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# Thermoelectric properties of the 3C, 2H, 4H, and 6H polytypes of the wide-band-gap semiconductors SiC, GaN, and ZnO

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We have investigated the thermoelectric properties of the 3C, 2H, 4H, and 6H polytypes of the wide-band-gap(n-type) semiconductors SiC, GaN, and ZnO based on first-principles calculations and Boltzmann transport theory. Our results show that the thermoelectric performance increases from 3C to 6H, 4H, and 2H structures with an increase of hexagonality for SiC. However, for GaN and ZnO, their power factors show a very weak dependence on the polytype. Detailed analysis of the thermoelectric properties with respect to temperature and carrier concentration of 4H-SiC, 2H-GaN, and 2H-ZnO shows that the figure of merit of these three compounds increases with temperature, indicating the promising potential applications of these thermoelectric materials at high temperature. The significant difference of the polytype-dependent thermoelectric properties among SiC, GaN, and ZnO might be related to the competition between covalency and ionicity in these semiconductors. Our calculations may provide a new way to enhance the thermoelectric properties of wide-band-gap semiconductors through atomic structure design, especially hexagonality design for SiC. © 2015 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution 3.0 Unported License. [http://dx.doi.org/10.1063/1.4931820]

## I. INTRODUCTION

Thermoelectric (TE) materials have attracted a lot of attention in recent years because of their ability to convert heat energy into electricity with reduced pollution.<sup>1–3</sup> The thermal–electricity conversion efficiency of TE materials is defined as the dimensionless figure of merit  $ZT = S^2\sigma T/\kappa$ , where  $T$  is the absolute temperature,  $S$  is the Seebeck coefficient,  $\sigma$  is the electrical conductivity, and  $\kappa$  is the thermal conductivity. The quantity  $S^2\sigma$  is the so-called power factor (PF) and is the key to achieving high thermoelectric performance. The thermal conductivity  $\kappa$  consists of the lattice thermal conductivity  $\kappa_l$  and the electronic component  $\kappa_e$ .<sup>3</sup> Because the Seebeck coefficient, electronic conductivity, and thermal conductivity are all related to the electronic structure, it is a great challenge to increase the  $ZT$  value. Various strategies have been proposed to solve this problem, such as the phonon-glass behavior found in caged compounds,<sup>4</sup> grain boundaries,<sup>5</sup> band convergence,<sup>6</sup> nanostructures,<sup>7,8</sup> strong electron–phonon coupling by charge density waves,<sup>9</sup> and the liquid-like state.<sup>10</sup>

Wide-band-gap semiconductors such as SiC, GaN and ZnO have attracted interest from scientists in the past decades because of their increasing applications in short-wavelength photonic devices and high-power high-frequency electronic devices.<sup>11–15</sup> Investigations of these materials show their potential in thermoelectric applications.<sup>16–19</sup> However, there is a lack of research on the

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thermoelectric dependence of the different structures of these materials, and polytypism is a common phenomenon in the process of synthesizing materials. Early experiments on GaAs combined with transmission electron microscopy showed that variation of the growth temperature changes the structure from zinc-blende-type to wurtzite-type.<sup>20</sup> Leitsmann *et al.* observed a phase transition between local zinc-blende and wurtzite geometries by changing the preparation conditions of the surfaces.<sup>21</sup> Group-IV SiC is a typical compound with more than 200 polytypes,<sup>22</sup> and many first-principles calculations have been performed on 3C-SiC, 2H-SiC, 4H-SiC, and 6H-SiC.<sup>23–25</sup> In this paper, we studied the 3C, 2H, 4H, and 6H structures of SiC, GaN, and ZnO to investigate the relationship between the polytypes and their thermoelectric properties.

