# 周健 (Jian ZHOU)

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School of Materials Science and Engineering
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Updated at June 9, 2026

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## I. Personal Information

Date of Birth: May 1986
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Citizenship: China
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Homepage: https://gr.xjtu.edu.cn/web/jianzhou

## II. Education

**Ph.D. in Mechanics**, COE, Peking University 2008.09–2013.07
Thesis: *Simulation Studies on the Property Modulations and Applications of Single Atomic Sheets.*
Supervisor: Prof. Qiang Sun

**B.Sc. in Theoretical Mechanics and Applications**, COE, Peking University 2004.09–2008.07

## III. Academic Appointments

Professor, School of MSE, Xi'an Jiaotong University 2018.09–Present
Postdoc (Prof. Ju Li), RLE, Massachusetts Institute of Technology 2017.09–2018.08
Postdoc (Prof. Puru Jena), Physics Dept, Virginia Commonwealth University 2013.10–2017.08

## IV. Recent Research Interests

Nonlinear optics driven ionic, electronic, spin, and orbital responses in quantum materials

## V. Honors and Recongnitions

研究生教学成果奖，陕西省学位与研究生教育学会 2025
World's Top 2% Scientists, both career life and yearly lists (Stanford) 2023–2025
Reviewer of the Year, *npj Computational Materials* 2023
小米青年学者 (Xiaomi Inc.) 2022
Most Cited Chinese Researcher, Elsevier 2020
Outstanding Editorial Youth Committee Member of *Acta Physico-Chimica Sinica* 2019
National One-Thousand Young Talent Program 2018
DMP Post-Doctoral Travel Award, American Physical Society 2017
Excellent Ph. D. Thesis, Peking University 2013
Excellent Graduate Student, Beijing, China 2013
Excellent Graduate Student, Peking University 2013

"Top-10 Academic" Award, Peking University 2012

## VI. Teaching Experience

| | |
|---|---|
| Solid State Physics (Graduate, in English) | Fall 2019 |
| Frontiers of Materials Science and Engineering (Graduate, in English) | Fall 2019 |
| Solid State Physics (Graduate, in English) | Fall 2020 |
| Frontiers of Materials Science and Engineering (Graduate, in English) | Fall 2020 |
| Solid State Physics (Graduate, in English) | Fall 2021 |
| Frontiers of Materials Science and Engineering (Graduate, in English) | Fall 2021 |
| 材料物理 (Undergraduate) | Fall 2023 |
| 量子力学导论 (Undergraduate) | Fall 2023 |
| Solid State Physics (Graduate, in English) | Fall 2023 |
| Frontiers of Materials Science and Engineering (Graduate, in English) | Fall 2023 |
| 材料物理 (Undergraduate) | Fall 2024 |
| 量子力学导论 (Undergraduate) | Fall 2024 |
| Solid State Physics (Graduate, in English) | Fall 2024 |
| 材料物理 (Undergraduate) | Fall 2025 |
| 量子力学导论 (Undergraduate) | Fall 2025 |
| Solid State Physics (Graduate, in English) | Fall 2025 |

## VII. Supervising Students

*Research Assistant*

- Yiwei Zhao (Jan 2023–Dec 2023), to National University of Singapore for postdoc, now at City University of Hong Kong.

*Ph.D. Students*

- Hafiz Muhammad Rizwan Ahmad (2017–2025), Finished study.
- Kun Liu (2019–2024, to Rocket Force University of Engineering), Thesis: *First-Principles Calculation Study of Photostriction Mechanisms in Chalcogenides and Nitrides*
- Qianqian Xue (2021–2025, to Guizhou Minzu University), Thesis: *Theory and First-Principles Calculations of Light-Driven Magnetic Moment Reorientation in Two-Dimensional Ferromagnetic Materials.*
- Xingchi Mu (2022–2026, to PengXinWei Corporation)
- Hanli Cui (2023–)
- Huimin Gao (2025–)
- Yiqian Zhang (2026–)

*Master Students*

- Yiming Pan (2018–2021, to Kiel University), Thesis: *First-Principles Study of Electronic and Optoelectronic Properties of 2D Ferroelectric Bi(110).*
- Xiao Li (2019–2022, to Xi'an Aero-Engine Corporation), Thesis: *First-Principles Study on the Structure and Properties of Boron-Based Electrolytes.*

- Yan Sun (2020–2023, to Huawei Technologies Co., Ltd. at Xi'an), Thesis: *First-Principles Study of Photomagnetization in Bilayer $In_2Se_3$.*
- Zihang Wu (2020–2023, to TP-Link Technologies Co., Ltd. at Shenzhen), Thesis: *First-Principles Study on Phase Transition of Two-Dimensional $In_2Se_3$ Antiferroelectric Structure via Light.*
- Cong Zhou (2021–2024, to Max Planck Institute for Polymer Research under Prof. Mischa Bonn), Thesis: *Light-induced Phase Transitions in Two-dimensional $MnBi_2Te_4$ and $MnBi_2Te_4/Bi_2Te_3$ Antiferromagnets.*
- Haoxiang Dong (2021–2024, to ZTE Corporation), Thesis: *First-Principles Study on Magnetoelectric Effect of Magnetic Polarized Bilayer $CrX_3$ (X = I, Br, Cl).*
- Xiantuo Zhao (2022–2025, to Yangtze Memory Technologies Co., Ltd. at Wuhan), Thesis: *First-Principles Study on Light-Induced Phase Transitions and Bulk Photovoltaic Current in Janus Transition Metal Dichalcogenides.*
- Zhiyuang Li (2024–)
- Hao Zuo (2024–)
- Yanrui Xu (2026–)

*Undergraduate Students*

- Jiashu Zheng, 2019
- Xilai Bao, 2021
- Zedong Huang, 2022
- Yurui Xu, 2025

## VIII. Ad hoc Reviewer for Scientific Journals

Nature, Nature Physics, Proceedings of National Academy of Sciences of the United State of the America, Physical Review Letters, Nature Communications, Advanced Materials, Advanced Science, Journal of the American Chemical Society, Nano Letters, Advanced Functional Materials, ACS Nano, npj Computational Materials, npj 2D Materials & Applications, Chemistry of Materials, Journal of Materials Chemistry A, Physical Review, The Journal of Physical Chemistry Letters, Inorganic Chemistry, ACS Applied Materials & Interfaces, Nano Research, Carbon, Small, Nanoscale, Chemical Communications, Journal of Materials Chemistry C, Scientific Reports, Physical Chemistry Chemical Physics, The Journal of Physical Chemistry, Applied Physics Letters, Chinese Physics B, New Journal of Physics, ACS Applied Electronic Materials, Nanomaterials, ChemPhysChem, AIP Advances, RSC Advances, Nanotechnology, International Journal of Hydrogen Energy, New Journal of Chemistry, Journal of Applied Physics, Journal of Magnetism and Magnetic Materials, Physics Letters A, Chemical Physics Letters, Physica Status Solidi, etc.

