# 贾帆豪

上海大学,材料科学与工程学院,博士后

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## 简介:

致力于功能材料基态或激发态的几何和电子结构性质预测和物性机理探索。应用密度泛函理论和量子多体微扰等计算方法,提出基于有机无机杂化钙钛矿实现长自旋寿命的柔性自旋电子学基础材料,收到PRL、AM等期刊的高质量引用;证明了用随机相近似精确描述关联能可以极大地提升对复杂氧化的铁电相关性质的预测精度;揭示了少层极性钙钛矿氧化物广泛存在的电子结构、电荷序和局域模式的基础特征;提出了一系列室温多铁二维材料。近五年发表论文31篇,被SCI检索27篇,被SCI引用380余次,H-index: 10;其中,一区论文7篇,封面论文1篇,高被引论文1篇。以第一作者或通讯作者分别在Materials Today Physics (IF 11.021, 1篇)、The Journal of Physical Chemistry Letters (IF 6.888, 封面)、Journal of Materials Chemistry C (IF 8.067, 1篇)、Physical Review B (IF 4.036, 3篇)、Physical Review Materials (IF 3.989, 1篇)等国际物理、材料领域期刊上发表工作。以访问学者方式先后在维也纳大学VASP开发组、香港大学和纽约州立大学布法罗分校物理系进行国际合作交流。曾获得国际晶体学会"2017年青年科学家奖",曾作为中国大陆25名青年学者之一参加"第69届林岛诺贝尔奖获得者大会"。申请发明专利1项。担任Applied Physics Letters等期刊审稿人。

#### 教育经历:

- (1) 2016-09 至 2021-06, Shanghai University, Condensed Matter Physics, 博士
- (2) 2012-09 至 2016-06, Zhejiang Normal University, Physics, 学士

### 博士后工作经历:

(1) 2021-07 至 2023-12, 在站, Shanghai University

#### 科研与学术工作经历:

- (1) 2019-11 至 2021-04, State University of New York at Buffalo, Department of Physics, with Prof. Peihong Zhang, 访问学者
- (2) 2018-03 至 2018-08, The University of Hong Kong, Department of Physics, with Prof. Jian Wang, 研究助理
- (3) 2017-11 至 2018-01, University of Vienna, Department of Physics, with Prof. Georg Kresse and Prof. Cesare Franchini, 访问学者

### 近五年主持或参加的国家自然科学基金项目/课题:

- (1) 国家自然科学基金委员会,面上项目,12074241,自旋耦合极化材料的电子结构设计和量子调控,2021-01-01 至 2024-12-31,62万元,在研,参与
- (2) 国家自然科学基金委员会,青年科学基金项目,11804216,基于二维磁性半导体的范

德华异质结的密度泛函理论研究, 2019-01-01 至 2021-12-31, 26万元, 结题, 参与

## 近五年主持或参加的其他科研项目/课题(国家自然科学基金项目除外):

(1) 鸿之微科技(上海)股份有限公司, 横向项目, 锂电关键材料数据库平台建设, 2021-09-01至 2022-12-31, 48万, 在研, 主持

#### 研究成果和学术奖励情况

## 一、论文列表(一作或通讯)

- [1] **Fanhao Jia**, Shunbo Hu\*, Shaowen Xu, Heng Gao, Guodong Zhao, P. Barone, A. Stroppa\*, and Wei Ren\*, Persistent Spin-Texture and Ferroelectric Polarization in 2D Hybrid Perovskite Benzylammonium Lead-halide. *J. Phys. Chem. Lett.*, 2020, 11(13): 5177-5183.
- [2] **Fanhao Jia**, Shaowen Xu, Guodong Zhao, C. Liu, and Wei Ren\*, Structural and Electronic Properties of Two-dimensional Freestanding BaTiO<sub>3</sub>/SrTiO<sub>3</sub> Heterostructures. *Phys. Rev. B*, 2020, 101(14): 144106.
- [3] **Fanhao Jia**, Georg Kresse, Cesare Franchini, Peitao Liu, Jian Wang, Alessandro Stroppa\*, Wei Ren\*, Cubic and Tetragonal Perovskites from The Random Phase Approximation. *Phys. Rev. Mater.*, 2019, 3(10): 103801.
- [4] **Fanhao Jia**, Yuting Qi, Shunbo Hu, Tao Hu, Musen Li, Guodong Zhao, Jihua Zhang, Alessandro Stroppa, Wei Ren\*, Structural Properties and Strain Engineering of a BeB<sub>2</sub> Monolayer from First-principles. *RSC Adv.*, 2017, 7(61): 38410-38414.
- [5] **贾帆豪**, 陈姝, 郝锐杰, 许少文, 任伟\*.钛酸盐 ATiO<sub>3</sub> 钙钛矿的铁电和反铁畸变. **低温物 理学报**, 2019, (2):88-96.
- [6] Shaowen Xu, Fanhao Jia\*, Xing Yu, Shunbo Hu, Heng Gao\*, Wei Ren\*, Intrinsic Multiferroic MnOF Monolayer with Room-Temperature Ferromagnetism. *Mater. Today Phys.*, 2022, 100775.
- [7] Shaowen Xu, **Fanhao Jia**\*, Xuli Cheng, Wei Ren\*, Predicting Intrinsic Antiferromagnetic and Ferroelastic MnF<sub>4</sub> Monolayer with Controllable Magnetization. *J. Mater. Chem. C*, 2021, 9(47): 17152-17157.
- [8] Xuli Cheng, Shaowen Xu, **Fanhao Jia**\*, Guodong Zhao, Minglang Hu, Wei Wu, and Wei Ren\*, Intrinsic Ferromagnetism with High Curie Temperature and Strong Anisotropy in a Ferroelastic VX monolayer (X= P, As). *Phys. Rev. B*, 2021, 104, 104417.
- [9] Jing Ni, Shunbo Hu\*, Musen Li, **Fanhao Jia\***, Guanhua Qin, Qiang Li, Zimo Zhou, Fangxing Zha\*, Wei Ren, Yin Wang, Accurate Band Offset Prediction of the  $Sc_2O_3/GaN$  and  $\theta$ -Al<sub>2</sub>O<sub>3</sub>/GaN Heterojunctions using Dielectric Dependent Hybrid Functional. *ACS Appl. Electron. Mater.*, 2022, 4, 6, 2747–2752.
- [10] Qinghe Zheng, Chao Liu, Heng Gao, **Fanhao Jia\***, Jisang Hong, Tao Hu\*, Zhongming Ren, Wei Ren\*, Ordered and Disordered Two-dimensional Tellurium-selenium Binary Compounds from Swarm Intelligence and First principles. *Mater. Today Commun.*, 2022, 31: 103409.
- [12] 焦志翔, **贾帆豪\***, 王永晨, 陈建国, 任伟, 程晋荣\*, 基于机器学习的 BiFeO<sub>3</sub>-PbTiO<sub>3</sub>-BaTiO<sub>3</sub> 固溶体居里温度预测. *无机材料学报*, 2022 (accepted)