## II. COMPUTATIONAL METHODS

The structures and electronic properties of SiC, GaN, and ZnO were investigated by first principles calculations. The ground-state properties, including full structural geometry optimization (variable-cell relaxation), were obtained by pseudopotential calculations, as implemented in the Quantum Espresso<sup>26</sup> code. The Perdew–Burke–Ernzerhof (PBE) parameterization of the generalized gradient approximation (GGA)<sup>27</sup> was used for the exchange–correlation potential. An energy cutoff of 60 Ry for the wave function and a  $10 \times 10 \times 10$  Monkhorst–Pack grid for Brillouin zone (BZ) sampling were used to ensure convergence of the self-consistent calculation. The thermoelectric transport properties were then determined using Boltzmann transport theory, as implemented in the BOLTZTRAP code<sup>28,29</sup> interfaced to the full-potential WIEN2K code.<sup>30</sup> A large number of  $k$  points (16,000) for the whole BZ was used in the calculations to achieve good convergence of the transport properties. In the full-potential calculations, the muffin-tin radii were selected to be 1.64 a.u. for Si, 1.82 a.u. for C, 1.92 a.u. for Ga, 1.66 a.u. for N, 1.96 a.u. for Zn, and 1.69 a.u. for O. The band gap obtained by GGA can be further improved by the quasiparticle GW method.<sup>31–33</sup> In this work, for simplicity, the band gap of the 2H structure was corrected based on available experimental data. The band gaps of the other structures were corrected using the so-called scissors correction. Because SiC, GaN, and ZnO are wide-band-gap materials, and considering that only the contribution of the band structure within an energy range of 0.5 eV from the Fermi energy is important for transport properties, the band gap correction has very little effect on the transport properties.

There are many methods that can be used for transport calculations. The choice of different computational methods may result in different values of the transport component, but the trend of the polytype-dependent transport properties, such as electronic conductivity and thermoelectric power, should be similar because they mainly depend on the band structure of the materials. In this work, we mainly focus on the effect of hexagonality on the thermoelectric performance of SiC, GaN, and ZnO, and the Boltzmann transport code was used because it serves our purpose well. Previously, we demonstrated the use of the Boltzmann transport code for other materials such as PbTe,<sup>34,35</sup> SnTe,<sup>35</sup> and GeTe,<sup>35</sup> as well as ZnO nanofilms,<sup>36</sup> and found good agreement between theory and the available experimental data. In this work, we focus on the n-type transport properties because electron doping can be realized in these three materials.

## III. RESULTS

Our calculations included four typical polytypes (3C, 2H, 4H, and 6H) of the three wide-band-gap semiconductors SiC, GaN, and ZnO. To determine the equilibrium lattice constants and calculate the bulk moduli of these compounds, we performed total energy calculations at various pressures (stresses) from  $-100$  to  $100$  GPa in steps of  $20$  GPa. After obtaining the energy–volume curve, the Murnaghan equation of state<sup>37</sup> was applied to determine the bulk modulus  $B_0$  and its pressure derivative  $B_0'$ . The calculated lattice constants and bulk moduli are listed in Table I, and compared with other calculations and experiments. Our calculations show that the hexagonal polytypes of each compound have similar basal lattice constants in the  $a$  direction and bulk moduli, and are in good agreement with available experimental and theoretical data.

TABLE I. Lattice constants and bulk moduli of the polytypes of SiC, GaN, and ZnO.

Compounds	Type	$a$ (Å)			$c/a$			$B_0$ (GPa)		
		Present	Other	Expt.	Present	Other	Expt.	Present	Other	Expt.
SiC	3C	4.3894	4.358 <sup>a</sup>	4.360 <sup>c</sup>				206.24	219 <sup>a</sup>	224 <sup>c</sup>
	2H	3.0989	3.072 <sup>a</sup>	3.076 <sup>b</sup>	1.6415	1.641 <sup>a</sup>	1.641 <sup>b</sup>	207.00	215.2 <sup>a</sup>	225 <sup>b</sup>
	4H	3.1010	3.069 <sup>a</sup>	3.073 <sup>b</sup>	3.2743	3.292 <sup>a</sup>	3.271 <sup>b</sup>	206.66	218 <sup>a</sup>	
	6H	3.1019	3.077 <sup>a</sup>	3.073 <sup>b</sup>	4.9070	4.910 <sup>a</sup>	4.907 <sup>b</sup>	206.54	204 <sup>a</sup>	
GaN	3C	4.5417	4.547 <sup>d</sup>	4.490 <sup>e</sup>				172.72	172 <sup>d</sup>	190 <sup>f</sup>
	2H	3.2141	3.217 <sup>d</sup>	3.190 <sup>g</sup>	1.6287	1.629 <sup>d</sup>	1.627 <sup>g</sup>	172.69	172.2 <sup>d</sup>	188 <sup>i</sup>
	4H	3.2126	3.158 <sup>j</sup>		3.2621	3.262 <sup>j</sup>		172.70	196 <sup>j</sup>	
	6H	3.2122	3.157 <sup>j</sup>		4.8949	4.895 <sup>j</sup>		171.33	194.5 <sup>j</sup>	
ZnO	3C	4.6261	4.508 <sup>k</sup>	4.620 <sup>l</sup>				129.49	161.7 <sup>k</sup>	
	2H	3.2855	3.199 <sup>k</sup>	3.2498 <sup>m</sup>	1.6137	1.614 <sup>k</sup>	1.602 <sup>m</sup>	128.43	162.3 <sup>k</sup>	142.6 <sup>m</sup>
	4H	3.2775			3.2488			128.32		
	6H	3.2752			4.8822			128.56		