Selected as Outstanding Reviewer (Reviewer of the Year) at *npj Computational Materials* in 2023

## IX. Academic Activities

- Editorial Youth Committee Member of *Acta Physico-Chimica Sinica* (2019-2024)
- Guest Editor, Special Issue "Optical Properties of Semiconductor Nanomaterials" in *Nanomaterials*

Organizer of the following conferences

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|---|---|---|
| 2023 | 第一届团簇物理学及能源信息应用研讨会 | 西安 |
| 2023 | 第四届结构材料及能源信息应用研讨会 | 西安 |
| 2024 | International Conference on Materials for Green Future | Phuket, Thailand |

## X. Membership in Professional Societies

- Chinese Physical Society
- Chinese Materials Research Society

## XI. Research Grants and Funding

| | | |
|---|---|---|
| 2012–2013 | New Excellent Ph.D. Candidate, Ministry of Education | ¥30,000 |
| 2018–2022 | National One-Thousand Young Talent Program | ¥2,000,000 |
| 2018–2021 | Young Talent Start-Up Program of Xi'an Jiaotong University (Class A) | ¥2,000,000 |
| 2019–2021 | Foreign Graduate Student Supervising Program | ¥40,000 |
| 2020–2022 | Optics driven phase transition in two-dimensional ferroelectric materials, NSFC-21903063 | ¥260,000 |
| 2020–2023 | Structural design and valleytronic topological properties of two-dimensional magnetic materials on group-IV semiconductor surfaces, NSFC-11974270 | ¥630,000 |
| 2020–2024 | Design of high aspect energy, high aspect power, and highly safe energy storage devices, 2019YFA0210600, (Co-PI) | ¥660,000 |
| 2024–2027 | Bulk photovoltaic effect in layered antiferromagnetic materials and its modulation, NSFC-12374065 | ¥530,000 |

## XII. Full Publication List

According to Google Scholar, total citation over 9,100 times, with *h*-index of 43.

* Corresponding author, = Equal contributor

1. Hydrogen storage in Al-N cage based nanostructures.
   X. Zhou, M. M. Wu, J. Zhou, Q. Sun*
   *Applied Physics Letters* 94, 103105 (2009).

2. Tuning electronic and magnetic properties of graphene by surface modification.
   J. Zhou, M. M. Wu, X. Zhou, Q. Sun*
   *Applied Physics Letters* 95, 103108 (2009).

3. Ferromagnetism in semihydrogenated graphene sheet.
   J. Zhou, Q. Wang, Q. Sun*, X. S. Chen, Y. Kawazoe, P. Jena
   *Nano Letters* 9, 3867 (2009).

4. Electric field enhanced hydrogen storage on polarizable materials substrates.
   J. Zhou, Q. Wang, Q. Sun*, P. Jena, X. S. Chen
   *Proceedings of National Academy of Sciences of U.S.A.* 107, 2801 (2010).
   Selected as "The Most Influential Interactional Academic Papers in China (2010)"

5. Electronic and magnetic properties of a BN sheet decorated with hydrogen and fluorine.
   Jian Zhou, Qian Wang, Qiang Sun*, Puru Jena
   *Physical Review B* 81, 085442 (2010).

6. Interaction of $C_{59}Si$ with Si based clusters: a study of Janus nanostructures.
Miao Miao Wu, Xiao Zhou, Jian Zhou, Qiang Sun*, Qian Wang, Puru Jena
*Journal of Physics: Condensed Matter* 22, 275303 (2010).

7. Stability and electronic structure of bilayer graphone.
J. Zhou, Q. Wang, Q. Sun*, P. Jena
*Applied Physics Letters* 98, 063108 (2011).

8. Enhanced Hydrogen Storage on Li Functionalized $BC_3$ Nanotube.
Jian Zhou, Qian Wang, Qiang Sun*, Puru Jena
*The Journal of Physical Chemistry C* 115, 6136 (2011).

9. Electronic structures and bonding of graphyne sheet and its BN analog.
Jian Zhou, Kun Lü, Qian Wang, Xiao Shuang Chen, Qiang Sun*, Puru Jena
*Journal of Chemical Physics* 134, 174701 (2011).

10. Tripyrrylmethane based 2D porous structure for hydrogen storage.
Xiao Zhou, Jian Zhou, Kun Lü, Qiang Sun*
*Fronters of Physics* 6, 220. (2011).

11. Intrinsic ferromagnetism in two-dimensional carbon structures: Triangular graphene nanoflakes linked by carbon chains.
Jian Zhou, Qian Wang, Qiang Sun*, Puru Jena
*Physical Review B* (Rapid Communication) 84, 081402(R) (2011).

12. Magnetism of Phthalocyanine-Based Organometallic Single Porous Sheet.
Jian Zhou, Qiang Sun*
*Journal of the American Chemical Society* 133, 15113 (2011).

13. Sc-phthalocyanine sheet: Promising material for hydrogen storage.
Kun Lü, Jian Zhou, Le Zhou, Qian Wang, Qiang Sun*, Puru Jena
*Applied Physics Letters* 99, 163104 (2011).

14. Tuning the band gap and magnetic properties of BN sheets impregnated with graphene flakes.
Min Kan, Jian Zhou, Qian Wang, Qiang Sun*, Puru Jena
*Physical Review B* 84, 205412 (2011).

15. Tuning magnetic properties of graphene nanoribbons with topological line defects: From antiferromagnetic to ferromagnetic.
Min Kan$^{=}$, Jian Zhou$^{=}$, Qiang Sun*, Qian Wang, Yoshiyuki Kawazoe, Puru Jena
*Physical Review B* 85, 155450 (2012).

16. Using carbon chains to mediate magnetic coupling in zigzag graphene nanoribbons.
Min Kan, Jian Zhou, Yawei Li, Qiang Sun*
*Applied Physics Letters* 100, 173106 (2012).

17. Pre-combustion $CO_2$ capture by transition metal ions embedded in phthalocyanine sheets.
Kun Lü, Jian Zhou, Le Zhou, Xiao Shuang Chen, Siew Hwa Chan, Qiang Sun*
*Journal of Chemical Physics* 136, 234703 (2012).

18. Magnetic properties of two-dimensional silicon carbide triangular nanoflakes-based kagome lattices.
Xiaowei Li, Jian Zhou, Qian Wang*, Puru Jena
*Journal of Nanoparticle Research* 14, 1056 (2012).

19. Magnetism of triangular nanoflakes with different compositions and edge terminations.
Shunhong Zhang, Jian Zhou, Xiaowei Li, Qian Wang*
*Journal of Nanoparticle Research* 14, 1171 (2012).