- [13] W. Yao, Shunbo Hu\*, **Fanhao Jia**\*, J. R Reimers, Y. Wang, D. J. Singh, and Wei Ren\*. Lattice Strain and Band Overlap of The Thermoelectric Composite Mg<sub>2</sub>Si<sub>1-x</sub>Sn<sub>x</sub>. *Phys. Rev. B*, 2022 (accepted)
- [14] Shaowen Xu<sup>†</sup>, **Fanhao Jia**<sup>†</sup>, Shunbo Hu, Athinarayanan Sundaresan, Nikita V Ter-Oganessian, Alexander P Pyatakov, Jinrong Cheng, Jincang Zhang, Shixun Cao, Wei Ren\*, Predicting the Structural, Electronic and Magnetic Properties of Few Atomic-Layer Polar Perovskite. *Phys. Chem. Chem. Phys.*, 2021, 23, 5578-5582.
- [15] Shaowen Xu, **Fanhao Jia\***, Guodong Zhao, Tao Hu, Shunbo Hu, Wei Ren\*, Tunable Magnetism and Insulator-Metal Transition in Bilayer Perovskites. *J. Phys. Chem. C*, 2021, 125(11), 6157–6162.

## 二、论文列表(共同作者)

- [1] Yabei Wu, Zhao Tang, Weiyi Xia, Weiwei Gao, **Fanhao Jia**, Yubo Zhang, Wenguang Zhu, Wenqing Zhang\*, Peihong Zhang\*. Prediction of protected band edge states and dielectric tunable quasiparticle and excitonic properties of monolayer MoSi<sub>2</sub>N<sub>4</sub>. *NPJ Comput. Mater.*, 2022, 8(1): 1-7.
- [2] Yongchen Wang, Fanhao Jia, Zhixiang Jiao, Jie Jian, Jianguo Chen, Yan Wang, Jinrong Cheng\*, Enhanced Insulation and Piezoelectric Properties of 0.57(Bi<sub>0.8</sub>La<sub>0.2</sub>)FeO<sub>3</sub>-0.43PbTiO<sub>3</sub> Solid Solutions with Fe Addition. *J. Am. Ceram. Soc.* 2022, 105(10): 6302-6310.
- [3] Zhao Tang, Greis J. Cruz, Yabei Wu, Weiyi Xia, **Fanhao Jia**, Wenqing Zhang, Peihong Zhang Giant Narrow-Band Optical Absorption and Distinctive Excitonic Structures of Monolayer C<sub>3</sub>N and C<sub>3</sub>B. *Phys. Rev. Appl.*, 2022, 17(3): 034068.
- [4] Yanna Chen, Osami Sakata, Hiroyuki Morita, Akifumi Matsuda, **Fanhao Jia**, Okkyun Seo, Loku Singgappulige Rosantha Kumara, Toshiaki Ina, Eiichi Kobayashi, Jaemyung Kim, Chulho Song, Satoshi Hiroi, Natalia Palina, Yanfang Lou, Wei Ren, Mamoru Yoshimoto, Electronic States of Gallium Oxide Epitaxial Thin Films and Related Atomic Arrangement. *Appl. Surf. Sci.*, 2022, 578: 151943.
- [5] Bing Luo, Xiaonan Ma, Junjie Liu, Wei Wu, Xing Yu, Shunbo Hu, Heng Gao, **Fanhao Jia**, Wei Ren, Enhanced Photogalvanic Effect in a 2D Ferroelectric ZrI<sub>2</sub> by Interlayer Sliding. *Physica E Low Dimens. Syst. Nanostruct.*, 2022, 142: 115297.
- [6] Shaowen Xu, **Fanhao Jia**, Guodong Zhao, Wei Wu, Wei Ren\*, A Two-dimensional Ferroelectric Ferromagnetic Half Semiconductor in a VOF Monolayer. *J. Mater. Chem. C*, 2021, 9, 9130-9136
- [7] Gabriel Lopez-Candales, Zhao Tang, Greis J Cruz, Weiyi Xia, Fanhao Jia, Peihong Zhang. Quasiparticle Band Structures of the 4d Perovskite Oxides SrZrO<sub>3</sub> and BaZrO<sub>3</sub>. *Phys. Rev. B*, 2021, 104(19): 195129.
- [8] Gabriel Lopez-Candales, Zhao Tang, Weiyi Xia, **Fanhao Jia**, Peihong Zhang\*, Quasiparticle Band Structure of SrTiO<sub>3</sub> and BaTiO<sub>3</sub>: A Combined LDA+U and G<sub>0</sub>W<sub>0</sub> Approach. *Phys. Rev. B*, 2021, 103(3): 035128.
- [9] Guo-Dong Zhao, Xingen Liu, Tao Hu, **Fanhao Jia**, Yaning Cui, Wei Wu, Myung-Hwan Whangbo, Wei Ren\*, Difference in Magnetic Anisotropy of the Ferromagnetic Monolayers VI<sub>3</sub> and CrI<sub>3</sub>. *Phys. Rev. B*, 2021, 103(1): 014438.

