Thermoelectric properties of two-dimensional topological insulators doped with nonmagnetic impurities

L. L. Li and W. Xu

Citation: Journal of Applied Physics 116, 013706 (2014); doi: 10.1063/1.4886176
View online: http://dx.doi.org/10.1063/1.4886176
View Table of Contents: http://scitation.aip.org/content/aip/journal/jap/116/1?ver=pdfcov
Published by the AIP Publishing

Articles you may be interested in
Design principles for HgTe based topological insulator devices

Devices with electrically tunable topological insulating phases
Appl. Phys. Lett. 102, 063503 (2013); 10.1063/1.4792275

Photomixing in topological insulator HgTe/CdTe quantum wells in terahertz regime

Two-dimensional electron systems in HgTe quantum wells
Low Temp. Phys. 35, 6 (2009); 10.1063/1.3064862

Electrical properties of in situ As doped Hg 1x Cd x Te epilayers grown by molecular beam epitaxy
J. Vac. Sci. Technol. B 19, 1488 (2001); 10.1116/1.1374628
Thermoelectric properties of two-dimensional topological insulators doped with nonmagnetic impurities

L. L. Li1,a) and W. Xu1,2,b)
1Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei 230031, China
2Department of Physics, Yunnan University, Kunming 650091, China

(Received 11 April 2014; accepted 18 June 2014; published online 3 July 2014)

We present a theoretical study on the thermoelectric properties of two-dimensional topological insulators (2DTIs) doped with nonmagnetic impurities. We develop a tractable model to calculate the electronic band structure without additional input parameters and to evaluate the thermoelectric properties of 2DTIs based on CdTe/HgTe quantum wells. We find that with increasing the doping concentration of nonmagnetic impurity, the edge states dominate the thermoelectric transport and the bulk-state conduction is largely suppressed. For typical sample parameters, the thermoelectric figure of merit $ZT$ (a quantity used to characterize the conversion efficiency of a thermoelectric device between the heat and electricity) can be much larger than 1, which is a great advance over conventional thermoelectric materials. Furthermore, we show that with decreasing the 2DTI ribbon width or the Hall-bar width, $ZT$ can be considerably further improved. These results indicate that the CdTe/HgTe 2DTIs doped with nonmagnetic impurities can be potentially applied as high-efficiency thermoelectric materials and devices. © 2014 AIP Publishing LLC. [http://dx.doi.org/10.1063/1.4886176]

I. INTRODUCTION

The thermoelectric effect can be utilized for mutual conversion between the heat energy and electric energy. The conversion of heat to electricity refers to the Seebeck effect, whereas the conversion of electricity to heat is called the Peltier effect. Such two effects have great technological applications in refrigeration and no-medium refrigeration.1 As a result, thermoelectrics is making an impact on the energy technology. For example, the Seebeck effect can be utilized to convert heat energy (i.e., the wasted heat from industry) into electricity for energy saving.2 It is known that the efficiency of thermoelectric conversion is one of the most challenging problems in solid-state electronics and material science. This property depends on the transport coefficients of a thermoelectric material through the figure of merit $ZT$, which is defined as

$$ZT = \frac{T \sigma S^2}{\kappa_e + \kappa_p}.$$  \hspace{1cm} (1)

Here, $\sigma$ is the electric conductivity, $S$ is the Seebeck coefficient (or thermopower), $T$ is the lattice temperature, and $\kappa_e$ and $\kappa_p$ are the electronic and phononic contributions to the thermal conductivity, respectively. The power factor is defined as $PF = \sigma S^2$, which characterizes the electric power output. For practical device applications, it is necessary to look for thermoelectric materials with larger $ZT$. There have been several proof-of-principle suggestions to improve the thermoelectric figure of merit. The most popular proposal is the electron conductor and phonon insulator.3 However, such two conditions often conflict with each other because the scattering centers felt by phonons are also felt by electrons at the same time, which makes it difficult to improve $ZT$. Another proposal to improve $ZT$ is to utilize the electronic systems with reduced dimensionality,4 in which the electronic density-of-states show a sharp peak structure and, thus, can achieve a large $S$.