20. Magnetism of two-dimensional triangular nanoflake-based kagome lattices.
Xiaowei Li, Jian Zhou, Qian Wang*, Xiaoshuang Chen, Yoshiyuki Kawazoe, Puru Jena
*New Journal of Physics* 14, 033043 (2012).

21. How to fabricate a semihydrogenated graphene sheet? A promising strategy explored.
Jian Zhou, Qiang Sun*
*Applied Physics Letters* 101, 073114 (2012).

22. Strain-Induced Spin Crossover in Phthalocyanine-Based Organometallic Sheets.
Jian Zhou, Qian Wang, Qiang Sun*, Yoshiyuki Kawazoe, Puru Jena
*The Journal of Physical Chemistry Letters* 3, 3109 (2012).

23. Tuning the properties of graphene using a reversible gas-phase reaction.
Lin Gan, Jian Zhou, Fen Ke, Hang Gu, Danna Li, Zonghai Hu, Qiang Sun, Xuefeng Guo*
*NPG Asia Materials* 4, e31 (2012).

24. Exfoliated graphene-supported Pt and Pt-based alloys as electrocatalysts for direct methanol fuel cells.
Wen Qian, Rui Hao, Jian Zhou, Micah Eastman, Beth A. Manhat, Qiang Sun, Andrea M. Goforth, Jun Jiao*
*Carbon* 52, 595 (2013).

25. Patterning Graphitic C-N Sheets into Kagome Lattice for Magnetic Materials.
Xiaowei Li, Jian Zhou, Qian Wang*, Yoshiyuki Kawazoe, Puru Jena
*The Journal of Physical Chemistry Letters* 4, 259 (2013).

26. Structure, Stability and Property Modulations of Stoichiometric Graphene Oxide.
Shunhong Zhang, Jian Zhou, Qian Wang*, Puru Jena
*The Journal of Physical Chemistry C* 117, 1064 (2013).

27. Absorption induced modulation of magnetism in two-dimensional metal phthalocyanine porous sheets.
Jian Zhou, Qiang Sun*
*Journal of Chemical Physics* 138, 204706 (2013).

28. The Intrinsic Ferromagnetism in a $MnO_2$ Monolayer.
Min Kan, Jian Zhou, Qiang Sun*, Yoshiyuki Kawazoe, Puru Jena
*The Journal of Physical Chemistry Letters* 4, 3382 (2013).

29. Self-consistent determination of Hubbard $U$ for explaining the anomalous magnetism of the $Gd_{13}$ cluster.
Kun Tao, Jian Zhou, Qiang Sun, Qian Wang, V. S. Stepanyuk, Puru Jena*
*Physical Review B* 89, 085103 (2014).

30. Carrier induced magnetic coupling transitions in phthalocyanine-based organometallic sheet.
Jian Zhou, Qiang Sun*
*Nanoscale* 6, 328 (2014).

31. Experimental and Theoretical Analysis of Fast Lithium Ionic Conduction in a $LiBH_4$-$C_{60}$ Nanocomposite.
Joseph A. Teprovich, Jr.*, Hector R. Colon-Mercado, Patrick A. Ward, Brent Peters, Santanab Giri, Jian Zhou, Scott Greenway, Robert N. Compton, Purusottam Jena, Ragaiy Zidan*
*The Journal of Physical Chemistry C* 118, 21755 (2014).

32. 18-Electron rule inspired Zintl-like ions composed of all transition metals.
Jian Zhou, Santanab Giri, Purusottam Jena*
*Physical Chemistry Chemical Physics* 16, 20241 (2014).

33. Tailoring Li adsorption on graphene.
Jian Zhou, Qiang Sun, Qian Wang, Puru Jena*
*Physical Review B* 90, 205427 (2014).

34. Intermediate Phases during Decomposition of Metal Borohydrides, $M(BH_4)_n$ ($M$ = Na, Mg, Y).
Yuzhen Liu, Santanab Giri, Jian Zhou, Puru Jena*
*The Journal of Physical Chemistry C* 118, 28456 (2014).

35. Self-assembly of metal atoms (Na, K, Ca) on graphene.
Jian Zhou, Shunhong Zhang, Qian Wang, Yoshiyuki Kawazoe, Puru Jena*
*Nanoscale* 7, 2352 (2015).

36. Electronic Structure and Stability of Mono- and Bi-metallic Borohydrides and Their Underlying Hydrogen-Storage Properties–A Cluster Study.
Yuzhen Liu, Jian Zhou, Puru Jena*
*The Journal of Physical Chemistry C* 119, 11056 (2015).

37. Penta-Graphene: A New Carbon Allotrope.
Shunhong Zhang, Jian Zhou, Qian Wang*, Xiaoshuang Chen, Yoshiyuki Kawazoe, Puru Jena
*Proceedings of National Academy of Sciences of U.S.A.* 112, 2372 (2015).
Included in Wikipedia (Penta-Graphene)

38. Unusual Stability of Multiply Charged Organo-Metallic Complexes.
Santanab Giri, Brandon Z. Child, Jian Zhou, and Puru Jena*
*RSC Advances* 5, 44003 (2015).

39. Giant magnetocrystalline anisotropy of $5d$ transition metal-based phthalocyanine sheet.
Jian Zhou*, Qian Wang, Qiang Sun, Yoshiyuki Kawazoe, Puru Jena*
*Physical Chemistry Chemical Physics* 17, 17182 (2015).

40. High-temperature superconductivity in heavily N- or B-doped graphene.
Jian Zhou*, Qiang Sun, Qian Wang, Puru Jena*
*Physical Review B* 92, 064505 (2015).

41. From Halogen to Superhalogen Behavior of Organic Molecules Created by Functionalizing Benzene.
Hongmin Zhao, Jian Zhou*, Hong Fang, Puru Jena*
*ChemPhysChem* 17, 184 (2016).

42. Stability of $B_{12}(CN)_{12}^{2-}$: Implications for Lithium and Magnesium Ion Batteries.
Hongmin Zhao[=], Jian Zhou[=,*], Puru Jena*
*Angewante Chemime International Edition* 55, 3704 (2016).

43. Beyond Graphitic Carbon Nitride: Nitrogen-Rich Penta-$CN_2$ Sheet.
Shunhong Zhang, Jian Zhou, Qian Wang*, Puru Jena
*The Journal of Physical Chemistry C* 120, 3993 (2016).

44. Strain and Carrier Induced Coexistence of Topologically Insulating and Superconducting Phase in Iodized Si(111) Films.
Jian Zhou*, Qian Wang, Qiang Sun, Puru Jena
*Nano Research* 9, 1578 (2016).