<sup>a</sup>Ref. 25 (local density approximation (LDA)).<sup>b</sup>Ref. 38.<sup>c</sup>Ref. 39.<sup>d</sup>Ref. 40 (GGA-PBE).<sup>e</sup>Ref. 41.<sup>f</sup>Ref. 42 (force balance method).<sup>g</sup>Ref. 43 (X-ray diffraction).<sup>h</sup>Ref. 44.<sup>i</sup>Ref. 45 (X-ray diffraction).<sup>j</sup>Ref. 46 (LDA).<sup>k</sup>Ref. 47 (LDA).<sup>l</sup>Ref. 48 (LDA).<sup>m</sup>Ref. 49.

The calculated energy-band structures of the polytypes of SiC, GaN, and ZnO are shown in Fig. 1. The energy bands of the hexagonal structures are represented versus the high-symmetry lines A-L-M- $\Gamma$ -A-H-K- $\Gamma$  within the BZ of the hexagonal system. From the 2H, 4H and 6H structures, there is more band folding because of the increase of the superlattice period along the  $c$  axis. GaN

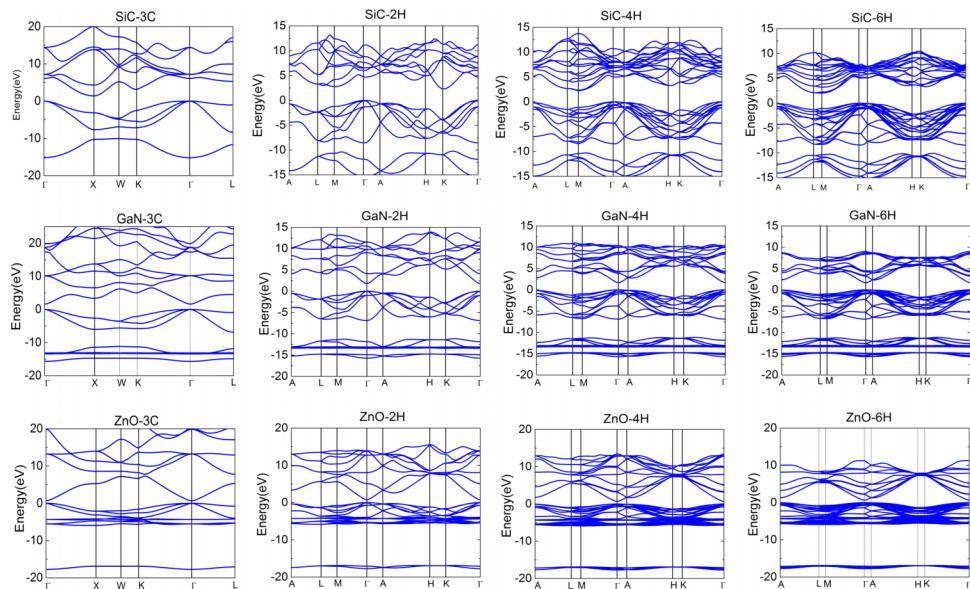


FIG. 1. Band structures of the polytypes of SiC, GaN, and ZnO. The energy bands of the hexagonal structures are represented versus the high-symmetry lines A-L-M- $\Gamma$ -A-H-K- $\Gamma$  within the BZ of the hexagonal systems.

