



Ruyi Song

Postdoctoral Scholar, Photon Science, SLAC

Bio

BIO

Ph.D. in Theoretical and Computational Chemistry / Materials Science

B.S. in Theoretical and Computational Chemistry / Chemical Biology

18+ high-profile publications (Nat. Chem., Nat. Commun., Phys. Rev., JACS, etc.) and 950+ citations.

Proficient in 1) quantum chemistry simulation; 2) quantum chemistry code development; 3) molecular mechanics simulation

6 years of research experience on DFT and solid-state materials/semiconductors;

5 years of research experience on MD and biological systems.

Recently march towards Machine-Learning-aided molecular simulation, property prediction, and material discovery.

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PROFESSIONAL EDUCATION

- Doctor of Philosophy, Duke University (2023)
- Bachelor of Science, Peking University (2017)
- Ph.D., Duke University , Theoretical and Computational Chemistry / Materials Science (2023)
- B.S., Peking University , Theoretical and Computational Chemistry / Chemical Biology (2017)

STANFORD ADVISORS

- Wendy Mao, Postdoctoral Faculty Sponsor

Publications

PUBLICATIONS

- **Thickness control of organic semiconductor-incorporated perovskites.** *Nature chemistry*
Park, J. Y., Song, R., Liang, J., Jin, L., Wang, K., Li, S., Shi, E., Gao, Y., Zeller, M., Teat, S. J., Guo, P., Huang, L., Zhao, et al
2023
- **Structure and electronic tunability of acene alkylamine based layered hybrid organic-inorganic perovskites from first principles** *PHYSICAL REVIEW MATERIALS*
Song, R., Liu, C., Kanai, Y., Mitzi, D. B., Blum, V.
2023; 7 (8)