45. Pressure-induced structural transition in copper pyrazine dinitrate and implications for quantum magnetism.
K. R. O'Neal, J. Zhou, J. G. Cherian, M. M. Turnbull, C. P. Landee, P. Jena, Z. Liu, J. L. Musfeldt
*Physics Review B* 93, 104409 (2016).

46. Intrinsic Quantum Spin Hall and Anomalous Hall Effect in h-Sb/Bi Epitaxial Growth on Ferromagnetic $MnO_2$ Thin Film.
Jian Zhou*, Qiang Sun, Qian Wang, Yoshiyuki Kawazoe, Puru Jena*
*Nanoscale* 8, 11202 (2016).

47. Quantum Phase Transition in Germanene and Stanene Bilayer: From Normal Metal to Topological Insulator.
Chengxi Huang, Jian Zhou, Haiping Wu, Kaiming Deng*, Puru Jena*, Erjun Kan*
*The Journal of Physical Chemistry Letters* 7, 1919 (2016).

48. Integrating superconducting phase and topological crystalline quantum spin Hall effect in hafnium intercalated gallium film.
Jian Zhou*, Shunhong Zhang, Qian Wang, Puru Jena*
*Applied Physics Letters* 108, 253102 (2016).

49. Two-dimensional topological nanomaterials and related Hall effects.
Jian Zhou, Puru Jena
*International Symposium on Clusters and Nanomaterials* (Proc. SPIE), 101740H, 242 (2016).

50. Logic Control of Interface-Induced Charge-Trapping Effect for Ultrasensitive Gas Detection with All-Mirror-Image Symmetry.
Chuancheng Jia, Qing Wang, Na Xin, Jian Zhou, Yao Gong, Lidong Li, Qiang Sun, Xuefeng Guo*
*Advances Materials Technologies* 1, 1600067 (2016).

51. Substituent-Stabilized Organic Dianions in the Gas Phase and Their Potential Use as Electrolytes in Lithium-Ion Batteries.
Hongmin Zhao, Jian Zhou, Puru Jena*
*ChemPhysChem* 17, 2992 (2016).

52. Like Charges Attract?
Tianshan Zhao, Jian Zhou, Qian Wang*, Puru Jena*
*The Journal of Physical Chemistry Letters* 7, 2689 (2016).

53. Valley contrasting in epitaxial growth of In/Tl homoatomic monolayer with anomalous Nernst conductance.
Jian Zhou*, Chengxi Huang, Erjun Kan, Puru Jena
*Physical Review B* 94, 035151 (2016).

54. A ferromagnetic and half-metallic $FeC_2$ monolayer containing $C_2$ dimers.
Tianshan Zhao, Jian Zhou, Qian Wang*, Yoshiyuki Kawazoe, Puru Jena*
*ACS Applied Materials & Interfaces* 8, 26207 (2016).

55. Investigation of hydrogen induced fluorescence in $C_{60}$ and its potential use in luminescent down shifting applications.
J. A. Teprovich Jr.*, A. L. Washington II, J. Dixon, P. A. Ward, J. H. Christian, B. Peters, J. Zhou, S. Giri, D. N. Sharp, J. A. Velten, R. N. Compton, P. Jena, R. Zidan*
*Nanoscale* 8, 18760 (2016).

56. Quantum anomalous Hall effect in ferromagnetic transition metal halides.
Chengxi Huang[=], Jian Zhou[=,*], Haiping Wu, Kaiming Deng, Puru Jena*, Erjun Kan*
*Physical Review B* 95, 045113 (2017).

57. Two-dimensional topological crystalline quantum spin Hall effect in transition metal intercalated compounds.
Jian Zhou*, Puru Jena
*Physical Review B* (Rapid Communication) 95, 081102(R) (2017).

58. Rational Design of Stable Dianions by Functionalizing Polycyclic Aromatic Hydrocarbons.
Mingmin Zhong, Jian Zhou, Puru Jena*
*ChemPhysChem* 18, 1937 (2017).

59. Role of ligands on the stability of $B_nX_n$ and $CB_{n-1}X_n$ ($n = 5 - 10$; $X$ = H, F, CN) and their potential as building blocks of electrolytes in lithium ion batteries.
Mingmin Zhong, Jian Zhou, Hong Fang, Purusottam Jena*
*Physical Chemistry Chemical Physics* 19, 17937 (2017).

60. Valley-Polarized Quantum Anomalous Hall Effect in Ferrimagnetic Honeycomb Lattices.
Jian Zhou*, Qiang Sun, Puru Jena*
*Physical Review Letters* 119, 046403 (2017).

61. Colossal Stability of Gas Phase Tri-anions: Super-pnictogens.
Tianshan Zhao, Jian Zhou, Qian Wang*, Puru Jena*
*Angewante Chemime International Edition* 56, 13421 (2017).

62. Giant Valley Splitting and Valley Polarized Plasmonics in Group-V Transition-Metal Dichalcogenide Monolayers.
Jian Zhou*, Puru Jena
*The Journal of Physical Chemistry Letters* 8, 5764 (2017).

63. Simultaneous Detection and Removal of Formaldehyde at Room Temperature: Janus Au@ZnO@ZIF-8 Nanoparticles.
Dawei Wang, Zhiwei Li, Jian Zhou, Hong Fang, Xiang He, Puru Jena, Jing-Bin Zeng*, Wei-Ning Wang*
*Nano-Micro Letters* 10, 4 (2018).

64. Effect of Coulomb Correlation on the Magnetic Properties of Mn Clusters.
Chengxi Huang, Jian Zhou, Kaiming Deng, Erjun Kan*, Puru Jena*
*The Journal of Physical Chemistry A* 122, 4350 (2018).

65. Atomically dispersed tungsten on metal halide monolayer as a ferromagnetic Chern insulator.
Chengxi Huang, Kaiming Deng, Jian Zhou*, Erjun Kan*
*Physical Review B* 98, 115424 (2018).

66. Electrochemically-mediated selective capture of heavy metal chromium and arsenic oxyanions from water.
Xiao Su, Akihiro Kushima, Cameron Halliday, Jian Zhou, Ju Li, T. Alan Hatton*
*Nature Communications* 9, 4701 (2018).

67. Opto-mechanics driven fast martensitic transition in two-dimensional materials.
Jian Zhou, Haowei Xu, Yifei Li, R. Jaramillo, Ju Li*
*Nano Letters* 18, 7794 (2018).

68. Super-alkalis as Building Blocks of One-Dimensional Hierarchical Electride.
Hong Fang[=,*], Jian Zhou[=], Puru Jena*
*Nanoscale* 10, 22963 (2018).

69. Lattice dynamic and instability in pentasilicene: A light single-element ferroelectric material with high Curie temperature.
Yaguang Guo, Cunzhi Zhang, Jian Zhou, Qian Wang*, Puru Jena
*Physical Review Applied* 11, 064063 (2019).

