

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.、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，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”。
- 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。
- **课题组目前已开展的研究方向**: 热电材料中的电/声子输运、储能材料中的电化学与离子输运、新型二维材料相关电/热/力/光等效应、以及相关计算程序的开发。
- **规划拓展的研究方向**: 机器学习、材料基因工程等。
- **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

2023

- 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.* accepted. (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. Materials*, In Press. (2023)

2022

- 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 tetrel metal halides: Ultra-long excitonic lifetimes, phase diagram and exciton dynamics, *Mater. Today Phys.* **22**, 100604 (2022).
- 5. Weijun Huang, Weijin Qian*, Haijun Luo, Mingliang Dong, **Hezhu Shao**, Yawei Chen, Xingzhen Liu, Changkun Dong*, Field emission enhancement from directly grown N-doped carbon nanotubes on stainless steel substrates, *Vacuum* **198**, 110900 (2022).
- 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, Kumpeng 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 Sb₂Te₂Se 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 MoTe₂, *npj 2D Mater. Appl.*, **4**,14 (2020).
- 4. Jun Zhang, Yiqun Xie*, Yibin Hu*, **Hezhu Shao***, Remarkable intrinsic ZT in the 2D PtX₂ (X = O, S, Se, Te) monolayers at room temperature, *Appl. Surf. Sci.* **532**, 147387 (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 PbI₂ from 300 K to 900 K, *Inorg. Chem. Front.* **6**, 920 (2019).
- 2. Shenghui Zhang, Xiaobin Niu, Yiqun Xie*, Kui Gong, **Hezhu Shao***, Yibin Hu*, Yin Wang, High intrinsic ZT in InP₃ monolayer at room temperature, *J. Phys.: Condens. Matter* **31**, 365501 (2019).
- 3. Hua jun 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-WTe₂, *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).
- 6. Xiaojian Tan, Guo-Qiang Liu^{*}, Haoyang Hu, **Hezhu Shao**, Jingtao Xu, Jun Jiang^{*}, Band engineering and crystal field screening in thermoelectric Mg₃Sb₂, *J. Mater. Chem. A* **7**, 8922 (2019).
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- 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).
- 11. Yue Hu, Zhen Zhu, Jiamin Xiao, **Hezhu Shao**, Li Zhao, Min Xu^{*}, Jun Zhuang^{*}, Atomic scale study of stress-induced misaligned subsurface layers in KDP crystals, *Sci. Rep.* **9**, 10399 (2019).
- 12. Hui Hua, Shaowei Feng, Zhongyu Ouyang, **Hezhu Shao**, Haiming Qin^{*}, Hui Ding, Qiping Du, Zhijun Zhang^{*}, Jun Jiang^{*}, Haochuan Jiang, YAGG:Ce transparent ceramics with high luminous efficiency for solid-state lighting application, *J. Adv. Ceram.* **8**, 389 (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).

- 2. Ke Xu, Yuanfeng Xu, Hao Zhang*, Bo Peng, **Hezhu Shao***, Gang Ni, Jing Li, Mingyuan Yao, Hongliang Lu, Heyuan Zhu*, Costas M. Soukoulis, The role of Anderson's rule in determining electronic, optical and transport properties of transition metal dichalcogenide heterostructures, *Phys. Chem. Chem. Phys.* **20**, 30351 (2018).
- 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).
- 5. Bo Peng, Hao Zhang*, **Hezhu Shao**, Ke Xu, Gang Ni, Jing Li, Heyuan Zhu and Costas M. Soukoulis, Chemical intuition for high thermoelectric performance in monolayer black phosphorus, α -arsenene and α -W-antimonene, *J. Mater. Chem. A* **6**, 2018 (2018).
- 6. Bo Peng, Hao Zhang*, **Hezhu Shao**, Ke Xu, Gang Ni, Liangcai Wu, Jing Li, Hongliang Lu, Qingyuan Jin, Heyuan Zhu, Room-Temperature Bound Exciton with Long Lifetime in Monolayer GaN, *ACS Photonics* **5**, 4081 (2018).
- 7. Bo Peng, Bohayra Mortazavi, Hao Zhang*, **Hezhu Shao**, Ke Xu, Jing Li, Gang Ni, Timon Rabczuk, Heyuan Zhu, Tuning Thermal Transport in C₃N Monolayers by Adding and Removing Carbon Atoms, *Phys. Rev. Applied* **10**, 034046 (2018).
- 8. Xiaofang Tan, Guoqiang Liu, Jingtao Xu*, Xiaojian Tan, **Hezhu Shao**, Haoyang Hu, Haochuan Jiang, Yalin Lu*, Jun Jiang*, Thermoelectric properties of In-Hg co-doping in SnTe: Energy band engineering, *J Materiomics* **4**, 62 (2018).
- 9. Xiaojian Tan, Hongxiang Wang, Guoqiang Liu*, Jacques G. Noudem, Haoyang Hu, Jingtao Xu, **Hezhu Shao**, Jun Jiang*, Designing band engineering for thermoelectrics starting from the periodic table of elements, *Materials Today Physics.* **7**, 35 (2018).
- 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).
- 11. Shaojun Liang, Jingtao Xu*, Jacques Guillaume Noudem, Hongxiang Wang, Xiaojian Tan, Guo-Qiang Liu, **Hezhu Shao**, Bo Yu, Song Yue*, Jun Jiang*, Thermoelectric properties of textured polycrystalline Na_{0.03}Sn_{0.97}Se enhanced by hot deformation, *J. Mater. Chem. A* **6**, 23730 (2018).
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Zhang, Jun Jiang*, Microstructure engineering beyond $\text{SnSe}_{1-x}\text{S}_x$ solid solution for high thermoelectric performance, *J. Materiomics* **4**, 321 (2018).

