邵　和　助

现任：温州大学电气与电子工程学院 副教授，硕士生导师.
Email: hzshao@wzu.edu.cn, 电话：0577-86590870,
地址: 浙江省温州市温州大学电气与电子工程学院, 325035.

工作经历

- 2010.4 – 2013.3 博士后，复旦大学物理流动站.
- 2013.3 – 2015.5 博士后，中国科学院宁波材料技术与工程研究所.
- 2015.5 – 2016.12 助理研究员，中国科学院宁波材料技术与工程研究所.
- 2016.12 – 2019.6 副研究员，中国科学院宁波材料技术与工程研究所.
- 2019.6 至今　副教授，温州大学电气与电子工程学院.

学位情况

- 07.01.2002　工学学士，微电子学，上海大学.
- 06.27.2006　理学硕士，光学，复旦大学.
- 04.28.2010　理学博士，无线电物理学，上海大学.

简介

- 近年来主要从事材料物理、化学性质的第一性原理计算研究，关注热电，储能，二维，拓扑等材料体系，与国内外多个课题组开展广泛而深入的合作。
- 已承担国家自然科学基金青年基金、浙江省自然科学基金、中国博士后基金、浙江省博士后科研择优项目、宁波市自然科学基金、温州市科技局工业项目等，参与国家自然科学基金面上基金、浙江省重点研发计划、宁波市2025重大科技创新等项目。
- 已在 Nature Commun.、Adv. Func. Mater.、ACS Nano、Phys. Rev. B、Mater. Today Phys.、J. Phys. Chem. Lett.、J. Mater. Chem. C 等期刊发表 SCI 论文 100 余篇，H-index 45，入选 2019 年度英国皇家化学会材料领域 “Top 1% 高被引中国作者”，2023 年获选国际先进材料协会会士(Fellow of IAAM)。
- 担任 Chemical Reviews、Adv. Mater.、Chem. Sci.、Nano Energy、J. Mater. Chem. A、J. Mater. Chem. C、ACS Applied Materials & Interfaces、J. Phys. Condens. Matter. 等期刊审稿人。

欢迎报考

欢迎物理、数学、计算机类专业本科生报考本课题组研究生。来这里你将经历：

- **能力培养**：科研方法的培养和科研习惯的建立，文献搜索、论文写作、口头汇报等能力的培养。
- **如何面对失败**：失败是科研活动中的常事，经历这些失败和打击之后，你会成长起来，比之前的自己强大和自信。
- **如何面对成功**：在这里你也可能会有新的发现，有若干创新的成果可以发表出来，那时候，世界会重新认识你，你也需要重新认识你自己；但记住，请保持低调，因为你的新成果很快就会被别人超越，这也是科研活动中的常事，因此不必自我膨胀或失落。

课题组文化

- **诚信**：不能弄虚作假。
- **劳动**：承担必要的日常服务，比如打扫实验室，日常报销等。
- **感恩**：尊重他人的时间和劳动。
- **合作**：共享技术，不对团队成员有保留。
- **竞争**：放眼世界，对于团队成员取得的成绩要羡慕而不要嫉妒，不和自己过不去，你们面对的是来自世界的竞争。

工作思路

- **基本思路**：重视学科基础，拓展计算技术，做以需求为牵引的科研。
- **研究方向**：材料电子、声子输运、材料高通量计算、基于机器学习的材料基因工程、基于神经演化方法的力场开发、具第一性原理精度的微纳器件模拟、以及相关计算程序的开发。
- **愿景**：积极拥抱新科技、学习新技术；努力在经营的领域往下扎根、向上结果。

论文发表

2024

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- 2. Ying Fang, **Hezhu Shao***, Wenzhou TE: AFirst-Principle-Calculated Thermoelectric Materials Database, Materials, **17**, 2200, 2024.