- **Chiral Perovskite Nanoplatelets with Tunable Circularly Polarized Luminescence in the Strong Confinement Regime** *ADVANCED OPTICAL MATERIALS*
Cao, Q., Song, R., Chan, C. S., Wang, Z., Wong, P., Wong, K., Blum, V., Lu, H.
2023
- **Large Scale Quantum Chemistry with Tensor Processing Units** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
Pederson, R., Kozlowski, J., Song, R., Beall, J., Ganahl, M., Hauru, M., Lewis, A. M., Yao, Y., Mallick, S., Blum, V., Vidal, G.
2022: 25-32
- **The Structural Origin of Chiroptical Properties in Perovskite Nanocrystals with Chiral Organic Ligands** *ADVANCED FUNCTIONAL MATERIALS*
Kim, Y., Song, R., Hao, J., Zhai, Y., Yan, L., Moot, T., Palmstrom, A. F., Brunecky, R., You, W., Berry, J. J., Blackburn, J. L., Beard, M. C., Blum, et al
2022; 32 (25)
- **Structural descriptor for enhanced spin-splitting in 2D hybrid perovskites** *NATURE COMMUNICATIONS*
Jana, M. K., Song, R., Xie, Y., Zhao, R., Sercel, P. C., Blum, V., Mitzi, D. B.
2021; 12 (1): 4982
- **Organic-to-inorganic structural chirality transfer in a 2D hybrid perovskite and impact on Rashba-Dresselhaus spin-orbit coupling** *NATURE COMMUNICATIONS*
Jana, M. K., Song, R., Liu, H., Khanal, D., Janke, S. M., Zhao, R., Liu, C., Vardeny, Z., Blum, V., Mitzi, D. B.
2020; 11 (1): 4699
- **Machine learning-empowered study of metastable CsPbI_3 under pressure and strain** *JOURNAL OF MATERIALS CHEMISTRY A*
Han, M., Peng, C., Song, R., Ke, F., Nashed, Y. G., Mao, W. L., Jia, C., Lin, Y.
2024
- **Extended Honeycomb Metal Chloride with Tunable Antiferromagnetic Correlations** *CHEMISTRY OF MATERIALS*
Xue, J., Song, R., Guo, Z., Sung, H. Y., Lortz, R., Williams, I. D., Lu, H.
2023; 36 (1): 551-560
- **Exploration, Prediction, and Experimental Verification of Structure and Optoelectronic Properties in $\text{I}_2\text{-Eu-IV-X}_4$ (I = Li, Cu, Ag; IV = Si, Ge, Sn; X = S, Se) Chalcogenide Semiconductors** *CHEMISTRY OF MATERIALS*
Wang, T., Mcwhorter, T. M., Wessler, G., Yao, Y., Song, R., Mitzi, D. B., Blum, V.
2023; 36 (1): 340-357
- **Chiral Cation Doping for Modulating Structural Symmetry of 2D Perovskites.** *Journal of the American Chemical Society*
Xie, Y., Morgenstein, J., Bobay, B. G., Song, R., Caturello, N. A., Sercel, P. C., Blum, V., Mitzi, D. B.
2023
- **Hybrid magnonics in hybrid perovskite antiferromagnets.** *Nature communications*
Comstock, A. H., Chou, C., Wang, Z., Wang, T., Song, R., Sklenar, J., Amassian, A., Zhang, W., Lu, H., Liu, L., Beard, M. C., Sun, D.
2023; 14 (1): 1834
- **Kinetically Controlled Structural Transitions in Layered Halide-Based Perovskites: An Approach to Modulate Spin Splitting** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Xie, Y., Song, R., Singh, A., Jana, M. K., Blum, V., Mitzi, D. B.
2022; 144 (33): 15223-15235
- **Highly Distorted Chiral Two-Dimensional Tin Iodide Perovskites for Spin Polarized Charge Transport** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Lu, H., Xiao, C., Song, R., Li, T., Maughan, A. E., Levin, A., Brunecky, R., Berry, J. J., Mitzi, D. B., Blum, V., Beard, M. C.
2020; 142 (30): 13030-13040
- **Molecular engineering of organic-inorganic hybrid perovskites quantum wells (vol 11, pg 1151, 2019)** *NATURE CHEMISTRY*
Gao, Y., Shi, E., Deng, S., Shiring, S. B., Snaider, J. M., Liang, C., Yuan, B., Song, R., Janke, S. M., Liebman-Pelaez, A., Yoo, P., Zeller, M., Boudouris, et al
2021; 13 (3): 290
- **Molecular engineering of organic-inorganic hybrid perovskites quantum wells** *NATURE CHEMISTRY*
Gao, Y., Shi, E., Deng, S., Shiring, S. B., Snaider, J. M., Liang, C., Yuan, B., Song, R., Janke, S. M., Liebman-Pelaez, A., Yoo, P., Zeller, M., Boudouris, et al
2019; 11 (12): 1151-1157

- **Unnatural Cytosine Bases Recognized as Thymines by DNA Polymerases by the Formation of the Watson-Crick Geometry** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*
Zeng, H., Mondal, M., Song, R., Zhang, J., Xia, B., Liu, M., Zhu, C., He, B., Gao, Y., Yi, C.
2019; 58 (1): 130-133

PRESENTATIONS

- Structural, Electronic and Optical Properties of 2D Perovskites from First Principles - Center for Hybrid Organic Inorganic Semiconductors for Energy (CHOISE) Annual Meeting (September 19, 2019)
- Transfer of Structural Asymmetry in Chiral 2D Hybrid Perovskites and Rashba-Dresselhaus Spin Splitting in Inorganic Bands - American Physical Society (APS) March Meeting 2021 (March 15, 2021)
- Structure-Property Control for Enhanced Spin-Splitting in 2D Hybrid Perovskites - EFRC-Hub-CMS-CCS Virtual Principal Investigators' Meeting 2021 (October 19, 2021)
- The Relationship between Structural Distortions and Spin-Splitting in Perovskites - American Physical Society (APS) March Meeting 2022 (March 14, 2022)
- First-Principles Structure Prediction and Chirality Transfer in Chiral Organic-Inorganic Perovskite Nanoplatelets - American Physical Society (APS) March Meeting 2023 (March 9, 2023)