In recent years, two-dimensional (2D) and three-dimensional (3D) topological insulators (TIs) have been theoretically predicted and experimentally observed.5–17 These new quantum states of matter are characterized by gapped insulating bulk states and gapless conducting edge/surface states. Rich and interesting physical properties, such as intrinsic spin Hall effect,18 finite-size effect,20 optical and transport phenomena,22 weak and anti-weak localizations,24,25 magneto-electric coupling and magneto-optic effect,26,27 and RKKY interactions between magnetic impurities,28,29 in TIs have been investigated. Recently, 3DTIs have been proposed as good thermoelectric materials.30–32 The results have shown that by utilizing the unique properties of TI, i.e., topologically protected surface states, combined with the methods to reduce the thermal conductivity, the thermoelectric efficiency of TI materials can be markedly improved. Although 2DTIs have also been proposed as novel thermoelectric materials,33,34 it was pointed out that the topologically robust edge states in 2DTIs do not improve the thermoelectric efficiency dramatically beyond the present-day materials.30 We notice that the previous theoretical results30–34 were obtained by taking a crude band structure model with additional free parameters such as the bulk electron effective mass, the bulk energy-gap and the edge (surface) subgap induced by the coupling of edge (surface) states. As is known, in 2DTIs realized from semiconductor quantum well (QW) structures,7 these parameters depend strongly on material and structure parameters such as the QW thickness6 and the width of the sample (or the Hall-bar width).20 Hence, it is necessary and worth to re-examine the thermoelectric properties of a 2DTI based on semiconductor heterostructures and to see how we can achieve a large $ZT$ in

---

a)Electronic mail: lllihfca@foxmail.com
b)Electronic mail: wenxu_issp@aliyun.com
The paper is organized as follows. In Sec. II, we present the theoretical approach to calculate the bulk- and edge-state energy spectra for a 2DTI and the corresponding thermoelectric properties such as the transport coefficients $\sigma$, $S$, $\kappa_e$, and the figure of merit $ZT$. In Sec. III, the numerical results are presented and discussed for the 2DTIs realized from CdTe/HgTe QWs. Finally, the concluding remarks are summarized in Sec. IV.

II. THEORETICAL APPROACH

A. Kane model for semiconductor QWs

We consider a symmetric CdTe/HgTe/CdTe QW with a thickness $L$ grown along the [001] direction (taken as the $z$-direction). Such a QW structure has a type-II band alignment, as illustrated in Fig. 1(a). The critical feature of type-II QWs is the band inversion: the barrier material such as CdTe has a normal band sequence with the lowest conduction band lying above the highest valence band, and the well material such as HgTe has an inverted band sequence with the lowest conduction band lying below the highest valence band due to strong intrinsic spin-orbit interactions.

In the set of the following basis state:

$$|1\rangle = |S - \frac{1}{2}\rangle = |iS - \uparrow\rangle, \quad (2a)$$
$$|2\rangle = \begin{pmatrix} \frac{1}{2} & \frac{3}{2} \\ -\frac{1}{2} & \frac{3}{2} \end{pmatrix} = -\frac{1}{\sqrt{2}}(X + iY) \downarrow\rangle,\quad (2b)$$
$$|3\rangle = \begin{pmatrix} 3 & 1 \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} = -\frac{1}{\sqrt{6}}(X + iY) \downarrow -2Z \rangle, \quad (2c)$$
$$|4\rangle = |S - \frac{1}{2}\rangle = |iS \downarrow\rangle, \quad (2d)$$
$$|5\rangle = \begin{pmatrix} 3 & -3 \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} = \frac{1}{\sqrt{2}}(X - iY) \downarrow\rangle, \quad (2e)$$
$$|6\rangle = \begin{pmatrix} 3 & 1 \rangle = \frac{1}{\sqrt{6}}(X - iY) \uparrow + 2Z \rangle, \quad (2f)$$

the six-band Kane Hamiltonian for unstrained bulk HgCdTe can be written as

$$H(K) = \begin{bmatrix} A - \sqrt{3} \nu' & \sqrt{2}U & 0 & 0 & \nu \\ -\sqrt{3} \nu & -\nu - Q & \sqrt{2}U & 0 & 0 \\ \sqrt{2}U & \sqrt{2}R & -\nu + Q & -\nu & S \\ 0 & 0 & -\nu' & A & \nu' \\ 0 & 0 & S' & \nu & -\nu \\ \nu' & S' & 0 & \sqrt{2}U & -\sqrt{2}R \\ \nu & 0 & 0 & -\sqrt{2}R & -\nu + Q \end{bmatrix}, \quad (3)$$