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- 1. **Hezhu Shao***, Daquan Ding, Ying Fang, Wei Song, Jielan Huang, Changkun Dong, and Hao Zhang*, Phonon transport in Cu_2GeSe_3: Effects of spin-orbit coupling and higher-order phonon-phonon scattering, Phys. Rev. B. **107**, 085202 (2023).
- 2. Ben Li, Juan Zhang, Yujie Xia, Ke Xu, Lei Peng, **Hezhu Shao***, Rui Yu*, Zengxu Wang, Yuanfeng Xu, Heyuan Zhu, and Hao Zhang*, Magnetic field effects and excitonic selection rules in monolayer palladium diselenide as a large-gap quantum spin Hall insulator, Phys. Rev. B. **107**, 155401 (2023).
- 3. Siqi Lin, Linlin Guo, Xianghu Wang, Yue Liu, Yuying Wu, Rongbin Li, **Hezhu Shao***, Min Jin*, Revealing the promising near-room-temperature thermoelectric performance in Ag_2Se single crystals, J. Materiomics, **9**, 754 (2023).
- 4. Yujie Xia, Le Shu, Yiming Zhang, Ying Chen, Lei Peng, Juan Zhang, Ben Li, **Hezhu Shao***, Yan Cen, Zhan Sui, Heyuan Zhu*, and Hao Zhang*, Full-Landscape Condensation Phases for Long-Lived Excitons in

2D Tellurium: Crystal-Field Splitting and Finite-Momentum Excitons, Adv. Funct. Mater. **33**, 2303779 (2023).

- 5. Jiayue Xu, Yunfang Pan, Tian Tian*, Chengling Mao, Haiwei Feng, Yunfeng Ma, **Hezhu Shao***, Effective enhancement of light yield achieved in $Bi_4Si_3O_{12}$ scintillation single crystals by doping with tantalum ions, J. Alloys Compd. **960**, 170754 (2023).
- 6. Yujie Xia, Ao Wu, Ben Li, Juan Zhang, Yiming Zhang, Lei Peng, **Hezhu Shao***, Yan Cen, Zengxu Wang, Shangdong Liu, Yimu Ji, Zhan Sui, HeyuanZhu*, and Hao Zhang*, Spin?Orbit-Coupling-Induced Topological Transition and Anomalously Strong Intervalley Scattering in Two-Dimensional Bismuth Allotropes with Enhanced Thermoelectric Performances, ACS Appl. Mater. Interfaces **15**, 19545 (2023).

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- 1. **Hezhu Shao***, Daquan Ding, Li Zhang, Chang-Kun Dong, Hao Zhang*, Thermoelectric performance in a Si allotrope with ultralow thermal conductivity: a first-principles study combining phonon-limited electronic transport calculations, Mater. Today Phys. **27**, 100756 (2022).
- 2. Cong Wang, Yue-Xing Chen*, Guoying Gao, Ke Xu, **Hezhu Shao***, Theoretical investigations of Janus WSeTe monolayer and related van der Waals heterostructures with promising thermoelectric performance, Appl. Surf. Sci. **593**, 153402 (2022).
- 3. Xia Cai, Yiming Zhang, Zejiao Shi, Ying Chen, Yujie Xia, Anran Yu, Yuanfeng Xu, Fengxian Xie, **Hezhu Shao**, Heyuan Zhu, Desheng Fu, Yiqiang Zhan*, Hao Zhang*, Discovery of Lead-Free Perovskites for High-Performance Solar Cells via Machine Learning: Ultrabroadband Absorption, Low Radiative Combination, and Enhanced Thermal Conductivities, Adv. Sci. **4**, 2103648 (2022).
- 4. Yiming Zhang, Bowen Hou, Yu Wu, Ying Chen, Yujie Xia, Haodong Mei, Mingran Kong, Lei Peng, **Hezhu Shao**, Jiang Cao, Wenjun Liu*, Heyuan Zhu*, Hao Zhang*, Towards high-temperature electron-hole condensate phases in monolayer tetrels metal halides: Ultra-long excitonic lifetimes, phase diagram and exciton dynamics, Mater. Today Phys. **22**, 100604 (2022).
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- 6. Sien Wang, Xiaowei Lu, Ankit Negi, Jixiong He, Kyunghoon Kim, **Hezhu Shao**, Peng Jiang, Jun Liu* and Qing Hao*, Revisiting the Reduction of Thermal Conductivity in Nano- to Micro-Grained Bismuth Telluride: The Importance of Grain-Boundary Thermal Resistance, Eng. Sci., **17**, 45 (2022).

- 7. Zheng Chang, Jing Ma, Kunpeng Yuan, Jiongzhi Zheng, Bin Wei, Mohammed Al-Fahdi, Yufei Gao, Xiaoliang Zhang*, **Hezhu Shao***, Ming Hu* and Dawei Tang*, Zintl Phase Compounds $Mg_3Sb_{2-x}Bi_x$ (x = 0, 1, and 2) Monolayers: Electronic, Phonon and Thermoelectric Properties From ab Initio Calculations, Front. Mech. Eng **8**, 876655 (2022).