70. Ultra-high-temperature Ferromagnetism in Intrinsic Tetrahedral Semiconductors.
Chengxi Huang[=], Junsheng Feng[=], Jian Zhou, Hongjun Xiang[*], Kaiming Deng, Erjun Kan[*]
*Journal of American Chemical Society* 141, 12413 (2019).

71. Optomechanical control of stacking patterns of h-BN bilayer.
Haowei Xu, Jian Zhou, Yifei Li, R. Jaramillo, Ju Li[*]
*Nano Research* 12, 2634 (2019).

72. Hydrogenated $C_{60}$ as high-capacity stable anode materials for Li-ion batteries.
Joseph A. Teprovich Jr.[*], Jason A. Weeks, Patrick A. Ward, Spencer C. Tinkey, Chengxi Huang, Jian Zhou, Ragaiy Zidan, Puru Jena[*]
*ACS Applied Energy Materials* 2, 6453 (2019).

73. Near-infrared optical properties and proposed phase-change usefulness of transition metal disulfides.
Akshay Singh, Yifei Li, Balint Fodor, Laszlo Makai, Jian Zhou, Haowei Xu, Austin J. Akey, Ju Li, Rafael Jaramillo[*]
*Applied Physics Letters* 115, 161902 (2019).

74. Normal-to-Topological Insulator Martensitic Phase Transition in Group-IV Monochalcogenides Driven by Light.
Jian Zhou[*], Shunhong Zhang, Ju Li[*]
*NPG Asia Materials* 12, 2 (2020).

75. Sub-Angstrom Characterization of Structural Origin for High In-Plane Anisotropy in 2D $GeS_2$.
Xudong Wang[=], Jieling Tan[=], Chengqian Han[=], Jiang-Jing Wang[*], Lu Lu, Hongchu Du, Chun-Lin Jia, Volker Deringer[*], Jian Zhou, Wei Zhang[*]
*ACS Nano* 14, 4456 (2020).

76. Intercalation induced ferromagnetism in group-V transition metal dichalcogenide bilayer.
H. M. R. Ahamd, Jian Zhou[*]
*AIP Advances* 10, 045323 (2020).

77. Noncontacting optostriction driven anisotropic and inhomogeneous strain in two-dimensional materials.
Jian Zhou[*], Sheng Mao, Shunhong Zhang
*Physical Review Research* (Rapid Communication) 2, 022059(R) (2020).

78. A Two-Plateaus Li-Se Chemistry for High-Volumetric-Capacity Se Cathodes.
Xiaoqun Qi, Ying Yang, Qiang Jin, Fengyi Yang, Yong Xie, Pengfei Sang, Kun Liu, Wenbin Zhao, Xiaobin Xu, Yongzhu Fu, Jian Zhou, Long Qie[*], Yunhui Huang[*]
*Angewante Chemime International Edition* 59, 13908 (2020).

79. Toggling valley-spin locking and nonlinear optical properties of single-element multiferroic monolayers via light.
Yiming Pan, Jian Zhou[*]
*Physical Review Applied* 14, 014024 (2020).

80. Giant Photonic Response of Mexican-Hat Topological Semiconductors for Mid-Infrared to THz Applications.
Haowei Xu, Jian Zhou, Hua Wang, Ju Li[*]
*The Journal of Physics Chemistry Letters* 11, 6119 (2020).

81. Tailoring geometric phases of two-dimensional functional materials under light: a brief review.
Jian Zhou[*]
*International Journal of Smart & Nano Materials* (invited review) 11, 191 (2020).

82. Tunable charge density wave in a black/blue phosphorene lateral heterostructure: A first-principles calculation.
Yan Li, Hongwei Bao, Jian Zhou*, Fei Ma*
*Physical Review B* 102, 165308 (2020).

83. Terahertz optics-driven phase transition in two-dimensional multiferroics.
Jian Zhou*, Shunhong Zhang*
*npj 2D Materials & Applications* 5, 16 (2021).

84. Colossal switchable photocurrents in topological Janus transition metal dichalcogenides.
Haowei Xu, Hua Wang, Jian Zhou, Yunfan Guo, Jing Kong, Ju Li*
*npj Computational Materials* 7, 31 (2021).

85. Layer number dependent ferroelasticity in 2D Ruddlesden-Popper organic-inorganic hybrid perovskites.
Xun Xiao, Jian Zhou, Kepeng Song, Jingjing Zhao, Yu Zhou, Peter Rudd, Yu Han, Ju Li*, Jinsong Huang*
*Nature Communications* 12, 1332 (2021).

86. Terahertz Driven Reversible Topological Phase Transition of Monolayer Transition Metal Dichalcogenides.
Jian Zhou*, Haowei Xu, Yongliang Shi, Ju Li*
*Advanced Science* 8, 2003832 (2021).

87. Pure bulk orbital and spin photocurrent in two-dimensional ferroelectric materials.
Xingchi Mu, Yiming Pan, Jian Zhou*
*npj Computational Materials* 7, 61 (2021).

88. Boosting oxygen reduction activity and enhancing stability through structural transformation of layered lithium manganese oxide.
Xuepeng Zhong, M'hamed Oubla, Xiao Wang, Yangyang Huang, Huiyan Zeng, Shaofei Wang, Kun Liu, Jian Zhou, Lunhua He, Haihong Zhong, Nicolas Alonso-Vante, Chin-Wei Wang, Wen-Bin Wu, Hong-Ji Lin, Chien-Te Chen, Zhiwei Hu*, Yunhui Huang*, Jiwei Ma*
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89. Light-induced static magnetization: nonlinear Edelstein effect.
Haowei Xu, Jian Zhou, Hua Wang, Ju Li*
*Physical Review B* 103, 205417 (2021).

90. Light-induced quantum anomalous Hall effect on the 2D surfaces of 3D topological insulators.
Haowei Xu, Jian Zhou, Ju Li*
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91. Pure spin photocurrent in non-centrosymmetric crystals: bulk spin photovoltaic effect.
Haowei Xu, Hua Wang Jian Zhou, Ju Li*
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92. Uranium In Situ Electrolytic Deposition with a Reusable Functional Graphene-Foam Electrode.
Chao Wang*, Ahmed S. Helal, Ziqiang Wang, Jian Zhou, Xiahui Yao, Zhe Shi, Yang Ren, Jinhyuk Lee, Jeng-Kuei Chang, Bunshi Fugetsu, Ju Li*
*Advanced Materials* 33, 2102633 (2021).

93. Designing stable *closo*-$B_{12}$ dianions in silico for Li- and Mg-ion battery applications.
Jianzhi Xu[=], Mengyang Li[=], Song Xu, Gerui Pei, Chuncai Kong, Xueguang Ren, Zhimao Yang, Tao Yang*, Jian Zhou*, Gao-Lei Hou*
*Inorganic Chemistry Frontiers* 8, 5201 (2021).

