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

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

Introduction

In the fields of green energy and intelligent sensing, two-dimensional (2D) thermoelectric and piezoelectric materials have gained unprecedented attention as bridges between energy and information [1–5]. Their value lies not only in their ability to directly convert widely distributed thermal and mechanical energy into electricity, but also in the vast performance controllable potential offered by their unique 2D structure, far exceeding that of traditional materials. Currently, research in this field has moved beyond simple evaluation of known material properties and entered a new phase characterized by "theory-first, design-on-demand." Computational simulations are playing a central role, revealing the microscopic mechanisms of energy conversion at the atomic scale and accurately predicting the performance limits achievable through strategies such as strain engineering, heterostructure construction, and bandgap manipulation. This "calculation first, experiment later" paradigm has greatly accelerated the discovery and application of new high-performance materials.

This Research Topic focuses on the breakthroughs driven by computational design in 2D thermoelectric and piezoelectric materials. A total of five articles have been collected for this Research Topic, covering research areas such as thermal transport, thermoelectrics, piezocatalysis, catalysis, photocatalysis, photovoltaic devices, and fusion materials. We hope this Research Topic will provide novel ideas to advance these materials and represent a key step toward their practical applications.

Thermoelectricity and thermal transport

Thermoelectric (TE) materials, which is capable of direct and pollution-free heat-to-electricity conversion, offer a promising solution to the challenges of energy scarcity and environmental pollution. Xiao et al. combined first-principles calculations with the Boltzmann transport equation to explore the thermoelectric and thermal transport properties of anti-perovskite M_3IO and M_4I_2O (M = K, Rb). By incorporating two-phonon scattering processes, they found that oxygen atoms within the M_6O octahedral frameworks undergo pronounced vibrational motion, yielding a Debye temperature well below 300 K and extremely low lattice thermal conductivity (0.30–0.89 $W\,m^{-1}\cdot K^{-1}$ at 300 K). M_4I_2O exhibits strong thermal transport anisotropy because of weak bonding along the zz direction, while M_3IO exhibits nearly isotropy. Rb_4OI_2 exhibits the lowest lattice thermal conductivity, with directional values of 0.47 (xx direction) and 0.30 (zz direction) $W\cdot m^{-1}\cdot K^{-1}$, compared to Rb_3OI's isotropic value of 0.52 $W\,m^{-1}\cdot K^{-1}$. This low conductivity is attributed to a short phonon relaxation time caused by the softening of transverse acoustic (TA) phonon branches. Electronically, multiple valleys at the valence band maximum in both materials contribute to high Seebeck coefficients, with p-type Rb_3OI reaching 527–684 $\mu V\,K^{-1}$. The thermoelectric performance peaks for p-type Rb_3OI at 900 K, with a maximum thermoelectric figure of merit (ZT) of 1.91 and a distinct peak of 1.41 along the zz direction, demonstrating its high potential as a p-type thermoelectric material.

Piezocatalysis, catalysis and photocatalysis

In the field of piezoelectric catalysis, the catalytic behavior of materials under mechanical stimulation has traditionally been explained at the macroscale based on semiconductor band theory. However, the microscopic mechanism linking piezoelectric properties to surface chemical reactivity remains incompletely understood. Recently, Sun et al. systematically investigate the electronic structure, electrostatic potential distribution, surface polarization, and chemical adsorption behavior under strain of tetragonal $PbTiO_3$ (PTO) based on density functional theory (DFT). Their study revealed that strain significantly modulates the band structure of PTO: bulk and few-layer PTO exhibit opposite trends in band gap changes, with the latter showing a nonmonotonic piezoelectric potential response under strain that directly correlates with the catalytic driving force. Furthermore, space charge and surface dipole moment analysis revealed that the ionic dipole plays a dominant role in polarization, while both compressive and tensile strain enhance the adsorption of $^*OH/^*H$ intermediates, revealing the critical influence of piezoelectric polarization on surface reaction thermodynamics. This work clarifies the piezoelectric catalytic mechanism of polar perovskites at the atomic scale, providing a theoretical basis for designing piezoelectric materials for efficient energy conversion and environmental remediation.