where

$$A = E_c + A_k, \quad \text{(4a)}$$
$$P = P_k - E_v, \quad \text{(4b)}$$
$$Q = Q_k, \quad \text{(4c)}$$
$$A_k = \lambda A_c(k^2 + k_z^2), \quad \text{(4d)}$$
$$P_k = \lambda \gamma_1(k^2 + k_z^2), \quad \text{(4e)}$$
$$Q_k = \lambda \gamma_2(k^2 - 2k_z^2), \quad \text{(4f)}$$
$$R = \lambda \sqrt{6} \gamma_3(k_i - k_z)k_z, \quad \text{(4g)}$$
Here, instead of a usual eight-band form, we use a six-band representation for the Kane Hamiltonian since the split-off-hole band is well separated from the heavy-hole and light-hole bands in HgCdTe systems. In the above equations, the symbols $|S\rangle$, $|X\rangle$, $|Y\rangle$, $|Z\rangle$ represent the Bloch atomic orbitals for the lowest conduction band and the highest valence bands; the labels $\uparrow$ and $\downarrow$ indicate the up and down spinors for each orbitals; $\lambda = \hbar^2/(2m_0)$; and $k^2 = k_x^2 + k_y^2$. $E_c$ and $E_v$ are the unstrained conduction- and valence-band edges, respectively; $A_k = 1 + E_p\beta(E_v - \Delta_m)$ relates to the electron effective mass via taking into account indirectly the coupling of the conduction band to the split-off-hole band to the conduction-band electron effective mass,\textsuperscript{35} with $E_g = E_v - E_c$ being the fundamental band-gap, $\Delta_m$ the spin-orbit splitting energy, and $P_0$ the Kane’s momentum matrix element; and $E_p$ is an energy parameter related to the Kane’s momentum matrix element $P_0$ by $E_p = 2m_0P_0^2/\hbar^2$, and $\gamma_j$ ($j = 1, 2, 3$) are three valence-band Luttinger parameters.

The energy spectrum and the corresponding wavefunction for electron in the QW are determined by the Schrödinger equation

$$H\Psi = E\Psi,$$

where $\Psi$ is the wave function and $E$ is the subband energy in the QW system. Within the envelope function theory (EFT),\textsuperscript{36} the total wave function $\Psi$ can be expanded as a linear combination of the zone center Bloch states $u(r)$ multiplied by a slowly varying envelope function $g(z)$, which reads

$$\Psi(R) = e^{ikz}\sum_{n=1}^{6} u_n(r)g_n(z),$$

where $R = (r, z) = (x, y, z)$, $k = (k_x, k_y)$ is the in-plane wave vector, and $n$ is the band index of the Bloch state. The EFT states that if $\Psi(R)$ is the solution of the Schrödinger equation, $g_n(z)$ is the solution of the following equation:

$$H(k_x, k_y)F(z) = EF(z),$$

where $F(z)$ is a six-component envelope function composed of different $g_n(z)$ ($n = 1, 2, \ldots, 6$). The Kane Hamiltonian can be expanded into its polynomial form for $k_z$ (the momentum operator along the $z$-direction) in the following way:

$$H(k_x, k_y) = H^{(2)}(k)k_z^2 + H^{(1)}(k)k_z + H^{(0)}(k),$$

where $H^{(2)}(k)$, $H^{(1)}(k)$, and $H^{(0)}(k)$ were documented previously.\textsuperscript{27} By replacing $k_z$ with $-i\partial/\partial z$, we can transform Eq. (6) into a set of coupled second-order differential equations

$$-H^{(2)}(k)\frac{d^2}{dz^2} - iH^{(1)}(k)\frac{d}{dz} + H^{(0)}(k)F(z) = EF(z).$$

This Hamiltonian equation can be numerically solved for the QW energy spectrum and corresponding wavefunction using the plane wave expansion method.\textsuperscript{38}

