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现任：温州大学电气与电子工程学院 副教授，硕士生导师。
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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。
- 在 Nature Commun.、J. Phys. Chem. Lett.、J. Mater. Chem. C、Phys. Rev. E、EPL 等期刊发表 SCI 论文 80 余篇，H因子22，入选 2018 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、Chemical Science、Nano Energy、J. Mater. Chem. A、J. Mater. Chem. C、ACS Applied Materials & Interfaces、J. Phys. Condens. Matter. 等期刊审稿人，担任国家自然科学基金委面上基金、青年基金评审专家。

欢迎报考

欢迎有志于继续深造（包括学术研究和通过研究生学习提升自己能力）的同学报考本课题组研究生。也欢迎校内优秀本科生进本组进行科研实践。成功来自积极和努力，本实验室将尽力为你提供成长所需环境，帮助学生成功是我们课题组的基本职责之一。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**: 量子计算、机器学习、材料基因工程、碳纳米管理论计算与实验。
- **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

2020

- 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)..

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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).
- 1. Shenghui Zhang, Xiaobin Niu, Yiqun Xie*, Kui Gong, **Hezhu Shao***, Yibin Hu*, Yin Wang, High intrinsic ZT in InP_3 monolayer at room temperature, *J. Phys.: Condens. Matter* **31**, 365501 (2019).
- 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-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).
- 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)₂Te₃ - 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).
- 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 aW-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).
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Zhang, Jun Jiang*, Microstructure engineering beyond SnSe_{1-x}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 sp₂-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 Bi_{0.48}Sb_{1.52}Te₃ 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 Sn_{0.97}Ag_{0.03}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).
- 6. X. J. Tan, G. Q. Liu*, **H. Z. Shao**, J. T. Xu, B. Yu, H. C. Jiang, J. Jiang*, Acoustic phonon softening and reduced thermal conductivity in Mg₂Si_{1-x}Sn_x solid solutions, *Appl. Phys. Lett.* **110**, 143903 (2017).
- 7. Bo Peng, Hao Zhang*, **Hezhu Shao**, Zeyu Ning, Yuanfeng Xu, Gang Ni, Hongliang Lu, David Wei Zhang, Heyuan Zhu, Stability and strength of atomically thin borophene from first principles calculations, *Mater. Res. Lett.* **5**, 399 (2017).

- 8. Bo Peng, Dequan Zhang, Hao Zhang*, **Hezhu Shao**, Gang Ni, Yongyuan Zhu, Heyuan Zhu, The conflicting role of buckled structure in phonon transport of 2D group-IV and group-V materials, *Nanoscale*, **9**, 7397 (2017).
- 9. Yuanfeng Xu, Bo Peng, Hao Zhang*, **Hezhu Shao**, Rongjun Zhang, Heyuan Zhu, First-principle calculations of optical properties of monolayer arsenene and antimonene allotropes, *Ann. Phys. (Berlin)* **529**, 1600152 (2017).
- 10. Yuanfeng Xu, Zeyu Ning, Hao Zhang*, Gang Ni, **Hezhu Shao**, Bo Peng, Xiangchao Zhang, Xiaoying He, Yongyuan Zhu, Heyuan Zhu, Anisotropic ultrahigh hole mobility in two dimensional penta-SiC₂ by strain-engineering: electronic structure and chemical bonding analysis, *RSC Adv.* **7**, 45705 (2017).
- 11. Xiaofang Tan, Xiaojian Tan, Guoqiang Liu*, Jingtao Xu*, **Hezhu Shao**, Haoyang Hu, Min Jin, Haochuan Jiang, Jun Jiang*, Optimizing the thermoelectric performance of In-Cd codoped SnTe by introducing Sn vacancies, *J. Mater. Chem. C* **5**, 7504 (2017).
- 12. Ling Wang, Xiaojian Tan*, Guoqiang Liu, Jingtao Xu, **Hezhu Shao**, Bo Yu, Haochuan Jiang, Song Yue*, Jun Jiang*, Manipulating Band Convergence and Resonant State in Thermoelectric Material SnTe by Mn²⁺In Codoping, *ACS Energy Lett.* **2**, 1203 (2017).
- 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).
- 14. Debo Li, Xiaojian Tan, Jingtao Xu*, Guoqiang Liu, Min Jin, **Hezhu Shao**, HuaJie Huang, Jianfeng Zhang*, Jun Jiang*, Enhanced thermoelectric performance in n-type polycrystalline SnSe by PbBr₂ doping, *RSC Adv.* **7**, 17906 (2017).
- 15. Ping Jiang, **Hezhu Shao**, Liang Chen*, Jiwen Feng, Zhaoping Liu*, Ion-selective copper hexacyanoferrate with an open-framework structure enables high-voltage aqueous mixed-ion batteries, *J. Mater. Chem. A* **5**, 16740 (2017).
- 16. Yongfu Liu*, Jack Silver*, Rong-Jun Xie, Jiahua Zhang, Huawei Xu, **Hezhu Shao**, Jun Jiang, Haochuan Jiang, An excellent cyan-emitting orthosilicate phosphor for NUV-pumped white LED application, *J. Mater. Chem. C* **5**, 12365 (2017).
- 17. Guoqing Wu, Haiming Qin*, Shaowei Feng, Xiaojian Tan, Zhaohua Luo, Yongfu Liu, **Hezhu Shao**, Jun Jiang*, Haochuan Jiang*, Ultra-fine Gd₂O₂S:Pr powders prepared via urea precipitation method using SO₂/SO₄²⁻ as sulfuration agent—A comparative study, *Powder Technology* **305**, 382 (2017).
- 18. Yajie Fu, Jingtao Xu, Guo-Qiang Liu, Xiaojian Tan, Zhu Liu, Xue Wang, **Hezhu Shao**, Haochuan Jiang, Bo Liang*, Jun Jiang*, Study on