- 13. Qiuju Zhang#, Mingzhi Dai#, **Hezhu Shao**, Ziqi Tian, Yichao Lin, Liang Chen*, Xiao Cheng Zeng, Insights into High Conductivity of the Two-Dimensional Iodine-Oxidized sp_2 -c-COF, *ACS Appl. Mater. Interfaces* **10**, 43595 (2018).
- 14. Shaojun Liang, Jingtao Xu*, Hongxiang Wang, Xiaojian Tan, Guo-Qiang Liu, **Hezhu Shao**, Bo Yu, Song Yue*, Jun Jiang*, Investigation on structure and thermoelectric properties in p-type $\text{Bi}_{0.48}\text{Sb}_{1.52}\text{Te}_3$ via PbTe incorporating, *J. Mater. Sci-Mater. EL* **29**, 7701 (2018).
- 15. Jiaran Li, Jingtao Xu*, Hongxiang Wang, Guo-Qiang Liu, Xiaojian Tan, **Hezhu Shao**, Haoyang Hu, Jun Jiang*, Enhanced thermoelectric performance in p-type polycrystalline SnSe by Cu doping, *J. Mater. Sci-Mater. EL* **29**, 18727 (2018).

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- 1. Min Jin*, **Hezhu Shao***, Haoyang Hu, Debo Li, Hui Shen, Jiayue Xu, Jun Jiang*, Growth and characterization of large size undoped p-type SnSe single crystal by Horizontal Bridgman method, *J. Alloy Compd.* **712**, 857 (2017).
- 2. Min Jin*, **Hezhu Shao***, Haoyang Hu, Debo Li, Jingtao Xu, Guoqiang Liu, Hui Shen, Jiayue Xu, Haochuan Jiang, Jun Jiang*, Single crystal growth of $\text{Sn}_{0.97}\text{Ag}_{0.03}\text{Se}$ by a novel horizontal Bridgman method and its thermoelectric properties, *J. Cryst. Growth* **460**, 112 (2017).
- 3. Xiaojian Tan, Ling Wang, **Hezhu Shao**, Song Yue, Jingtao Xu, Guoqiang Liu,* Haochuan Jiang, Jun Jiang*, Improving Thermoelectric Performance of α -MgAgSb by Theoretical Band Engineering Design, *Adv. Energy Mater.* **7**, 1700076 (2017).
- 4. Yuanfeng Xu, Hao Zhang*, **Hezhu Shao**, Gang Ni, Jing Li, Hongliang Lu, Rongjun Zhang, Bo Peng, Yongyuan Zhu, Heyuan Zhu*, Costas M. Soukoulis, First-principles study on the electronic, optical, and transport properties of monolayer α - and β -GeSe, *Phys. Rev. B* **96**, 245421 (2017).
- 5. Ning Liu, Shifeng Jin, Liwei Guo, Gang Wang, **Hezhu Shao**, Liang Chen*, Xiaolong Chen*, Two-dimensional semiconducting gold, *Phys. Rev. B* **95**, 155311 (2017).
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- 13. Xue Wang, Jingtao Xu*, Guo-Qiang Liu, Xiaojian Tan, Debo Li, **Hezhu Shao**, Tianya Tan, Jun Jiang*, Texturing degree boosts thermoelectric performance of silver-doped polycrystalline SnSe, *NPG Asia Mater.* **9**, e426 (2017).
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