2021

- 1. Yu Wu, Bowen Hou, Ying Chen, Jiang Cao, **Hezhu Shao***, Yiming Zhang, Congcong Ma, Heyuan Zhu, Rongjun Zhang* & Hao Zhang*, Strong electron phonon coupling influences carrier transport and thermoelectric performances in group-IV/V elemental monolayers, npj Comput. Mater. **7**, 145 (2021).
- 2. Ting Hai, Guoqiang Xie*, Jie Ma, **Hezhu Shao***, Zhen Qiao, Zhipeng Qin, Yue Sun, Fengqiu Wang, Peng Yuan, Jingui Ma, and Liejia Qian, Pushing Optical Switch into Deep Mid-Infrared Region: Band Theory, Characterization, and Performance of Topological Semimetal Antimonene, ACS Nano **15**, 7430 (2021).
- 3. Yu Wu, Bowen Hou, Congcong Ma, Jiang Cao, Ying Chen, Zixuan Lu, Haodong Mei, **Hezhu Shao**, Yuanfeng Xu*, Heyuan Zhu, Zhilai Fang, Rongjun Zhang* and Hao Zhang*, Thermoelectric performance of 2D materials: the band-convergence strategy and strong intervalley scatterings, Mater. Horiz. **8**, 1253 (2021).
- 4. Ying Chen, Yu Wu, Bowen Hou, Jiang Cao, **Hezhu Shao**, Yiming Zhang, Haodong Mei, Congcong Ma, Zhilai Fang*, Heyuan Zhu* and Hao Zhang*, Renormalized thermoelectric figure of merit in a band-convergent Sb_2Te_2Se monolayer: full electron phonon interactions and selection rules, J. Mater. Chem. A **9**, 16108 (2021).
- 5. Bo Yin, Shuquan Liang*, Dongdong Yu, Boshi Cheng, Ishioma L. Egun, Jiande Lin, Xuefang Xie, **Hezhu Shao**, Haiyong He*, Anqiang Pan*, Increasing Accessible Subsurface to Improving Rate Capability and Cycling Stability of Sodium-Ion Batteries, Adv. Mater. **33**, 2100808 (2021).

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- 1. Bowen Hou, Yiming Zhang, Hao Zhang*, **Hezhu Shao***, Congcong Ma, Xintong Zhang, Ying Chen, Ke Xu, Gang Ni*, Heyuan Zhu, Room Temperature Bound Excitons and Strain-Tunable Carrier Mobilities in Janus Monolayer Transition-Metal Dichalcogenides, J. Phys. Chem. Lett. **11**, 3116 (2020).
- 2. Xiaoxia Yu, **Hezhu Shao**, Xueyun Wang, Yingcai Zhu, Daining Fang and Jiawang Hong*, Anomalous lattice thermal conductivity in layered MNCl (M = Zr, Hf) materials driven by lanthanide contraction, J. Mater. Chem. A **8**, 3128 (2020).