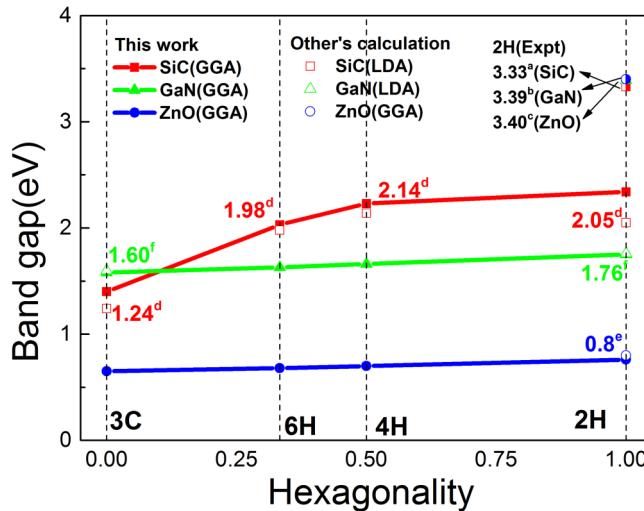


FIG. 2. Calculated band gaps (eV) of the polytypes of SiC, GaN, and ZnO. Available experimental (Exp) values and theoretical data (obtained by LDA or GGA) from the literature are shown for comparison. The superscript labels are as follows: a, Ref. 39; b, Ref. 50; c, Ref. 51; d, Ref. 25; e, Ref. 53; and f, Ref. 52.

and ZnO are direct-gap semiconductors in all structures, and their strong localization in the range of the valence band near the Fermi energy is because of the contributions of  $3d$  orbitals, with the valence-band maximum(VBM) and conduction-band minimum(CBM) both located at the  $\Gamma$  point. However, for SiC, because hexagonality increases from 3C to 2H, the CBM state changes from the X point to the M point, and then to the K point.

A comparison between the calculated and experimental band gaps of the 2H structure is shown in Fig. 2. For GaN and ZnO, variation of the calculated band gaps of the different polytypes is not obvious, with a modulation of less than 0.2 eV. However, for SiC, the largest difference of the band gaps of the polytypes is about 1.0 eV.

By solving the Boltzmann transport equations with the relaxation time approximation, the thermoelectric transport coefficients can be expressed as<sup>54</sup>

$$\sigma = e^2 X_0 \quad (1)$$

$$S = \frac{-1}{eT} \left( \frac{X_1}{X_0} - \mu \right) \quad (2)$$

where  $e$  is the magnitude of the elementary charge,  $T$  is the absolute temperature,  $\mu$  is the chemical potential, and the integrals  $X_n$  ( $n = 0$  or  $1$ ) are functionals of the transport distribution function,<sup>55,56</sup> which are determined by the electronic structure and the electron scattering mechanisms of the material. Therefore, using the electronic structure, it is possible to calculate  $\sigma/\tau$  and  $S$  as a function of carrier concentration and temperature  $T$ . In this work, we focus on n-type materials, but it is worth pointing out that their p-type counterpart materials can also exhibit good or even better thermoelectric properties. The relaxation time  $\tau$  was assumed to be the same value for the polytypes of each compound, because our aim was to determine the relationship between the polytypes and the thermoelectric properties. Temperatures of 400, 600, 800, 1000, 1200, and 1400K were chosen to investigate the relationship between the power factor and hexagonality, and the relaxation time  $\tau$  of the same compound was set to be a constant at 10fs. Figure 3 shows the relationships between power factor and hexagonality for the three compounds at 1000K. In Fig. 3(a), the line shape of each power factor curve of the SiC polytype is different with the peaks appearing at different electron concentrations. The 4H structure has the highest power factor within the electron concentration range  $10^{20}$ – $10^{21}$  cm $^{-3}$ , and the 2H structure has the second highest power factor at  $5 \times 10^{21}$  cm $^{-3}$ . In Fig. 3(b), the relationships between the electron concentration and the power factor are almost the same for the GaN-3C, 2H, and 4H structures, with a slightly steeper decrease for the 6H structure. Interestingly, the power factor curves of the ZnO polytypes follow exactly the same trend as those of

