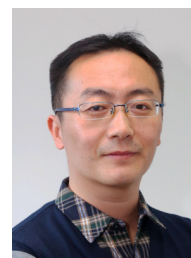


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## Research Interests

Theoretical and computational biophysics on membrane proteins, in particular:

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

## Education

Shandong University, China

- PhD, Condensed Matter Physics, 2002 to 2007
- BSc, Physics, 1998 to 2002

## Academic Experience

- Peking University, Beijing, China
  - Assistant Professor & Principal Investigator, Since 2016
- University of Oxford (Sansom Group), Oxford, United Kingdom
  - Marie Curie Research Fellow, Jan 2014 to Dec 2015
  - Newton International Fellow, Jan 2013 to Dec 2013
- Max Planck Institute for Biophysical Chemistry (de Groot Group), Göttingen, Germany
  - Max-Planck Postdoc Fellow, Feb 2012 to Dec 2012
  - Alexander von Humboldt Postdoc Fellow, Dec 2009 to Jan 2012
- University of Western Australia (Corry Group), Perth, Australia
  - Postdoc Research Associate, Jul 2007 to Jul 2009

## International Awards and Honors

- 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

## External Grants and Funding

- 2021-2024, Developing new models and methods for computational studies of membrane proteins, International Collaboration Grant, National Key Program of MOST, 2,640k RMB, Lead PI.
- 2021-2025, The gating and permeation mechanism of the mechanosensitive ion channel NompC, General Program of NSFC, 700k RMB, Sole PI.
- 2019-2023, Development of new calcium ion models for computational studies of biosystems, General Program of NSFC, 800k RMB, Sole PI.
- 2016-2021, Molecular machines for transmembrane signaling and transport, National Key Program of MOST, 2,000k (out of 34.5M) RMB, Co-PI.
- 2016-2019, The Global Recruitment Program, 2,000k RMB, Sole PI.

## 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 (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
- Biotechnology and Biological Sciences Research Council, UK
- Natural Science Foundation of Beijing

## Referee Assistance for Journals

- Nature Communications
- Journal of the American Chemical Society
- eLife
- Journal of Physical Chemistry Letters
- Journal of Chemical Theory and Computation
- Biophysical Journal
- ...

## Presentations

### International Talks

1. Invited Talk: Prediction of lipid contacting residues based on the simulation data of membrane proteins, The HECBioSim Seminar, UK (virtual), April 26, 2021.
2. Oral Presentation: Molecular Dynamics Simulations on the Mechanosensitive Ion Channel NompC, The 20<sup>th</sup> Hünfeld Workshop of Computer Simulation and Theory of Macromolecules, Germany (virtual), April 24, 2021.
3. Invited Talk: Combining Physics-based and Knowledge-based Computational Methods for the Study of Membrane Proteins, The 65<sup>th</sup> Annual Meeting of the Biophysical Society (**The Future of Biophysics Symposium**, virtual), Feb 24, 2021.
4. Invited Talk: Multiscale molecular dynamics simulations for antimicrobial peptides study, Multiscale Modeling for Biotherapeutics Symposium (virtual), Schrödinger, Inc., Nov 19, 2020.
5. Invited Talk: The Ca<sup>2+</sup> permeation mechanism of the open-state ryanodine receptor 1, University of California Irvine, Feb 5, 2020.
6. Invited Talk: Computational Studies of Ca<sup>2+</sup>-permeable channels, Riken, Japan, Aug 27, 2019.
7. Invited Talk: How Do Calcium Ions Permeate through the Ryanodine Receptor 1, The 1<sup>st</sup> KIAS-Beijing Workshop on Biological Sciences, Seoul, Korea, July 3-5, 2019.

8. Invited Talk: Activation of the mechanosensitive ion channel OSCA. Victor Chang Cardiac Research Institute, Sydney, Australia, Feb 15, 2019.
9. Invited Talk: To understand, predict and design membrane proteins. Australian National University, Canberra, Australia, Feb 6, 2019.
10. Invited Talk: Ion permeation and gating mechanism of the mechanosensitive ion channel OSCA revealed by molecular dynamics simulations. The 18<sup>th</sup> KIAS Conference on Protein Structure and Function, Seoul, Korea, November 15-17, 2018.
11. Invited Talk: "Multiscale MD simulations on PSI and ion channel X", The 101<sup>st</sup> Canadian Chemistry Conference and Exhibition, Edmonton, Canada, May 27-31, 2018.
12. 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.
13. 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.
14. Oral Presentation: Dermcidin oligomer in action, presented at the Workshop on Computer Simulation and Theory of Macromolecules, Huenfeld, Germany, Apr 21, 2012.