- 3. Bo Peng, Hao Zhang, Weiwen Chen, Bowen Hou, Zhi-Jun Qiu, **Hezhu Shao**, Heyuan Zhu, Bartomeu Monserrat, Desheng Fu, Hongming Weng and Costas M. Soukoulis, Sub-picosecond photo-induced displacive phase transition in two-dimensional $MoTe_2$, npj 2D Mater. Appl., **4**,14 (2020).
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- 1. Bo Peng, Haodong Mei, Hao Zhang*, **Hezhu Shao***, Ke Xu, Gang Ni, Qingyuan Jin, Costas M. Soukoulis, Heyuan Zhu, High thermoelectric efficiency in monolayer PbI_2 from 300 K to 900 K, Inorg. Chem. Front. **6**, 920 (2019).
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- 3. Huajun Tian, **Hezhu Shao**, Yi Chen, Xiaqin Fang, Pan Xiong, Bing Sun, Peter H.L. Notten, Guoxiu Wang, Ultra-stable sodium metal-iodine batteries enabled by an in-situ solid electrolyte interphase, Nano Energy **57**, 692 (2019).
- 4. Yu Chen$^{\#}$, Bo Peng$^{\#}$, Chunxiao Cong*, Jingzhi Shang, Lishu Wu, Weihuang Yang, Jiadong Zhou, Peng Yu, Hongbo Zhang, Yanlong Wang, Chenji Zou, Jing Zhang, Sheng Liu, Qihua Xiong, **Hezhu Shao**, Zheng Liu*, Hao Zhang*, Wei Huang, Ting Yu*, In-Plane Anisotropic Thermal Conductivity of Few-Layered Transition Metal Dichalcogenide Td-WTe_2, Adv. Mater. **31**, 1804979 (2019).
- 5. Huajun Tian, Xuechao Yu, **Hezhu Shao**, Liubing Dong, Yi Chen, Xiaqin Fang, Chengyin Wang, Weiqiang Han*, Guoxiu Wang*, Unlocking Few-Layered Ternary Chalcogenides for High-Performance Potassium-Ion Storage, Adv. Energy Mater. **9**, 1901560 (2019).
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- 7. Sichen Duan, Na Man, Jingtao Xu*, Qingsong Wu, Guo-qiang Liu, Xiaojian Tan, **Hezhu Shao**, Kai Guo, Xinxin Yang*, Jun Jiang*, Thermoelectric $(Bi,Sb)_2Te_3$ $Ge_{0.5}Mn_{0.5}Te$ composites with excellent mechanical properties, J. Mater. Chem. A **7**, 9241 (2019).
- 8. Jiahua Zhang, Jingtao Xu*, Xiaojian Tan, Hongxiang Wang, Guo-Qiang Liu, **Hezhu Shao**, Bo Yu, Song Yue*, Jun Jiang*, Optimized orientation and enhanced thermoelectric performance in $Sn_{0.97}Na_{0.03}Se$ with Te addition, J. Mater. Chem. C, **7**, 2653, (2019).
- 9. Shi-Xin Lin, Xiaojian Tan, **Hezhu Shao**, Jingtao Xu, Qingsong Wu, Guo-Qiang Liu*, Wen-Hua Zhang*, Jun Jiang*, Ultralow Lattice Thermal

Conductivity in SnTe by Manipulating the Electron Phonon Coupling, J. Phys. Chem. C **123**, 15996 (2019).

- 10. Ping Jiang, Liang Chen*, **Hezhu Shao**, Shaohua Huang, Qiushi Wang, Yuebin Su, Xiaoshuang Yan, Xinmiao Liang, Jiujun Zhang, Jiwen Feng*, Zhaoping Liu*, Methylsulfonylmethane-Based Deep Eutectic Solvent as a New Type of Green Electrolyte for a High-Energy-Density Aqueous Lithium-Ion Battery, ACS Energy Lett. **4**, 1419, (2019).
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- 1. **Hezhu Shao***, Min Jin, Bo Peng, Hao Zhang*, Xiaojian Tan, Guo-Qiang Liu, Haochuan Jiang, Jun Jiang*, First-Principles Study of Manipulating the Phonon Transport of Molybdenum Disulfide by Sodium Intercalating, J. Phys. Chem. C **122**, 2632 (2018).
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- 3. Min Jin, Zhiwei Chen, Xiaojian Tan*, **Hezhu Shao**, Guoqiang Liu, Haoyang Hu, Jingtao Xu, Bo Yu, Hui Shen, Jiayue Xu, Haochuan Jiang, Yanzhong Pei*, Jun Jiang*, Charge Transport in Thermoelectric SnSe Single Crystals, ACS Energy Lett. **3**, 689 (2018).
- 4. Bo Peng, Ke Xu, Hao Zhang*, Zeyu Ning, **Hezhu Shao**, Gang Ni, Jing Li, Yongyuan Zhu, Heyuan Zhu, and Costas M. Soukoulis, 1D SbSeI, SbSI, and SbSBr With High Stability and Novel Properties for Microelectronic, Optoelectronic, and Thermoelectric Applications, Adv. Theory Simul. **1**, 1700005 (2018).
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- 10. Hong-Xiang Wang[#], Li-Sha Mao[#], Xiaojian Tan, Guo-Qiang Liu*, Jingtao Xu*, **Hezhu Shao**, Hao-Yang Hu, Jun Jiang*, Nontrivial thermoelectric behavior in cubic SnSe driven by spin-orbit coupling, Nano Energy **51**, 649 (2018).
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