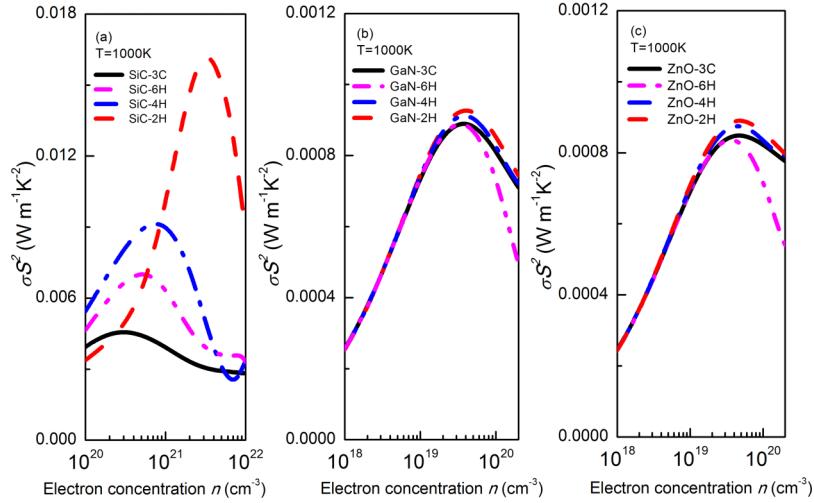


FIG. 3. Power factors of the different polytypes of (a) SiC, (b) GaN, and (c) ZnO at 1000K as a function of electron concentration.

the GaN polytypes, that is, their power factors show much weaker dependence on hexagonality than those of SiC.

We set the peak power factor of the 3C structure as a reference (set to be a unit). The relationships between the relative peak power factors at 1000K and hexagonality for the different polytypes are shown in Fig. 4(a). In the SiC polytypes, the relative peak power factor and the real peak power factor increase as the hexagonality increases. For GaN and ZnO, the peak power factors of their polytypes at 1000 K are almost the same. Figure 4(b) shows plots of the carrier concentration of the peak power factor against hexagonality, and the change of the peak positions follows the same trend.

Because it is usually difficult to achieve heavy doping, it is reasonable to choose  $n = 10^{18}$ – $10^{20} \text{ cm}^{-3}$  as a typical carrier concentration range. In this range, the 4H structure exhibits the highest power factor for SiC, while the 2H structures are the best for ZnO and GaN. Their thermoelectric properties at different temperatures were also investigated to determine the trends between the structures and temperature. Because it is relatively difficult to obtain a precise relaxation time  $\tau$  and thermal conductivity  $\kappa$  through calculations, we used an approximation approach to determine the figure of merit ( $ZT$ ). For ZnO, Ong *et al.*<sup>53</sup> estimated the relaxation time of 2H-ZnO as  $\tau = (2.53 \times 10^{-5})T^{-1}n^{-1/3}$  with  $\tau$  in s,  $T$  in K, and  $n$  in  $\text{cm}^{-3}$ , and calculated the thermal conductivity

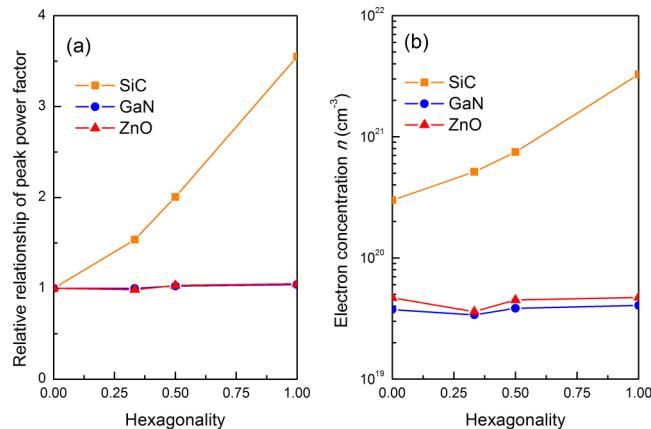


FIG. 4. (a) Plots of relative power factor against hexagonality at 1000K. (b) Plots of carrier concentration of the peak power factor against hexagonality at 1000K. The hexagonalities of 3C, 6H, 4H and 2H are 0, 0.33, 0.5, and 1, respectively.