94. Coherence control of directional nonlinear photocurrent in spatially symmetric systems.
Yongliang Shi, Jian Zhou*
*Physical Review B* 104, 155146 (2021).

95. A Multiferroic Iron Arsenide Monolayer.
Xiaoyu Xuan, Tingfan Yang, Jian Zhou, Zhuhua Zhang*, Wanlin Guo
*Nanoscale Advances* 4, 1324 (2022).

96. Photo-magnetization in two-dimensional sliding ferroelectrics.
Jian Zhou*
*npj 2D Materials & Applications* 6, 15 (2022).

97. Screening transition metal-based polar pentagonal monolayers with large piezoelectricity and shift current.
Yaguang Guo, Jian Zhou, Huanhuan Xie, Yanyan Chen, Qian Wang*
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98. A $\pi$-Conjugated Polyimide-Based High-Performance Aqueous Potassium-Ion Asymmetric Supercapacitor.
Yaoyao Zhao$^{=}$, Shicong Zhang$^{=}$, Shumao Xu$^{=}$, Xiao Li, Yifan Zhang, Yang Xu, Jian Zhou, Hui Bi*, Fuqiang Huang*, Tianquan Lin*
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99. Tailoring photoinduced nonequilibrium magnetizations in $In_2Se_3$ bilayers.
Yan Sun, Xingchi Mu, Qianqian Xue, Jian Zhou*
*Advanced Optical Materials* 10, 2200428 (2022).

100. On-demand quantum spin Hall insulators controlled by two-dimensional ferroelectricity.
Jiawei Huang, Xu Duan, Sunam Jeon, Youngkuk Kim, Jian Zhou, Jian Li*, Shi Liu*
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101. Synergetic ligand and size effects of boron cage based electrolyte in Li-ion battery.
Xiao Li, Tao Yang*, Jian Zhou*
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102. Anisotropic terahertz optostriction in group-IV monochalcogenide compounds.
Kun Liu, Jian Zhou*
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103. Rational Design of Endohedral Superhalogens without Using Metal Cations and Electron Counting Rules.
Qianqian Xue, Mingmin Zhong*, Jian Zhou*, Puru Jena
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104. Optical generation and electric control of pure spin photocurrent in ferroelectric Ruddlesden-Popper perovskite $(MA)_2Pb(SCN)_2I_2$ monolayer.
Yue Zhao, Xingchi Mu, Gaoyang Gou*, Jian Zhou*, Xiaoli Lu, Yue Hao*
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105. Toward Room-temperature Electrical Control of Magnetic Order in Multiferroic van der Waals Materials.
Chengxi Huang, Jian Zhou, Huasheng Sun, Fang Wu, Yusheng Hou*, Erjun Kan*
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Chunmei Zhang[=,*], Hanqi Pi[=], Liqin Zhou[=], Si Li, Jian Zhou, Aijun Du, Hongming Weng[*]
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107. Designing inorganic semiconductors with cold-rolling processability.
Xu-Dong Wang[=], Jieling Tan[=], Jian Ouyang, Hangming Zhang, Jiang-Jing Wang, Yuecun Wang, Volker L. Deringer, Jian Zhou, Wei Zhang[*], En Ma[*]
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108. Photoinduced Rippling of Two-Dimensional Hexagonal Nitride Monolayers.
Kun Liu, Sheng Mao, Shunhong Zhang, Jian Zhou[*]
*Nano Letters* 22, 9006 (2022).

109. Tailoring Bulk Photovoltaic Effects in Magnetic Sliding Ferroelectric Materials.
Chunmei Zhang, Ping Guo, Jian Zhou[*]
*Nano Letters* 22, 9297 (2022).

110. Carrier driven magnetic and topological phase transition in two-dimensional III-V semiconductors.
Yan Li, Xinru Ma, Hongwei Bao, Jian Zhou[*], Fei Ma[*], Jingbo Li[*]
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111. Magnetic proximity enabled bulk photovoltaic effects in van der Waals heterostructures.
Xingchi Mu, Qianqian Xue, Yan Sun, Jian Zhou[*]
*Physical Review Research* 5, 013001 (2023).

112. Renormalizing Antiferroelectric Nanostripes in $\beta'$-$In_2Se_3$ via Optomechanics.
Zihang Wu, Kun Liu, Xingchi Mu, Jian Zhou[*]
*The Journal of Physical Chemistry Letters* 14, 677 (2023).

113. A general thermodynamics-triggered competitive growth model to guide the synthesis of two-dimensional nonlayered materials.
Zijing Zhao[=], Zhi Fang[=], Xiaocang Han[=], Shiqi Yang, Cong Zhou, Yi Zeng, Biao Zhang, Wei Li, Zhan Wang, Ying Zhang, Jian Zhou, Jiadong Zhou, Yu Ye, Xinmei Hou, Xiaoxu Zhao[*], Song Gao, Yanglong Hou[*]
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114. Shift current response in elemental two-dimensional ferroelectrics.
Zhuang Qian, Jian Zhou, Hua Wang, Shi Liu[*]
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115. Spin glass behavior in amorphous $Cr_2Ge_2Te_6$ phase-change alloy.
Xiaozhe Wang[=], Suyang Sun[=], Jiang-Jing Wang[*], Shuang Li, Jian Zhou, Oktay Aktas, Ming Xu, Volker L. Deringer, Riccardo Mazzarello, En Ma, Wei Zhang[*]
*Advanced Science* 10, 2302444 (2023).

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Qianqian Xue, Xingchi Mu, Yan Sun, Jian Zhou[*]
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117. Vibrational-anharmonicity-assisted phase transitions in perovskite oxides under terahertz irradiation.
Cong Zhou, Jian Zhou[*]
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Youxuan Wu[=], Shiyuan Wang[=], Chuoqi Chen, Cong Zhou, Kun Chen, Jian Zhou, Zhi Wang, Ya-Qing Bie[*], Shaozhi Deng
*Advanced Optical Materials* 12, 2301747 (2024).

119. $d_z^2$ Band Links Frontier Orbitals and Charge Carrier Dynamics of Single-Atom Cocatalyst-Aided Photocatalytic $H_2$ Production.
Yiwei Fu[=], Kejian Lu[=], Anlan Hu, Jie Huang, Liejin Guo, Jian Zhou, Jin Zhao, Oleg V. Prezhdo*, Maochang Liu*
*Journal of the American Chemical Society* 145, 28166 (2023).

120. Collective octahedral tilting in ultrathin Ruddlesden-Popper perovskite under terahertz light.
Kun Liu, Jian Zhou*
*Applied Physics Letters* 124, 022902 (2024).