Thermoelectric Properties of Polycrystalline SnSe by Ge Doping, *J. Elect. Mater.* **46**, 3182 (2017).

- 19. Dewen Xie, Jingtao Xu*, Zhu Liu, Guoqiang Liu, **Hezhu Shao**, Xiaojian Tan, Haochuan Jiang, Jun Jiang*, Stabilization of Thermoelectric Properties of the Cu/Bi_{0.48}Sb_{1.52}Te₃ Composite for Advantageous Power Generation, *J. Elect. Mater.* **46**, 2746 (2017).

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- 1. **Hezhu Shao***, Xiaojian Tan, Jun Jiang*, Haochuan Jiang*, First-principles study on the elastic properties of Cu₂GeSe₃, *EPL* **113**, 26001 (2016).
- 2. **Hezhu Shao***, Hao Zhang, Bo Peng, Xiaojian Tan, Guo-Qiang Liu, Jun Jiang*, Haochuan Jiang, A first-principles study on the intrinsic phonon transport of Cu₂GeSe₃, *EPL* **115**, 26002 (2016).
- 3. **Hezhu Shao***, Xiaojian Tan, Guo-Qiang Liu, Jun Jiang*, Haochuan Jiang*, A first-principles study on the phonon transport in layered BiCuOSe, *Sci. Rep.* **6**, 21035 (2016).
- 4. Liang Chen*#, **Hezhu Shao**#, Xufeng Zhou, Guoqiang Liu, Jun Jiang, Zhaoping Liu*, Water-mediated cation intercalation of open-framework indium hexacyanoferrate with high voltage and fast kinetics, *Nature Commun.* **7**, 11982 (2016).
- 5. Bo Peng, Hao Zhang*, **Hezhu Shao***, Yuanfeng Xu, Rongjun Zhang, Heyuan Zhu, The electronic, optical, and thermodynamic properties of borophene from first-principles calculations, *J. Mater. Chem. C* **4**, 3592 (2016).
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- 9. Bo Peng, Hao Zhang*, **Hezhu Shao**, Yuanfeng Xu, Rongjun Zhang, Hongliang Lu, David Wei Zhang, Heyuan Zhu*, First-Principles Prediction of Ultralow Lattice Thermal Conductivity of Dumbbell Silicene: A Comparison with Low-Buckled Silicene, *ACS Appl. Mater. Interfaces* **8**, 20977 (2016).
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group-IV materials from ab initio calculations, *Phys. Rev. B.* **94**, 245420 (2016).

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- 15. Dewen Xie , Jingtao Xu*, Guoqiang Liu, Zhu Liu, **Hezhu Shao**, Xiaojian Tan, Jun Jiang*, Haochuan Jiang, Synergistic Optimization of Thermoelectric Performance in p-Type Bi_{0.48}Sb_{1.52}Te₃/Graphene Composite, *Energies* **9**, 236 (2016).
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