- [10] 许少文, **贾帆豪**, 乔磊, 任伟\*, 稀土六硼化物的研究进展. *中国材料进展*, 2020, (2):124-132.
- [11] Shaowen Xu, **Fanhao Jia**, Yali Yang, Lei Qiao, Shunbo Hu, David J Singh, Wei Ren\*, Interplay of Electronic, Magnetic, and Structural Properties of GdB<sub>6</sub> from First Principles. *Phys. Rev. B*, 2019, 100(10): 104408.
- [12] Kangying Wang, Tao Hu, **Fanhao Jia**, Guodong Zhao, Yuyu Liu, Igor V Solovyev, Alexander P Pyatakov, Anatoly K Zvezdin, Wei Ren\*, Magnetic and Electronic Properties of Cr<sub>2</sub>Ge<sub>2</sub>Te<sub>6</sub> Monolayer by Strain and Electric-field Engineering. *Appl. Phys. Lett.*, 2019, 114(9): 092405.
- [13] Tao Hu, **Fanhao Jia**, Guodong Zhao, Jiongyao Wu, Alessandro Stroppa, Wei Ren\*, Intrinsic and Anisotropic Rashba Spin Splitting in Janus Transition-metal Dichalcogenide Monolayers. *Phys. Rev. B*, 2018, 97(23): 235404.
- [14] Yabei Wu, Weiyi Xia, Weiwei Gao, **Fanhao Jia**, Peihong Zhang\*, Wei Ren\*, Quasiparticle Electronic Structure of Honeycomb C<sub>3</sub>N: from Monolayer to Bulk. *2D Mater.*, 2018, 6(1): 015018.
- [15] Brendan J Kennedy, Qingdi Zhou, Shipeng Zhao, **Fanhao Jia**, Wei Ren\*, Kevin S Knight\*, Low-temperature Structure and The Ferroelectric Phase Transitions in The CdTiO<sub>3</sub> Perovskite. *Phys. Rev. B*, 2017, 96(21): 214105.
- [16] Shunbo Hu, **Fanhao Jia**, Cornelia Marinescu, Fanica Cimpoesu, Yuting Qi, Yongxue Tao, Alessandro Stroppa\*, Wei Ren\*, Ferroelectric Polarization of Hydroxyapatite from Density Functional Theory. *RSC Adv.*, 2017, 7(35): 21375-21379.

#### 三、论著之外的代表性研究成果和学术奖励、邀请报告

- (1) 程 晋 荣; 焦 志 翔; 贾 帆 豪; 一 种 新 型 四 元 系 压 电 陶 瓷, 2022-05-31, 中 国, CN202210162927.X (专利)
- (2) 2019-6-30至2019-7-5,参加第69届诺贝尔奖物理学获得者大会,德国林岛,会议共汇聚了28位诺贝尔物理学奖得主、9位诺贝尔化学奖得主以及2位图灵奖得主,另外还有来自89个不同国家和地区共580位优秀的青年学者,其中中国大陆入选25名(会议)
- (3) 贾帆豪;国际晶体学会青年科学家奖(2017年), IUCr Journals (奖励)
- (4) Electronic Behavior of Few-Layer Ferroic Perovskites, 国际纳米技术与材料大会(2022,中国,厦门)(学术报告)