121. Driving and detecting topological phase transition in noncentrosymmetric systems via an all-optical approach.
Mengtong Yang, Xiaoyan Miao, Si Li, Jian Zhou*, Chunmei Zhang*
*Physical Review B* 109, 125101 (2024).

122. Current Induced Spin and Orbital Polarization in Magnetic Sliding Ferroelectrics.
Haoxiang Dong, Jian Zhou*
*Physica Status Solidi-Rapid Research Letters* 2400062 (2024).

123. Assembly-inspired multiferroicity with nontrivial Chern insulating phase from exohedral metallofullerenes.
Feiyang Huang, Mo Xiong, Jian Zhou*, Tao Yang*
*Journal of Chemical Physics* 160, 184302 (2024).

124. Light-Induced Topological Phase Transition with Tunable Layer Hall Effect in Axion Antiferromagnets.
Cong Zhou, Jian Zhou*
*Nano Letters* 24, 7311 (2024).

125. Bulk photovoltaic effects in helimagnets.
Chunmei Zhang, Hanqi Pi, Jian Zhou*
*Physical Review B* (Letter) 110, L041104 (2024).

126. Ionic Photovoltaics-in-Memory in van der Waals Material.
Dongyan Li[=], Zexin Li[=], Chen Pan[=], Yan Sun, Jian Zhou, Xingjian Yangdong, Xiang Xu, Lixin Liu, Haoyun Wang, Yunxin Chen, Xingyu Song, Pengbin Liu, Xing Zhou*, Shi-Jun Liang*, Feng Miao*, Tianyou Zhai*
*Advanced Materials* 36, 2406984 (2024).

127. In-Sublattice Carrier Transition Enabled Polarimetric Photodetectors with Reconfigurable Polarity Transition.
Dongyan Li[=], Zexin Li[=], Yan Sun, Jian Zhou, Xiang Xu, Haoyun Wang, Yunxin Chen, Xingyu Song, Pengbin Liu, Zhengtang Luo, Su-Ting Han, Xing Zhou*, Tianyou Zhai*
*Advanced Materials* 36, 2407010 (2024).

128. Nonlinear Optics-Driven Spin Reorientation in Ferromagnetic Semiconductors.
Qianqian Xue, Yan Sun, Jian Zhou*
*ACS Nano* 18, 24317 (2024).

129. Band-Edge Mixture Engineered Giant and Switchable Shift Current Generation.
Yue Gao, Mengtong Yang, Wenli Zou, Jian Zhou*, Chunmei Zhang*
*Nano Letters* 24, 12560 (2024).

130. Quasi-Solid-State Conversion with Fast Redox Kinetics Enabled by A Sulfonamide-Based Electrolyte in Li-Organic Batteries.

Huang Cai, Xinke Cui, Yonghao Shi, Yuxin Zhang, Xinran Chen, Linghan Fan, Jian Zhou, Chuanjin Tian*, Weijiang Xue*
*ACS Nano* 18, 32723 (2024).

131. 20-electron exohedral alkaline-earth-metallofullerenes $M(C_{60})_3$ ($M$ = Ca, Sr, Ba).
Feiyang Huang, Jian Zhou*, Tao Yang*
*Physical Chemistry Chemical Physics* 26, 29475 (2024).

132. Light-induced pure spin transportation in twisted atomic wires of transition metal trichalcogenides.
Chanjuan Shang, Haoxiang Dong, Yanyan Zhao, Wei Pei, Jijun Zhao, Jian Zhou*, Si Zhou*
*Physical Review B* 110, 235428 (2024).

133. Nonvolatile Ferroic and Topological Phase Control under Nonresonant Light.
Jian Zhou*, Hanli Cui
*The Journal of the Physical Chemistry Letters* (invited Perspective) 16, 222 (2025).

134. Ultrafast Photocurrent Hysteresis in Photoferroelectric $\alpha$-$In_2Se_3$ Diagnosed by Terahertz Emission Spectroscopy.
Zhen Lei, Jiawei Chang, Qiyi Zhao, Jian Zhou, Yuanyuan Huang*, Qihua Xiong*, Xinlong Xu*
*Science Advances* 11, eads8786 (2025).

135. Prediction of high Chern number and bulk photovoltaic current in Janus $1T'$ transition metal dichalcogenides under circularly polarized light.
Xiantuo Zhao, Hong Wang, Jian Zhou*
*Physica Status Solidi-Rapid Research Letters* 19, 2500014 (2025).

136. 2D edge-seeded heteroepitaxy of ultrathin high-$\kappa$ dielectric textCaNb$_2$O$_6$ for 2D field-effect transistors.
Xiulian Fan$^=$, Jiali Yi$^=$, Bin Deng, Cong Zhou, Zejuan Zhang, Jia Yu, Weihan Li, Cheng Li, Guangcheng Wu, Xilong Zhou, Tulai Sun, Yihan Zhu, Jian Zhou, Juan Xia, Zenghui Wang, Keji Lai, Zheng Peng, Dong Li*, Anlian Pan*, Yu Zhou*
*Nature Communications* 16, 2585 (2025).

137. Unraveling phase transformation with phononic hyperbolicity using off-resonant terahertz light.
Hanli Cui, Jian Zhou*
*Physical Review Materials* 9, 034602 (2025).

138. Valley-dependent giant orbital moments and transport features in rhombohedral graphene multilayers.
Xingchi Mu, Jian Zhou*
*Physical Review B* 111, 165102 (2025).
Selected as Editors' Suggestion

139. Contrasting Light-Induced Spin Torque in Antiferromagnetic and Altermagnetic Systems.
Jian Zhou*, Chunmei Zhang*
*Physical Review Letters* 134, 176902 (2025).

140. Reversing Néel Vector in Parity-Time Antiferromagnets by Nonreciprocal Light Scattering.
Qianqian Xue, Jian Zhou*
*Nano Letters* 25, 9054 (2025).

141. Achieving High-Yield Conversion of Janus Transition Metal Dichalcogenides on Diverse Substrates.
Xueqiu Zheng$^=$, Kunyan Zhang$^=$, Xiantuo Zhao, Jian Zhou, Hongzhi Shen, Jing Kong, Yunfan Guo*
*ACS Nano* 19, 20744 (2025).

142. Pure spin and orbital bulk photovoltaic effect in topological screw dislocations.
Mengtong Yang, Chunmei Zhang*, Jian Zhou*
*Physical Review B* 112, 035152 (2025).

143. Nonresonant Raman control of ferroelectric polarization.
Jiaojian Shi*, Christian Heide, Haowei Xu, Yuejun Shen, Meredith Henstridge, Isabel Sedwick, Anudeep Mangu, Xinyue Peng, Shangjie Zhang, Mariano Trigo, Tony F. Heinz, Ju Li, Keith A. Nelson, Edoardo Baldini, Jian Zhou, Shambhu Ghimire, David A. Reis, Aaron M. Lindenberg*
*Advanced Materials* 37, e10524 (2025).

