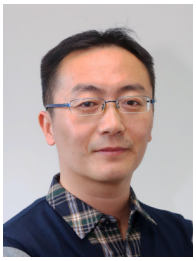
Personal Information



Full Name: SONG, Chen
Gender: Male
Nationality: Chinese

Post and Contact

Associate Professor with Tenure, PI
Center for Quantitative Biology
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Research Interests

Theoretical and computational biophysics on membrane proteins, in particular:

- Development and application of computational methods in biophysics
- Function mechanisms of ion channels
- Antimicrobial peptides and their potential as new antibiotics

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. Xue, L.; Yan, N.; **Song, C.*** Deciphering Ca^{2+} Permeation and Valence Selectivity in Ca_V1: Molecular Dynamics Simulations Reveal the Three-Ion Knock-On Mechanism. *Proc. Natl. Acad. Sci. U.S.A.* 2025, 122, e2424694122.

2. 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.

3. 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.

4. Zhou, D.; Chen, N.; Huang, S.; **Song, C.**; Zhang, Z.* Mechanistic Insights into the Acetyl-CoA Recognition by SLC33A1. *Cell Discov.* 2025, 11, 36.

5. 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.

6. 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.

7. 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.

8. 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.

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

9. 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.

10. Duan, J.; **Song, C.*** Twist Is the Key to the Gating of Mechanosensitive Ion Channel NOMPC. *eLife* 2024, 13, RP102941. https://doi.org/10.7554/eLife.102941.1

11. 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.

12. 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.

13. 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.

14. 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.

15. 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.

16. 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.

17. 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.

18. 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.

19. 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.

20. 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.

21. 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.

22. 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.

23. 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.

24. 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.

25. 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.

26. 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.

27. Liu, C.; Zhang, A.; Yan, N.; **Song, C.*** Atomistic Details of Charge/Space Competition in the Ca^{2+} Selectivity of Ryanodine Receptors. *J. Phys. Chem. Lett.* 2021, 12, 4286.

28. 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.

29. 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.

30. 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.

31. Zhang, A.; Yu, H.; Liu, C.; **Song, C.*** The Ca^{2+} Permeation Mechanism of the Ryanodine Receptor Revealed by a Multi-Site Ion Model. *Nat. Commun.* 2020, 11, 922.

32. 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)

33. 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.

34. 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.

35. **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.

36. 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.

37. 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.

38. 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.

39. 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.

40. 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.

41. 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.

42. 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, please visit my google scholar.

Oral Presentations

International Talks

1. 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.

2. Invited Presentation: Showcase of AI-assisted class in computational biology, Global MOOC and Online Education Conference 2024, London, UK, Dec 12, 2024.

3. Invited Talk: CTGoMartini: Simulating Protein Conformational Transitions with Gō-Martini Models, 2024 Frontier Symposium in Computational Chemistry, Biophysics, and Biological Sciences, Seoul, Korea, Nov 8, 2024.

4. 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.

5. 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.

6. Invited Talk: Molecular dynamics simulations of Ca^{2+} ion channels. The Molecular Modelling Conference 2023, Wollongong, Australia, Dec 8, 2023.

7. Invited Talk: Molecular dynamics simulations of Ca^{2+} ion channels with a multisite Ca^{2+} model. The 10^{th} Federation of the Asian and Oceanian Physiological Societies Congress, Daegu, Korea, Nov 1, 2023.

8. Invited Talk: From K^{+} to Ca^{2+}: Continuing computational studies of ion channels. The 20^{th} Anniversary Symposium at the Department of Theoretical and Computational Biophysics, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany, Oct 13, 2023.

9. Invited Talk: Prediction and simulation of protein conformation transitions. RIKEN Seminar, Wakō, Japan, Sep 15, 2023.

10. 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.

11. Invited Talk: Push to open: the gating mechanism of the mechanosensitive ion channel NOMPC. The 15^{th} World Congress on Computational Mechanics, Japan (virtual), Aug 2, 2022.

12. Invited Talk: Prediction of lipid contacting residues based on the simulation data of membrane proteins, The HECBioSim Seminar, UK (virtual), April 26, 2021.

13. Oral Presentation: Molecular Dynamics Simulations on the Mechanosensitive Ion Channel NOMPC, The 20^{th} Hünfeld Workshop of Computer Simulation and Theory of Macromolecules, Germany (virtual), April 24, 2021.

14. Invited Talk: Combining Physics-based and Knowledge-based Computational Methods for the Study of Membrane Proteins, The 65^{th} Annual Meeting of the Biophysical Society, *The Future of Biophysics Symposium*, USA (virtual), Feb 24, 2021.

15. Invited Talk: Multiscale molecular dynamics simulations for antimicrobial peptides study, Multiscale Modeling for Biotherapeutics Symposium (virtual), Schrödinger, Inc., Nov 19, 2020.

16. Invited Talk: The Ca^{2+} permeation mechanism of the open-state ryanodine receptor 1, University of California, Irvine, Feb 5, 2020.

17. Invited Talk: Computational Studies of Ca^{2+}-permeable channels, Riken, Japan, Aug 27, 2019.

18. Invited Talk: How Do Calcium Ions Permeate through the Ryanodine Receptor 1, The 1^{st} KIAS-Beijing Workshop on Biological Sciences, Seoul, Korea, July 3-5, 2019.

19. Invited Talk: Activation of the mechanosensitive ion channel OSCA. Victor Chang Cardiac Research Institute, Sydney, Australia, Feb 15, 2019.

