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Editorial: Calculation and design of two-dimensional thermoelectric and piezoelectric materials

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Editorial on the Research Topic
Calculation and design of two-dimensional thermoelectric and piezoelectric materials

Introduction

Two-dimensional (2D) materials have been widely applied in various fields from science to engineering due to their fascinating physical and chemical properties [1–3]. 2D thermoelectric/piezoelectric materials could directly convert thermal/mechanical energy into electrical energy, which could solve the energy problems and relieve environmental pollution. Though the thermoelectric or piezoelectric properties of a large amount 2D materials including graphene, hexagonal boron nitride, arsenene, metal carbides and nitrides (MXenes), and transition metal dichalcogenides (TMDs) have been detailedly investigated, these performance has not yet met the requirements for commercial applications. Usually, the thermoelectric/piezoelectric properties could be improved by developing 2D material, doping, straining engineering, chemical functionalization, *etc.* [4–7] Furthermore, some novel physical properties including magnetism, topology, and valley may appear in some 2D materials. The combination of thermoelectricity/piezoelectricity with other unique properties may lead to novel device applications or scientific breakthroughs in new physics. Combining the advantages of thermoelectricity/piezoelectricity with other unique properties may result in new physical breakthroughs or novel device applications. Thus, designing and developing novel thermoelectric/piezoelectric materials is full of significance.

In this Research Topic "*Calculation and design of two-dimensional thermoelectric and piezoelectric materials*," we have collected a total of 13 articles including the recent progress

in thermoelectricity, magnetism, topology, photocatalysis, and noise reduction. Next, we briefly summarize the research highlights about these fascinating studies.

Thermoelectricity

The thermoelectric effect could convert mechanical energy into electrical energy, thus providing a considerable solution to address environmental and energy issues. With the help of first-principles calculations and Boltzmann transport theory, Li et al. predicted the electronic and thermoelectric properties of pentagonal PdX_2 (X = Se, Te) monolayers (MLs). The maximum thermoelectric figure of merit (ZT) reaches 6.6 (or 4.4) for p-type (or n-type) $PdTe_2$, which is a potential thermoelectric candidate. Yin et al. theoretically predicted 2D $TlInSe_3$ to be a promising thermoelectric material with a high ZT value of 4.15 at 500 K. Cui et al. explored the thermal properties of biphenylene by non-equilibrium molecular dynamics calculations, and they found that the thermal conductivity of biphenylene is isotropic and sensitive to size and temperature. The graphene/biphenylene lateral heterojunction possesses an interface thermal conductance of about 2.84×10^9 $WK^{-1}m^{-2}$. Furthermore, the interface thermal conductance could be obviously tuned by strain.

Magnetism

2D ferromagnetic and antiferromagnetic materials provides a novel platform for the application of spintronics. Tu et al. summarized the recent progress of 2D intrinsic Cr-based ferromagnetic semiconductors from the theoretical perspective, and showcased the importance of first-principles calculations in designing new 2D ferromagnetic semiconductors. Wang et al. summarized the magnetic, electronic, topological, spin-transport properties, and potential applications of a series of spin-gapless semiconductors including 2D oxalate-based metal-organic frameworks (MOFs), Fe_2I_2 ML, Cr_2X_3 (X = S, Se, and Te) ML, $CrGa_2Se_4$ ML, HK Mn-cyanogen lattice, MnNF ML, and Fe_4N_2 pentagon crystal. Kang et al. found that $Cr_2Ge_2Te_6$ switches from semiconductor to metal by adsorption Ti or Fe atoms, while $Cr_2Ge_2Te_6$ changes from semiconductor to half-metal by adsorption of Sc, V, Co., Ni, or Cu atoms. Moreover, the adsorption of 3d transition metal atoms obviously enhance the Curie temperature $Cr_2Ge_2Te_6$. Chen et al. predicted $MnSi_2N_4$ ML to be an antiferromagnetic semiconductor, and external strain could effectively tune its antiferromagnetic coupling. Furthermore, $MnSi_2N_4$ ML shows half-metallic ferromagnetism when an external magnetic field is applied. Wang et al. predicted 2D ferromagnetic GdScSi and GdScGe MLs to possess good dynamical, thermal, and mechanical stabilities. More excitingly, the Curie temperatures of GdScSi ML (470 K) and GdScGe ML (495 K) are above room temperature. Zhang et al. found that Ti and Ge doped 2D SiC systems are nonmagnetic semiconductors, Sc and Al doped 2D SiC systems are magnetic metals, and V, Cr, Mn, Fe, Co., and Zn doped 2D SiC systems are magnetic semiconductors. Yang et al. summarized the electronic, magnetic, and transport properties of Mn_2CoAl bulk and Mn_2CoAl-based films including Mn_2CoAl bulk, Mn_2CoAl 001 surface, various types of Mn_2CoAl films, $Mn_2CoAl/GaAs$, $MgO/Mn_2CoAl/Pd$, $Mn_2CoAl/Ag/Mn_2CoAl$.

Topology, photocatalysis, and noise reduction

Yang et al. demonstrated tetragonal $Na_2Zn_2O_3$ to host charge-two Dirac point phonons and charge-two Weyl point phonons at high-symmetry points. Shen et al. prepared a three-dimensional porous structured ZnO/graphene/graphene oxide/multi-walled carbon nanotube (ZnO/G/GO/MCNT) composite aerogels and reported its photocatalytic efficiency for Rhodamine B (RhB) degradation is 3.3 times higher than that of ZnO. Ren et al. performed a structural model of a stranding machine to obtain the first eight orders of inherent frequencies and vibration patterns, and found that the resonant frequency could be avoided and the vibration reduction could be achieved by increasing the wall thickness of the bearing seat.

We hope that this Research Topic could provide guidance for developing novel thermoelectric, magnetic, topological, photocatalytic materials, and reducing noise. Finally, we thank to all the authors, reviewers, and editors who have made contributions to this Research Topic.

Author contributions

GW and HY prepared the first draft, while S-DG and YSA revised the manuscript. All authors contributed to the article and approved the submitted version.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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