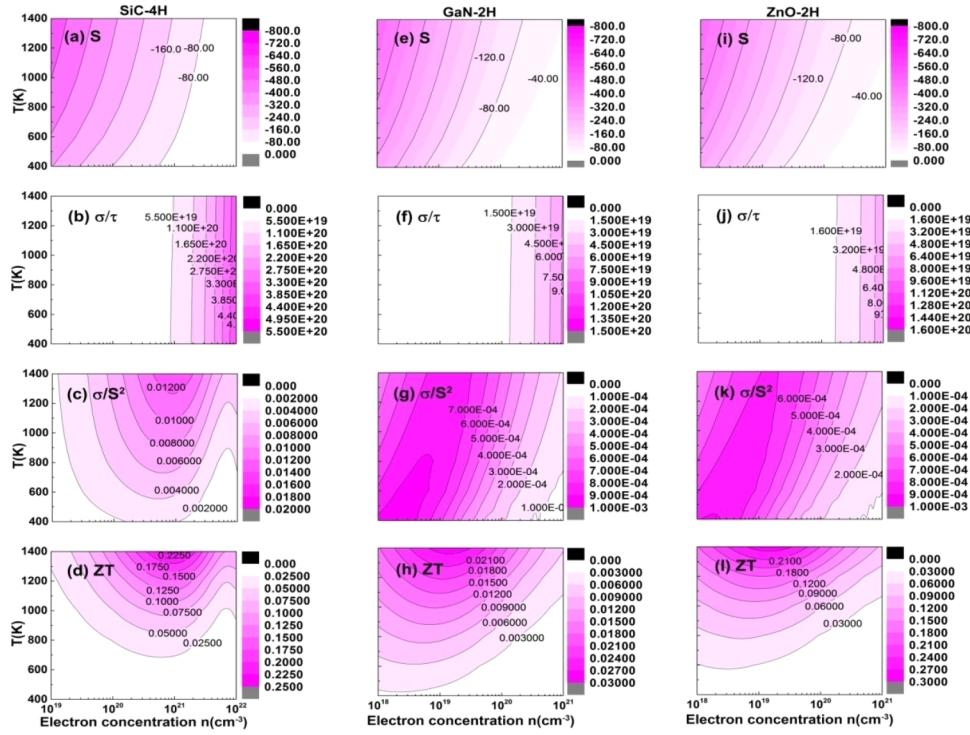


FIG. 5. Contour plots of the transport properties as a function of temperature and carrier concentration. (a)–(d) SiC-4H: Seebeck coefficient  $S(\mu\text{VK}^{-1})$ , electrical conductivity with respect to relaxation time  $\sigma/\tau(\Omega^{-1}\text{m}^{-1}\text{s}^{-1})$ , power factor  $\sigma S^2$  ( $\text{Wm}^{-1}\text{K}^{-2}$ ), and ZT value. (e)–(h)GaN-2H: Seebeck coefficient  $S(\mu\text{VK}^{-1})$ , electrical conductivity with respect to relaxation time  $\sigma/\tau(\Omega^{-1}\text{m}^{-1}\text{s}^{-1})$ , power factor  $\sigma S^2$  ( $\text{Wm}^{-1}\text{K}^{-2}$ ), and ZT value. (i)–(l)ZnO-2H:Seebeck coefficient  $S(\mu\text{VK}^{-1})$ , electrical conductivity with respect to relaxation time  $\sigma/\tau(\Omega^{-1}\text{m}^{-1}\text{s}^{-1})$ , power factor  $\sigma S^2$  ( $\text{Wm}^{-1}\text{K}^{-2}$ ),and ZT value.

by  $\kappa = (A - BT)/T$  with  $A = 12800 \text{ Wm}^{-1}$  and  $B = 5.2 \text{ Wm}^{-1}\text{K}^{-1}$ . These formulas were used by another group<sup>57</sup> to calculate the thermoelectric properties of GaN:  $\tau(T, n) = (2.55 \times 10^{-5})T^{-1}n^{-1/3}$  ( $\tau$  in s,  $T$  in K,  $n$  in  $\text{cm}^{-3}$ ) and  $\kappa = (5.85 \times 10^4)/T$  ( $\kappa$  in  $\text{Wm}^{-1}\text{K}^{-1}$ ,  $T$  in K). For 4H SiC, we set  $\tau = 10^{-14}$  s, and  $\kappa$  to follow a simple function:  $\kappa = B/T$ .<sup>53</sup> To obtain the constant  $B$ , we used previous data ( $T = 300\text{K}$ ,  $\kappa = 370\text{Wm}^{-1}\text{K}^{-2}$ ),<sup>58</sup> which gave  $B = 1.11 \times 10^5\text{Wm}^{-1}$ . The main purpose was to obtain a rough trend, which is shown in Fig. 5, where a darker color indicates a higher physical quantity. The carrier concentrations are extended to show the peak location. It is clear that ZT strongly increases with  $T$  up to the highest  $T$  in the range, which is consistent with the report of Ong *et al.*<sup>53</sup> One reason for the strong dependence of ZT on  $T$  dependence is that the three compounds investigated all possess large band gaps, and the power factor increases with  $T$ . Conversely, the electronic thermal conductivity has only a weak  $T$  dependence, while the lattice thermal conductivity strongly decreases with  $T$ . Our results show that it is possible to optimize the ZT of SiC, GaN, and ZnO by selecting a suitable carrier concentration range at high temperature. The significantly enhanced thermoelectric performance at high temperature and the high melting temperature of these three compounds indicate their potential high-temperature applications.