Following the discovery of graphene, research on 2D materials has intensified. Constructing heterostructures through van der Waals interactions has emerged as a key approach for tailoring material properties and expanding their functional applications. Tao et al. demonstrated that van der Waals heterostructures composed of MXene Zr_2CO_2 and 2D semiconductor monolayers (SiC and GeC) exhibit excellent thermal stability at 300 K while retaining the inherent electronic band structures of their components. These heterostructures exhibit a typical type-I band alignment, rendering them suitable for light-emitting device applications. Significant charge transfer (0.1459 |e| in Zr_2CO_2/SiC) and interfacial potential drops (6.457 eV and 3.712 eV, respectively) effectively promote the separation of photogenerated carriers. Notably, the Zr_2CO_2/SiC heterostructure exhibits high carrier mobility along the transport direction (~3,656 $cm^2\,V^{-1}\cdot s^{-1}$) and excellent light absorption, demonstrating its broad potential for applications in photocatalysis and photovoltaics. This research provides a theoretical basis for the rational design of 2D heterostructures for energy and optoelectronic devices.

The unique electronic structures and catalytic properties of 2D materials make them highly promising for nanodevices. Recently, Du et al. predicted a new class of wrinkled 2D materials, X_2B_6 (X = K, Na, Rb), designed through elemental mutation, with their dynamical and thermal stability confirmed theoretically. Mechanically, these materials exhibit anisotropic behavior, with Young's moduli ranging from 296 to 406 N/m and Poisson's ratios from 0.35 to 0.36. Lectronically, K_2B_6 and Rb_2B_6 are metallic, whereas Na_2B_6 is an ultra-narrow bandgap semiconductor (~0.42 eV) with ultrahigh electron mobility (~9,942 $cm^2\,V^{-1}\cdot s^{-1}$) and strong light absorption. More notably, X_2B_6 monolayers exhibit low Gibbs free energies for both the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER), indicating promising electrocatalytic activity. This work systematically reveals the potential of X_2B_6 monolayers for high-speed electronic devices and high-efficiency energy conversion catalysts, providing a theoretical basis for designing and developing novel 2D materials.

Fusion materials

Tungsten is an important candidate material for plasma-facing components in fusion devices, making the study of its damage mechanisms under high-energy irradiation crucial. However, the influence of electron excitation on its irradiation damage behavior is not fully understood. To address this, Sheng et al. employed a two-temperature molecular dynamics (2T-MD) model to demonstrate that electronic effects significantly regulate the formation of irradiation defects in tungsten, particularly under high-energy conditions (~150 keV). Compared with classical molecular dynamics simulations, the 2T-MD model predicts a substantial reduction in both the peak and residual defect numbers. Further analysis shows that while the peak defect number increases with rising irradiation temperature, the residual defect number remains largely unchanged. Increasing the electron density suppresses peak defects but has little effect on residual defects. Conversely, delaying the activation of electron-phonon coupling results in more defects. These phenomena are attributed to the local energy dissipation and atomic energy redistribution induced by electron-phonon coupling, which promotes defect recombination and suppresses defect formation. This study provides mechanistic insights into the role of electron excitation in the irradiation damage of metals

and offers theoretical guidance for evaluating and designing fusion materials for high-energy irradiation environments.

The contributions within this Research Topic aim to offer valuable insights for the development of novel thermal transport, thermoelectrics, piezocatalysis, catalysis, photocatalysis, photovoltaic devices, and fusion materials. Finally, we thank to all the authors, reviewers, and editors who have made contributions to this Research Topic.

Author contributions

GW: Writing – original draft. HY: Writing – original draft. S-DG: Writing – review and editing. YA: Writing – review and editing.

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