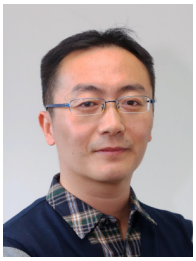

Personal Information

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

Post and Contact

Assistant Professor, PI
Center for Quantitative Biology
& Peking-Tsinghua Center for Life Sciences
Academy for Advanced Interdisciplinary Studies
Peking University
Beijing 100871, China
Tel: +86-10-62759559
Email: c.song@pku.edu.cn
Web: http://cqb.pku.edu.cn/songgroup/

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

- 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

Peer-reviewed Publications since Joining Peking University

1. Wang, D.[†]; Li, J.[†]; Wang, L.; Cao, Y.; Kang, B.; Meng, X.; Li, S.[*]; **Song, C.**[*] Toward Atomistic Models of Intact SARS-CoV-2 via Martini Coarse-Grained Molecular Dynamics Simulations. *Quant. Biol. (in press)*, posted on *bioRxiv*, https://doi.org/10.1101/2022.01.31.478415.

2. 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.

3. 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.

4. 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.

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

5. 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.

6. 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.

7. 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.

8. 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.

9. 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.

10. 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.

11. 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.

12. 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.

13. 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)

14. 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.

15. 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.

16. **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.

17. 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.

18. 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.

19. 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.

20. 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.

21. 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.

22. 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.

23. 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 101st 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: Prediction of the alternative conformation of proteins based on deep learning, The 33rd Chinese Chemical Society Congress, Qingdao, June 19, 2023.

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

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

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

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

6. 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.

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

8. 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.

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

10. 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.

11. 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.

12. 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.

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

14. 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.

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

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

17. 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.

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

19. 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.

20. 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.

21. 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.

22. 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–)
- *Selected Lectures for Systems Biology* (2 hours/year): part of a joint graduate and undergraduate course (Spring, 2018–)
- *Discussion on Integrated Sciences* (2 hours/year): part of an undergraduate course (Autumn, 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)

Grants and Funding

- Jul 2021 – Jun 2024, Developing new models and methods for computational studies of membrane proteins, International Collaboration Grant, National Key Program from Ministry of Science and Technology of China, 2.64M CNY, Lead PI, on-going.
- 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, on-going.
- 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, The Global Recruitment Program, 2M CNY, Sole PI, completed.
- Jul 2016 – Jun 2021, Molecular machines for transmembrane signaling and transport, National Key Program from National Science Foundation of China, 2M (out of 34.5M) CNY, Co-PI, completed.

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 committee member of the ICAM-China Branch
- Biophysical Society of China, and committee member of the panel on Molecular Biophysics
- Chinese Society for Bioinformatics, and committee member of the panel on Structure Prediction and Simulation of Biomolecules
- Biophysical Society
- American Chemical Society
- Chinese Chemical Society

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 Physical Chemistry Letters
- Journal of Chemical Theory and Computation
- Biophysical Journal