一、个人简介



雷文，男，博士，讲师。研究内容包括：通过第一性原理计算研究材料的电子/声子输运、热电等性质，以及利用机器学习方法进行材料筛选等。2024年毕业于武汉大学，获博士学位。先后参与国家自然科学基金项目2项，广西自然科学基金等省部级科研项目2项。先后在 “Phys. Rev. B”、“Appl. Phys. Lett.”、“Nanoscale”“J. Mater. Chem. C”、“J. Phys. Chem. C”等期刊以第一作者或通讯作者身份发表学术论文7篇。

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二、代表性的项目

1. 利用机器学习高通量筛选高性能热电材料（62074114 国家自然科学基金面上项目），已结题，参与

2. 六角结构的Sr4IrO6及相关4*d*/5*d*过渡金属氧化物的电子结构和物理性质研究（11864008国家自然科学基金地区基金项目），已结题，参与

3. 纳米光伏太阳能电池材料的理论设计与器件优化研究（2018AD19200 广西科技基地和人才专项项目），已结题，参与

4. 铁电Rashba半导体材料的第一性原理设计与基础物理研究（2018GXNSFAA138185 广西自然科学基金面上项目），已结题，参与

三、代表性的成果

1. Ke Peng, Feng Xiao, Bowen Chen, **Wen Lei\***, Xing Ming\*, Ultra-high carrier mobility and ultra-low lattice thermal conductivity in PdSSe monolayers with fully Stone–Wales defects. ***Applied Physics Letters***, 2024, 125(25), 253102.
2. **Wen Lei**, Yufeng Luo, Haibin Cao, Hongmei Yuan, Wenyan Jiao, Mengke Li, Huijun Liu\*, Unique mass-dependent lattice thermal conductivities of orthorhombic MX2 (M = Pd, Pt; X = S, Se): a comparative study. ***Physics Letters A***, 2024, 526, 29970.
3. **Wen Lei**, Rui Hu, Shihao Han, Hongmei Yuan, Wenyan Jiao, Yufeng Luo, Huijun Liu\*, Directional control of the electronic and phonon transport properties in the ferroelastic PtSe2. ***The Journal of Physical Chemistry C***, 2024, 128(1), 543-548.
4. **Wen Lei**, Rui Hu, Shihao Han, Hongmei Yuan, Wenyan Jiao, Huijun Liu\*, The TiNI monolayer: a two-dimensional system with promising ferroelastic, topological, and thermoelectric properties. ***Physical Chemistry Chemical Physics***, 2022, 24(46), 28134-28140.
5. **Wen Lei**, Wei Wang, Xing Ming\*, Shengli Zhang\*, Gang Tang, Xiaojun Zheng, Huan Li, Carmine Autieri, Structural transition, metallization and superconductivity in quasi 2D layered PdS2 under compression. ***Physical Review B***, 2020, 101, 205149.
6. **Wen Lei**, Bo Cai, Huanfu Zhou, Gunter Heymann, Xin Tang, Shengli Zhang\*, Xing Ming\*, Ferroelastic lattice rotation and band-gap engineering in quasi 2D layered-structure PdSe2 under uniaxial stress. ***Nanoscale***, 2019, 11, 12317-12325.
7. **Wen Lei**, Shengli Zhang\*, Gunter Heymann, Xin Tang, Jianfeng Wen, Xiaojun Zheng, Guanghui Hu, Xing Ming\*, A new 2D high-pressure phase of PdSe2 with high-mobility transport anisotropy for photovoltaic applications. ***Journal of Materials Chemistry C***, 2019, 7, 2096-2105.