B. Reduced effective Hamiltonian

After obtaining the QW subband energies and corresponding wavefunctions at the center of Brillouin zone (the $\Gamma$ point), we can construct the reduced effective Hamiltonian or effective two-dimensional (2D) Hamiltonian for the system. At the $\Gamma$ point, the six-component wavefunctions can be written in the form of column vector as $F_j(z) = [g^{(1)}_j(z), g^{(2)}_j(z), g^{(3)}_j(z), g^{(4)}_j(z), g^{(5)}_j(z), g^{(6)}_j(z)]^T$, which satisfy the following Schrödinger equation:

$$H\left(k = 0, -i\frac{d}{dz}\right)F_j(z) = E_jF_j(z),$$

where $E_j$ is the energy level for the $j$th subband at the $\Gamma$ point. Here, we choose the zone-center envelope functions $F_{j,\uparrow}(z)$, $F_{j,\downarrow}(z)$, $F_{j,\uparrow\uparrow}(z)$, and $F_{j,\downarrow\downarrow}(z)$ as the basis functions, with $E$ and $H$ labeling the lowest electron and the highest hole subbands and $\uparrow/\downarrow$ denoting the spin up/down states. By averaging the $z$-component of six-band Kane Hamiltonian under such basis functions, we obtain an effective 2D Hamiltonian

$$H^\ddagger_{\text{eff}}(k) = \int_{-\infty}^{+\infty} dzF_j^\dagger(z)H(k, -i\frac{d}{dz})F_j(z),$$

where $i$ and $j$ represent the electron and hole subband indices in the basis functions. In the absence of structure and bulk inversion asymmetries, the effective 2D Hamiltonian consists of two decoupled blocks, which as related by the TR symmetry. The matrix form of such an effective Hamiltonian is given by

$$H^\ddagger_{\text{eff}}(k) = \begin{bmatrix}
E_e + Bk^2 & Ak_+ & 0 & 0 \\
A^*k_- & E_h + Ck^2 & 0 & 0 \\
0 & 0 & E_e + Bk^2 & -Ak_- \\
0 & 0 & -A^*k_+ & E_h + Ck^2
\end{bmatrix},$$

where $k_\pm = k_x \pm i k_y$, $E_e$ and $E_h$ are the lowest electron and the highest hole subband energies at the zone center, respectively. $B$ and $C$ are related to the electron and heavy-hole effective masses, and $A$ is determined by the overlap of zone-center wavefunctions for the lowest electron and the highest hole subbands. These parameters depend sensitively on the QW thickness and the temperature.

To calculate the 2DTI band structure including the bulk-state and edge-state energy spectra, we should consider a Hall-bar structure in the QW plane [see Fig. 1(b)], which is commonly used in the magneto-transport measurements. The Hall-bar width is $W$ along the $y$-direction, which corresponds just to the ribbon width of the 2DTI. Furthermore, we
assume the periodic boundary condition in the \(x\)-direction and hard-wall boundary condition in the \(y\)-direction. In this case, \(k_x\) is a good quantum number but \(k_y\) should be replaced by \(-id/dy\).

The energy spectrum and wavefunction for the 2DTI are determined by the following Schrödinger equation associated with the effective 2D Hamiltonian:

\[
H_{\text{eff}}(k_x, -i d/dy) \Phi_{k_y}(r) = E(k_x) \Phi_{k_y}(r),
\]

(13)

where \(E(k_x)\) is the energy dispersion and \(\Phi_{k_y}(r) = e^{ik_yy} [\phi_1(y), \phi_2(y), \phi_3(y), \phi_4(y)]^T\) is a four-component wave function with \(\phi_j(y)\) being the envelope function along the \(y\)-direction satisfying the hard-wall boundary condition

\[
\phi_j(y)|_{y = \pm W/2} = 0 \quad (j = 1, 2, 3, 4).
\]

(14)

To solve this effective 2D Hamiltonian equation, a finite difference method with the hard-wall boundary condition is used.\(^{39}\)

### C. Thermoelectric transport coefficients

In the linear response regime, the low-field transport coefficients for thermoelectric materials are described by the following Onsager relations:

\[
J_E = \sigma L_0 E + \frac{e L_1}{T} \nabla T
\]

(15a)

and

\[
J_T = -e L_1 E - \frac{L_2^2}{T} \nabla T,
\]

(15b)

where \(J_E/J_T\) are the electric/thermal current densities, \(\sigma\) is the electron charge, and \(E\) is the electric field. The electronic conductivity \(\sigma\), the Seebeck coefficient \(S\), and the thermal conductivity \(\kappa_e\) can be expressed in terms of the transport coefficients \(L_j\) \((j = 0, 1, 2)\) as follows:

\[
\sigma = e^2 L_0, \quad S = -\frac{1}{eT} L_1, \quad \kappa_e = \frac{1}{T} \frac{L_0 L_2 - L_1^2}{L_0},
\]

(16a-16c)

It should be noted that Eqs. (16a)-(16c) only take into account of electronic contributions to thermoelectric transport and phononic contributions are neglected. Inserting these expressions into Eq. (1), the figure of merit \(ZT\) can be written as

\[
ZT = \frac{L_1^2}{L_0 L_2 - L_1^2 + \kappa_p T L_0}.
\]

(17)

where \(\kappa_p\) is the phononic thermal conductivity.