### Domestic Talks

1. Invited Talk: On the gating mechanisms of mechanosensitive ion channels, Xiamen Soft Matter Forum & ICAM-China Autumn Workshop, Xiamen, China, Dec 10, 2021.
2. 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.
3. Invited Talk: The Gating Mechanisms of Two Mechanosensitive Ion Channels, International Symposium of Biophysics and Soft Matter Frontiers, Jinan, China, Dec 19, 2020.
4. 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.
5. 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.
6. Invited Talk: Visualizing Ca<sup>2+</sup> Permeation through the Ryanodine Receptor by Molecular Dynamics Simulations, International Workshop on Multiscale Biological Imaging, Shanghai, China. Nov 9-10, 2019.
7. Invited Talk: Computational studies of mechanosensitive ion channels, The 6<sup>th</sup> Structural Biology Conference of China, Jixi, Anhui, China. Oct 11-14, 2019.

8. 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.
9. Invited Talk: How Do Calcium Ions Permeate through the Ryanodine Receptor 1, Songshan Lake Workshop and Summer School, Dongguan, Guangdong, China. Aug 1, 2019.
10. Invited Talk: Molecular details of gating in mechanosensitive ion channels, NYU Shanghai, China, May 31, 2019.
11. 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.
12. Invited Talk: “Studying Ion Channel Permeation with Molecular Dynamics Simulations”, The 16th Chinese Biophysics Congress, Chengdu, China, Aug 24-27, 2018.
13. 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.
14. Invited Talk: Development of  $\text{Ca}^{2+}$  Model for Simulating Biological Systems, The 2nd Worldwide Chinese Computational Biology and Molecular Simulation Conference, Guangzhou, China, Jun 10, 2018.
15. 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.
16. Invited Talk: Computational Electrophysiology in Ion Channel Research, Workshop on Modeling and Analysis in Molecular Biology and Electrophysiology, Suzhou, China, Jun 16, 2016.

## Selected Publications

1. Wang, D.#; Li, J.#; Wang, L.; Cao, Y.; Li, S.\*; **Song, C.\*** Toward an Atomistic Model of SARS-CoV-2. [Preprint](#).
2. 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. [Preprint](#) (accepted by *PLoS Comput. Biol.*).
3. 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.
4. 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.
5. Liu, C.; Zhang, A.; Yan, N.; **Song, C.\*** Atomistic Details of Charge/Space Competition in the  $\text{Ca}^{2+}$  Selectivity of Ryanodine Receptors. *J. Phys. Chem. Lett.* 2021, 12, 4286.

6. 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 (43), 14548. (**Editor's Picks & Cover Story**)
7. 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.
8. Zhang, A.; Yu, H.; Liu, C.; **Song, C.\*** The Ca<sup>2+</sup> Permeation Mechanism of the Ryanodine Receptor Revealed by a Multi-Site Ion Model. *Nat. Commun.* 2020, 11 (1), 1.
9. **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 (9), 1658.
10. 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 (9), 850.
11. 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 (1), 16985.
12. Köpfer, D. A.#; **Song, C.#,\***; Gruene, T.; Sheldrick, G. M.; Zachariae, U.\*; de Groot, B. L.\* Ion Permeation in K<sup>+</sup> Channels Occurs by Direct Coulomb Knock-On. *Science* 2014, 346 (6207), 352. (co-first and co-corresponding author)
13. **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 (12), 4586.
14. **Song, C.**; Corry, B.\* Testing the Applicability of Nernst-Planck Theory in Ion Channels: Comparisons with Brownian Dynamics Simulations. *PLoS One* 2011, 6 (6), e21204–e21204.
15. **Song, C.**; Corry, B.\* Ion Conduction in Ligand-Gated Ion Channels: Brownian Dynamics Studies of Four Recent Crystal Structures. *Biophys. J.* 2010, 98 (3), 404–411.
16. **Song, C.**; Corry, B.\* Intrinsic Ion Selectivity of Narrow Hydrophobic Pores. *J. Phys. Chem. B* 2009, 113 (21), 7642–7649.

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