborations between dry and wet experiments, 2024 Annual Meeting of Innovative Research Groups of NSFC, Chengdu, Dec 29, 2024.
9. Invited Talk: Multiple gating mechanisms of mechanosensitive ion channel NOMPC, Symposium of Quantitative Biology and Complex Systems, Hangzhou, Nov 17, 2024.
10. Invited Talk: ProtRAP-LM: Fast and accurate protein relative accessibility prediction and membrane protein screening through protein language model embeddings, The 13th National Conference on Bioinformatics and Systems Biology, Haikou, Oct 10, 2024.
11. Invited Talk: Computer simulation of ion permeation through ion channels: the effect of THz electromagnetic stimuli, The 2024 Chinese Biophysics Congress, Lanzhou, Jul 26, 2024.
12. Invited Talk: Computational Microscope in the Study of Integrative and Quantitative Biology, NSFC ShuangQing Forum, Beijing, Apr 2, 2024.

13. Invited Talk: Prediction and Simulation of Protein Dynamics and Function, Microsoft Research Asia, Beijing, Dec 1, 2023.
14. Invited Talk: Prediction and simulation of protein conformation transitions, Shandong University, Qingdao, Oct 31, 2023.
15. Invited Talk: Multiscale computer simulation on Ca^{2+} -membrane interactions, The 17th National Conference on Computer Chemistry of China, Xining, July 22, 2023.
16. Invited Talk: Prediction of the alternative conformation of proteins based on deep learning, The 33rd Chinese Chemical Society Congress, Qingdao, June 19, 2023.
17. Invited Talk: Membrane Contact Probability and Lipid Accessibility Prediction, The 12th Chinese National Conference on Chemical Biology, Dalian, Apr 17, 2023.
18. Invited Talk: Molecular Dynamics Simulations of Calcium Ion Channels, Forum on Biomolecular Simulations, virtual, Mar 10, 2023.
19. Invited Talk: Computational Biophysics and Chemistry on Membrane Proteins, Forum on Chemical Biology, virtual, Mar 4, 2023.
20. Oral Presentation: Quantitative Computation of Ca^{2+} in Biophysics, Quantitative Biology Symposium 2022, Beijing, Dec 4, 2022.
21. Invited Talk: Combination of AI with molecular dynamics simulations for the study of biomolecules, World AI Conference 2022, Shanghai (virtual), China, Sep 2, 2022.
22. Invited Talk: On the gating mechanisms of mechanosensitive ion channels, Xiamen Soft Matter Forum & ICAM-China Autumn Workshop, Xiamen (virtual), China, Dec 10, 2021.
23. Invited Talk: On the Valence Selectivity of Ryanodine Receptors, The First Greater Bay Area Biophysics and New Drug Discovery Forum, Zhuhai, China, April 10, 2021.
24. Invited Talk: The Gating Mechanisms of Two Mechanosensitive Ion Channels, International Symposium of Biophysics and Soft Matter Frontiers, Jinan, China, Dec 19, 2020.
25. Invited Talk: The Gating Mechanism of the Tethered Mechanosensitive Ion Channel NOMPC, The Ninth National Conference on Bioinformatics and Systems Biology, Shanghai, Sep 28, 2020.
26. Invited Talk: Lipid contact probability: an essential property of (membrane) proteins, Tsinghua Sanya International Mathematics Forum: Computational and Mathematical Bioinformatics and Biophysics, Sanya, China. Dec 9-13, 2019.
27. Invited Talk: Visualizing Ca^{2+} Permeation through the Ryanodine Receptor by Molecular Dynamics Simulations, International Workshop on Multiscale Biological Imaging, Shanghai, China. Nov 9-10, 2019.
28. Invited Talk: Computational studies of mechanosensitive ion channels, The 6th Structural Biology Conference of China, Jixi, Anhui, China. Oct 11-14, 2019.
29. Invited Talk: Simulating the gating mechanism of the mechanosensitive ion channels in biological systems, Nationwide Mechanics Forum for PhD Students, Beijing, China. Sep 22, 2019.
30. Invited Talk: How Do Calcium Ions Permeate through the Ryanodine Receptor 1, Songshan Lake Workshop and Summer School, Dongguan, Guangdong, China. Aug 1, 2019.

31. Invited Talk: Molecular details of gating in mechanosensitive ion channels, NYU Shanghai, China, May 31, 2019.
32. Invited Talk: Understanding dimerization of kinases with computer simulations. Workshop on the Methods of Protein Structure and Dynamics, CSRC, Beijing, China, December 12-13, 2018.
33. Invited Talk: "Studying Ion Channel Permeation with Molecular Dynamics Simulations", The 16th Chinese Biophysics Congress, Chengdu, China, Aug 24-27, 2018.
34. Invited Talk: Computational Study on the Dimerization of the Fam20 Kinases, The Fifth National Conference on Biological Physical Chemistry, Taiyuan, China, Jul 22-25, 2018.
35. Invited Talk: Development of Ca^{2+} Model for Simulating Biological Systems, The 2nd World-wide Chinese Computational Biology and Molecular Simulation Conference, Guangzhou, China, Jun 10, 2018.
36. Oral Presentation: Computational Studies on the Function Mechanisms of Two Antimicrobial Peptides, Quantitative Biology 2017: Computational and Single-Molecule Biophysics, Beijing, China, Jun 25, 2017.
37. Invited Talk: Computational Electrophysiology in Ion Channel Research, Workshop on Modeling and Analysis in Molecular Biology and Electrophysiology, Suzhou, China, Jun 16, 2016.