To understand the physical origin of the difference in the thermoelectric performance of the different polytypes of these three wide-band-gap semiconductors, the density of states (DOS) and ionicity were analyzed. For ZnO and GaN, the DOS for the various polytypes, as shown in Fig. 6, almost overlap and the difference is hard to distinguish. For SiC, the DOS of the 3C structure gradually increases while those of the hexagonal structures all exhibit a sharp increase. The diverse lines lead to the distinction of the power factors. The electronic differences among those compounds may have resulted from their different ionicity.<sup>59</sup> According to the model developed by Phillips,<sup>60</sup> the ionicities of SiC, GaN, and ZnO are 0.177, 0.500, and 0.616, respectively.<sup>61</sup> The 6H structure can be regarded as a stack of several 2H cells with special rotation, and the cubic structure (3C) also exhibits a hexagonal form in the [111] direction. To simplify the relationship between ionicity and

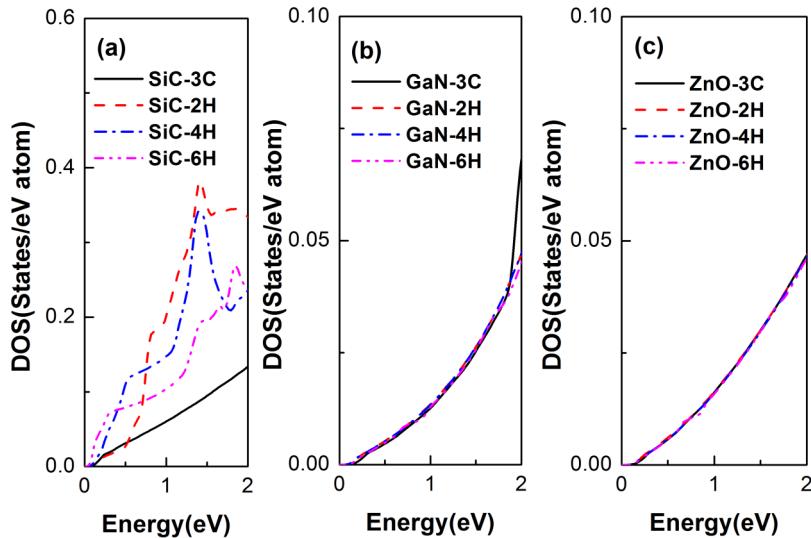


FIG. 6. DOS of the conduction band of different polytypes: (a) SiC, (b) GaN, and (c) ZnO. The conduction band minimum is set to zero eV.

polytype, we consider the polytypes as repetitive units of the 2H structure with angular deflection. Obviously, the thermoelectric performance shows a weaker dependency on the rotation offset for compounds with higher ionicity, such as GaN and ZnO. Covalent interactions decrease as ionicity increases, and the percentage of ionic bonds might influence the thermoelectric behavior of the polytypes. This is an interesting qualitative relationship, although the quantitative results are yet to be investigated.

#### IV. CONCLUSIONS

In summary, the thermoelectric properties of the polytypes of the wide-band-gap semiconductors SiC, GaN, and ZnO were investigated by first-principles calculations and Boltzmann transport theory. Compared with SiC, the power factors of GaN and ZnO show a very weak dependence on the polytype. Their figure of merit strongly increases with increasing temperature. The variation of the density of states in the polytypes leads to their different thermoelectric performance, which might be related to the competition between covalency and ionicity. Our results may provide a new way to enhance the thermoelectric properties of wide-band-gap semiconductors.

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