20. Invited Talk: To understand, predict and design membrane proteins. Australian National University, Canberra, Australia, Feb 6, 2019.

21. Invited Talk: Ion permeation and gating mechanism of the mechanosensitive ion channel OSCA revealed by molecular dynamics simulations. The 18^{th} KIAS Conference on Protein Structure and Function, Seoul, Korea, November 15-17, 2018.

22. Invited Talk: "Multiscale MD simulations on PSI and ion channel X", The 101^{st} Canadian Chemistry Conference and Exhibition, Edmonton, Canada, May 27-31, 2018.

23. 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.

24. 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.

25. 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: Ca^{2+} permeation and selectivity mechanisms of voltage-gated ion channel Ca_V, The 8^{th} National Conference on Statistical Physics and Complex Systems, Ningbo, Jul 30, 2025.

2. Invited Talk: Multiscale Simulations of Membrane Proteins, The 3^{rd} National Conference on Biomolecular Structure Prediction and Simulation, Changchun, Jun 15, 2025.

3. Invited Talk: Virtual Directed Evolution of Antimicrobial Peptides through Deep Reinforcement Learning, The 18^{th} Chinese Chemical Society National Conference on Computer Chemistry of China, Xi'an, Apr 27, 2025.

4. Invited Talk: Mechanism-driven screening of antimicrobial peptides, The 7^{th} National Conference of Protein & Peptide Chemical Biology, Qingdao, Apr 19, 2025.

5. 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.

6. Invited Talk: Multiple gating mechanisms of mechanosensitive ion channel NOMPC, Symposium of Quantitative Biology and Complex Systems, Hangzhou, Nov 17, 2024.

7. Invited Talk: ProtRAP-LM: Fast and accurate protein relative accessibility prediction and membrane protein screening through protein language model embeddings, The 13^{th} National Conference on Bioinformatics and Systems Biology, Haikou, Oct 10, 2024.

8. 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.

9. Invited Talk: Computational Microscope in the Study of Integrative and Quantitative Biology, NSFC ShuangQing Forum, Beijing, Apr 2, 2024.

10. Invited Talk: Prediction and Simulation of Protein Dynamics and Function, Microsoft Research Asia, Beijing, Dec 1, 2023.

11. Invited Talk: Prediction and simulation of protein conformation transitions, Shandong University, Qingdao, Oct 31, 2023.

12. Invited Talk: Multiscale computer simulation on Ca^{2+}-membrane interactions, The 17^{th} National Conference on Computer Chemistry of China, Xining, July 22, 2023.

13. Invited Talk: Prediction of the alternative conformation of proteins based on deep learning, The 33rd Chinese Chemical Society Congress, Qingdao, June 19, 2023.

14. Invited Talk: Membrane Contact Probability and Lipid Accessibility Prediction, The 12th Chinese National Conference on Chemical Biology, Dalian, Apr 17, 2023.

15. Invited Talk: Molecular Dynamics Simulations of Calcium Ion Channels, Forum on Biomolecular Simulations, virtual, Mar 10, 2023.

16. Invited Talk: Computational Biophysics and Chemistry on Membrane Proteins, Forum on Chemical Biology, virtual, Mar 4, 2023.

17. Oral Presentation: Quantitative Computation of Ca^{2+} in Biophysics, Quantitative Biology Symposium 2022, Beijing, Dec 4, 2022.

18. Invited Talk: Combination of AI with molecular dynamics simulations for the study of bio-molecules, World AI Conference 2022, Shanghai (virtual), China, Sep 2, 2022.

19. Invited Talk: On the gating mechanisms of mechanosensitive ion channels, Xiamen Soft Matter Forum & ICAM-China Autumn Workshop, Xiamen (virtual), China, Dec 10, 2021.

20. 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.

21. Invited Talk: The Gating Mechanisms of Two Mechanosensitive Ion Channels, International Symposium of Biophysics and Soft Matter Frontiers, Jinan, China, Dec 19, 2020.

22. 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.

23. 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.

24. 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.

25. Invited Talk: Computational studies of mechanosensitive ion channels, The 6th Structural Biology Conference of China, Jixi, Anhui, China. Oct 11-14, 2019.

26. 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.

27. Invited Talk: How Do Calcium Ions Permeate through the Ryanodine Receptor 1, Songshan Lake Workshop and Summer School, Dongguan, Guangdong, China. Aug 1, 2019.

28. Invited Talk: Molecular details of gating in mechanosensitive ion channels, NYU Shanghai, China, May 31, 2019.
29. 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.
30. Invited Talk: "Studying Ion Channel Permeation with Molecular Dynamics Simulations", The 16th Chinese Biophysics Congress, Chengdu, China, Aug 24-27, 2018.
31. 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.
32. Invited Talk: Development of Ca^{2+} Model for Simulating Biological Systems, The 2nd Worldwide Chinese Computational Biology and Molecular Simulation Conference, Guangzhou, China, Jun 10, 2018.
33. 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.
34. 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–)
- *Quantitative Biology Techniques* (6 hours/year): part of a graduate course for the CLS program (Spring, 2023–)
- *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, 2018–2023)
- *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, Science Fund for Innovative Research Groups from 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

- 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

- Institute for Complex Adaptive Matter (ICAM), and committee member of the ICAM-China Branch
- 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

Referee Assistance for Journals

I have been invited to review papers for many journals, including:

- Nature Communications
- Journal of the American Chemical Society
- Proceedings of the National Academy of Sciences USA
- eLife
- Journal of Chemical Theory and Computation
- Journal of Physical Chemistry Letters
- Journal of General Physiology
- Biophysical Journal