Teaching Activities

- *Mechanics* (48 hours/year): an undergraduate course for the Integrated Science Program (ISP) of Yuanpei College (Autumn, 2017-)
- *Molecular Dynamics Simulations of Biosystems and Practicals* (32 hours/year): a graduate course (Spring, 2019-2025)
- *Quantitative Biology Techniques* (6 hours/year): part of a graduate course for the CLS program (Spring, 2023-2025)
- *Discussion on Integrated Sciences* (2 hours/year): part of an undergraduate course (Autumn, 2018-)
- *Selected Lectures for Systems Biology* (2 hours/year): part of a joint graduate and undergraduate course (Spring, 2018-)
- *Advances in Theoretical and Systems Biology* (32 hours/year): a graduate course (Autumn, 2017-2020)
- *Theoretical and Systems Biology* (32 hours/year, Lab Rotations): a graduate course (Autumn, 2017)
- *Introduction to Computational Biology* (4 hours/year): module course for the PTN (Peking University-Tsinghua University-National Institute Biological Sciences) Graduate Program (Autumn, 2019 & 2021)

External Grants and Funding

- Dec 2025 – Nov 2029, Design principles of membrane proteins as functional elements, National Key R&D Program of China, 20M CNY, Lead PI, ongoing.
- Jan 2024 – Dec 2028, Quantitative biology of complex living systems, The Innovative Research Group Project of the National Natural Science Foundation of China, 1.5M CNY, Co-PI, ongoing.
- Nov 2023 – Oct 2026, Regulation and design of biomolecular machinery driven by structural dynamics, National Key R&D Program of China, 1.5M CNY, Co-PI, ongoing.
- Jul 2021 – Jun 2024, Developing new models and methods for computational studies of membrane proteins, International Collaboration Grant, National Key R&D Program of China, 2.64M CNY, Lead PI, completed.
- Jan 2021 – Dec 2024, The gating and permeation mechanism of the mechanosensitive ion channel NOMPC, General Program from National Science Foundation of China, 696k CNY, Sole PI, ongoing.
- Jan 2019 – Dec 2022, Development of new calcium ion models for computational studies of biosystems, General Program from National Science Foundation of China, 780k CNY, Sole PI, completed.
- Jan 2017 – Dec 2019, National Talent Program, 2M CNY, Sole PI, completed.
- Jul 2016 – Jun 2021, Molecular machines for transmembrane signaling and transport, National Key R&D Program of China, 2M CNY, Co-PI, completed.

Professional Service

Editorial Services

- Assistant Editor-in-Chief and Associate Editor, *Quantitative Biology*, since Jan 2024.
- Guest Editor, Proceedings of the National Academy of Sciences of the United States of America.

Academic Events Organized

- SMART Symposium: 2025 Frontier in Computational Chemistry, Biophysics, and Biological Sciences, Shenzhen, China, Oct 24–26, 2025.
- 2025 Hong Kong Symposium on Molecular Modeling and Simulation, Hong Kong, China, May 23–26, 2025.
- 2024 Frontier Symposium in Computational Chemistry, Biophysics, and Biological Sciences, Seoul, Korea, 8–10 Nov 2024.
- Symposium on Computer Simulations and Cryo-ET/EM of Complex Biomolecular Systems, international (virtual), 18–19 Nov 2021.
- The 3rd Worldwide Chinese Computational Biology Conference, international (virtual), 3–6 August 2020.

- International Biophysical Society Networking Meeting: Youth Workshop of Biophysics, Beijing, 7 Dec 2019.
- Songshan Lake Workshop and Summer School: Theoretical and Computational Biology: from Molecules to Systems, Guangdong-Hong Kong-Macao Center for Interdisciplinary Sciences, Guangdong, 1–4 August 2019.
- Annual Meeting of Quantitative Biology: Computational and Single-Molecule Biophysics, Beijing, 23–27 June 2017.

Academic Society Services

- Biophysical Society, Ambassador for China (since 2026).
- Biophysical Society of China, and committee member of the panels on Molecular Biophysics and Calcium Signaling.
- Chinese Society for Bioinformatics, and committee member of the panel on Structure Prediction and Simulation of Biomolecules.

Referee Assistance for Funding Agencies

- National Science Foundation of China.
- Biotechnology and Biological Sciences Research Council, UK
- French National Research Agency, France