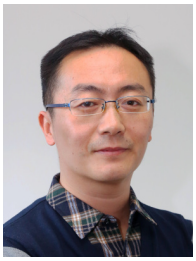
Personal Information



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Post and Contact

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Research Interests

Theoretical and computational biophysics on membrane proteins, in particular:

- Function mechanisms of ion channels
- Development and application of computational methods in biophysics
- 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

- Apr 2016 – Now, Assistant Professor & Principal Investigator

– University of Oxford (Sansom Group), Oxford, United Kingdom

- Jan 2014 – Dec 2015, Marie Curie Research Fellow
- Jan 2013 – Dec 2013, Newton International 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

International Awards and Honors

- Nominated and Selected Speaker at the *Future of Biophysics Symposium*, Biophysical Society, 2021
- The Marie-Curie Fellowship, European Commission, 2014-2015
- The Newton International Fellowship, UK, 2013
- The BPS International Travel Awards, USA, 2012
- The DAAD Travel Grant, Germany, 2012
- The Alexander von Humboldt Fellowship, Germany, 2010-2012

Publications

Preprints and/or Manuscripts under Review

1. Li, J.; Wang, L.; Zhu, Z.; **Song, C.*** Exploring the Alternative Conformation of a Known Protein Structure Based on Contact Map Prediction. *bioRxiv* 2022, https://doi.org/10.1101/2022.06.07.495232.

2. Liu, C.; **Song, C.*** Calcium Binding and Permeation in TRPV Channels: Insights From Molecular Dynamics Simulations. *bioRxiv* 2022, https://doi.org/10.1101/2022.09.07.506889.

3. Kang, K.†; Wang L.†; **Song, C.*** ProtRAP: Predicting Lipid Accessibility Together with Solvent Accessibility of Proteins in One Run. *ChemRxiv* 2022, https://doi.org/10.26434/chemrxiv-2022-3tdq5.

4. Liu, C.; Zhong, Q.; Kang, K.; Ma, R.*; **Song, C.*** Asymmetrical Ca^{2+} Induced Stress and Remodeling in Lipid Bilayer Membranes. *ChemRxiv* 2022, https://doi.org/10.26434/chemrxiv-2022-24qv4.

5. Wang, D.; Li, J.; Wang, L.; Cao, Y.; Li, S.*; **Song, C.*** Toward Atomistic Models of Intact SARS-CoV-2 via Martini Coarse-Grained Molecular Dynamics Simulations. *bioRxiv* 2022, https://doi.org/10.1101/2022.01.31.478415.

†: co-first authorship; *: co-corresponding authorship.

6. Wu, Z.†; Liu, C.†; Yu, H.†; Kang, D.†; Ma, Y.; Li, X.; Zhang, L.; Fan, C.; Li, X.-Z.*; Song, C.*; Yin, C.-C.*; Mao, Y.* Chemistry of Cation Hydration and Conduction in a Skeletal Muscle Ryanodine Receptor. *bioRxiv* 2019 (rewriting), https://doi.org/10.1101/732172.

7. 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. *ChemRxiv* 2022, https://doi.org/10.26434/chemrxiv-2022-x73hl-v2.

Peer-reviewed Publications since Joining Peking University

1. 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.

2. 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.

3. 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.

4. 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.

5. 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.

6. 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.

7. 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.

8. 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)

9. 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.

10. 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.

11. **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.

12. 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.

13. 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.

14. 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.

15. 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.

16. 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.

17. 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.

18. 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: Exploring the alternative conformation of a known protein structure based on deep learning predictions. Frontier of Dynamic Structural Biology, Japan (Virtual), Oct 18, 2022.

2. 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.

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

4. 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.

5. 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.

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

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

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

9. 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.

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

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

12. 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.

13. 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.

14. 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.

15. 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.

Domestic Talks

1. 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.

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

3. 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.

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

5. 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.

6. 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.

7. 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.

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

9. 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.

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

11. Invited Talk: Molecular details of gating in mechanosensitive ion channels, NYU Shanghai, China, May 31, 2019.

12. 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.

13. Invited Talk: "Studying Ion Channel Permeation with Molecular Dynamics Simulations", The 16th Chinese Biophysics Congress, Chengdu, China, Aug 24-27, 2018.

14. 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.

15. 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.

16. 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.

17. 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–)

- Introduction to Computational Biology (8 hours/year): module course for the PTN (Peking University-Tsinghua University-National Institute Biological Sciences) Graduate Program, Autumn, 2018–2021.
- Advances in Theoretical and Systems Biology (32 hours/year): a graduate course (Spring, 2017–2020)
- Theoretical and Systems Biology (32 hours/year, Rotations): a graduate course (Autumn, 2017)

Grants and Funding

- 2022-2026, Peking-Tsinghua Joint Center for Life Sciences, 6M CNY, PI.
- 2021-2024, Developing new models and methods for computational studies of membrane proteins, International Collaboration Grant, National Key Program of MOST, 2.64M CNY, Lead PI.
- 2021-2024, The gating and permeation mechanism of the mechanosensitive ion channel NompC, General Program of NSFC, ~700k CNY, Sole PI.
- 2019-2022, Development of new calcium ion models for computational studies of biosystems, General Program of NSFC, ~800k CNY, Sole PI.
- 2016-2021, Molecular machines for transmembrane signaling and transport, National Key Program of MOST, 2M (out of 34.5M) CNY, Co-PI.
- 2016-2019, The Global Recruitment Program, 2M CNY, Sole PI.
- 2016-2021, Peking-Tsinghua Joint Center for Life Sciences, 6M CNY, PI.

Professional Service

Academic Events Organized

- 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.

Professional Society Affiliations

- Institute for Complex Adaptive Matter (ICAM), and board member of the ICAM-China branch
- Biophysical Society of China, and board member of the molecular biophysics panel
- Biophysical Society
- American Chemical Society
- Chinese Chemical Society

Referee Assistance for Funding Agencies

- National Science Foundation of China. *I served not only as a letter reviewer, but also as a panel referee for multiple disciplines (Chemistry and Biology)*.
- Biotechnology and Biological Sciences Research Council, UK

Referee Assistance for Journals

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