144. Layer-dependent disorder controlling shift current generation in two-dimensional centrosymmetric systems.
Yiwei Zhao, Xiantuo Zhao, Chunmei Zhang, Jian Zhou*
*Physical Review B* 112, 115112 (2025).

145. Recent Advances of Bulk Photovoltaic Effect in Exotic Quantum Materials: Progress and Challenges.
Yiwei Zhao, Qianqian Xue, Xingchi Mu, Hanli Cui, Jian Zhou*
*Advanced Materials* (invited review) 38, e17783 (2026).

146. Strain-modulated bulk photovoltaic effect in negative piezoelectrics.
Yue Gao, Jian Zhou*, Chunmei Zhang*
*Frontiers of Physics* 21, 125204 (2026).

147. Magnetic precession induced spin accumulation in collinear antiferromagnets.
Qianqian Xue, Jian Zhou*
*Physical Review B* 113, 214425 (2026).

148. Light-Driven Ferroic Switching Enables Reversible Control of Hydrogen Adsorption Thermodynamics.
Xueqing Wan, Zhenlong Zhang, Charles Paillard, Jian Zhou, Jinyang Ni*, Chuanlu Yang*, Zhijun Jiang*, Laurent Bellaiche
*Nano Letters* in press (2026).

## XIII. Invited Talks at Conferences

| | | |
|---|---|---|
| 2016.11 | APS Southeast Section Meeting | Charlottesville, USA |
| 2018.03 | International Conference on Low-Dimensional Quantum Materials | Snowbird, USA |
| 2019.07 | The 10th General Conference of the Asian Consortium on Computational Materials Science (ACCMS-10) | Hong Kong |
| 2019.08 | The 6th Int'l Conference on Condensed Matter & Materials Physics | Xi'an, China |
| 2019.09 | 中国物理大会-2019，M 计算物理 | 郑州 |
| 2019.1 | The 5th International Conference on 2D Materials and Technology (ICON-2DMAT 2019) | Suzhou, China |
| 2019.11 | 第二届先进结构材料实验设计和计算模拟论坛 | 成都 |
| 2019.11 | The 10th International Symposium on Clusters and Nanomaterials (ISCAN-10) (declined) | Richmond, USA |
| 2019.11 | 西安交大物质科学计算研讨会 | 西安 |
| 2020.08 | 第一届西安交大-南科大材料学院双边论坛 | 西安 |
| 2020.12 | 东南地区物理力学青年学者论坛 (declined) | 广州 |
| 2021.07 | 中国材料大会，Z 计算材料 | 厦门 |
| 2021.07 | 第十三届计算纳米科学与新能源材料国际研讨会 | 呼和浩特 |
| 2021.07 | 首届微纳米表征与测量研讨会 | 成都 |

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|---|---|---|
| 2021.09 | 中国物理大会-2021，M 计算物理 (online) | 兰州 |
| 2021.1 | The 10th International Conference on Advanced Fibers and Polymer Materials | Shanghai, China |
| 2021.11 | 2021 IEEE The 9th International Conference on Information, Communication and Networks | Xi'an, China |
| 2021.11 | 北京高精尖论坛 | 北京 |
| 2021.12 | 2021 材料微观量子特性与计算凝聚态物理研讨会 | 重庆 |
| 2022.08 | 2021 先进结构材料实验设计与计算模拟论坛 | 太原 |
| 2022.07 | 第二届计算纳米科学与新能源材料（线上）国际研讨会 (declined) | 西安 |
| 2022.08 | 第三届团簇科学与原子制造研讨会 | 太原 |
| 2022.1 | The 13th APCTP Workshop on Multiferroics | Nanjing, China |
| 2023.04 | 第四届团簇科学与原子制造研讨会 | 西安 |
| 2023.05 | 第四届半导体青年学术会议 | 上海 |
| 2023.05 | 生命健康交叉研究论坛 | 武汉 |
| 2023.07 | 中国材料大会，Z-材料的模拟计算 | 深圳 |
| 2023.07 | 第十四届计算纳米科学与新能源材料国际研讨会 | 西安 |
| 2023.07 | The International Symposium on Computational Structure Prediction and Advanced Materials 2023 | Xi'an, China |
| 2023.08 | 中国物理大会-2023，M 计算物理 | 银川 |
| 2023.1 | 全国凝聚态理论与统计物理学术会议 | 济南 |
| 2023.11 | The 13th Asian Meeting on Ferroelectrics; The 13th Asian Meeting on Electroceramics | Macau, China |
| 2023.12 | 第十九届全国电介质物理、材料与应用学术会议 | 南京 |
| 2023.12 | The First International Workshop on Materials Frontiers | Zhuhai, China |
| 2024.03 | Materials for Green Future (keynote) | Phuket, Thailand |
| 2024.04 | 第八届全国磁性材料与器件大会 | 杭州 |
| 2024.06 | 第十八届全国磁学理论会议 | 成都 |
| 2023.07 | 中国材料大会，D02-多铁性材料；Z-材料的模拟计算；D38-无机光电功能材料 | 广州 |
| 2024.09 | The 22nd International Conference on Ternary and Multinary Compounds (ICTMC-22) | Beijing, China |
| 2024.1 | The 8th International Conference on Electronic Materials and Nanotechnology for Green Environment (declined) | Jeju, Korea |
| 2024.11 | 第五届半导体青年学术会议 | 武汉 |
| 2024.11 | 第十五届计算纳米科学与新能源材料国际研讨会 | 福州 |
| 2025.05 | 中国化学会第一届全国表界面科学会议 | 成都 |
| 2025.05 | The 11th General Conference of the Asian Consortium on Computational Materials Science (ACCMS-11) | Yokohama, Japan |
| 2025.07 | 中国材料大会，D54-超晶格材料；Z-材料的模拟计算 | 厦门 |
| 2025.07 | 第十九届全国磁学理论会议 | 呼和浩特 |
| 2025.07 | 中国物理大会，磁学分会 | 哈尔滨 |
| 2025.12 | 非平衡态开放系统物理研讨会 | 杭州 |
| 2026.03 | APS Summit Meeting at Hong Kong | Hong Kong |
| 2026.06 | 第十七届计算纳米科学与新能源材料国际研讨会 | 昆明 |
| 2026.07 | 中国材料大会，Z-材料的模拟计算 | 武汉 |
| 2026.07 | 2026 中国扫描探针显微学大会（ChinaSPM 2026）暨第三届先进材料及量子科学国际研讨会（3rd AMQS） | 乌鲁木齐 |