Because the edge states in a 2DTI are perfectly conducting, they can be considered as 1D ballistic transport channels. Thus, the electronic transport for edge states can be described by the Landauer-Büttiker formula. The transport coefficients \(L^\text{edge}_j\) \((j = 0, 1, 2)\) are given by\(^{13}\)

\[
L^\text{edge}_j = \frac{n \hbar}{\eta} \int_{-\Delta/2}^{\Delta/2} dE (E - \mu)^j \left( -\frac{\partial f}{\partial E} \right),
\]

(18)

where \(\eta = 2\) accounts for the spin degeneracy, \(l\) and \(s\) represent the sample’s length and the cross-section area of the sample, \(h\) is the Plank’s constant, \(T(E)\) is the energy-dependent transmission coefficient, \(\mu\) is the chemical potential in the system, and \(f(E)\) is the Fermi-Dirac distribution function. In a 2DTI, the energy spectrum is characterized by gapped bulk states and gapless edge states. When the electron energy \(E\) lies inside the bulk energy-gap \(\Delta\), the transmission probability \(T(E) = 1\), which reflects the perfect conduction of the edge states. Under above considerations, the transport coefficients for gapless edge states can be written as

\[
L^\text{edge}_j = \frac{n \hbar}{\eta} \int_{-\Delta/2}^{\Delta/2} dE (E - \mu)^j \left( -\frac{\partial f}{\partial E} \right),
\]

(19)

where \(\Delta/2 (\sim \Delta/2)\) denotes the bottom (top) of bulk conduction (bulk valence band).

When the finite-size effect is taken into account, the edge states on the two boundaries of the Hall-bar can couple together to produce a subgap \(\delta\) in the energy spectrum.\(^{20}\) Due to the presence of such a subgap, the range of integral in \(L^\text{edge}_j\) no longer includes the energy region between \(-\delta/2\) and \(\delta/2\). Furthermore, the transmission coefficient for gapped edge states becomes \(T(E) = f(1 - \delta/2 - \mu)/k_BT - f(1 - \delta/2 - \mu)/k_BT + 1\), as given by the previous work.\(^{20}\) Consequently, the transport coefficients for gapped edge states can be written as

\[
L^\text{edge}_j = \frac{n \hbar}{\eta} \int_{-\delta/2}^{\delta/2} dE (E - \mu)^j \left( -\frac{\partial f}{\partial E} \right),
\]

(20)

where \(F_j(E) = T(E)(E - \mu)^j (-\partial f/\partial E)\).

Applying the relaxation time approximation to the Boltzmann equation, the transport coefficients \(L^\text{bulk}_j\) \((j = 0, 1, 2)\) for gapped bulk states are given by

\[
L^\text{bulk}_j = \frac{n \hbar}{s} \int_{-\infty}^{\infty} d\varepsilon \Pi(\varepsilon)(\varepsilon - \mu)^j \left( -\frac{\partial \varepsilon}{\partial \varepsilon} \right),
\]

(21)

where \(\Pi(\varepsilon)\) is a function depending on the band structure of specific material system. For the bulk states in the 2DTI, the function \(\Pi(\varepsilon)\) is given by\(^{40}\)

\[
\Pi(\varepsilon) = \sum_{k_x} v(k_x) v(k_x) \tau(k_x) \delta[\varepsilon - E(k_x)],
\]

(22)

where \(\tau(k_x)\) is the relaxation time, which is assumed to be a constant \(\tau\) and \(v(k_x)\) is the group velocity related to the band structure, which is given by

\[
v(k_x) = \frac{1}{\hbar} \frac{\partial E(k_x)}{\partial k_x} = \frac{1}{\hbar} \left( \Phi_{k_x} \left| \frac{\partial H^\text{eff}(k)}{\partial k_x} \right| \Phi_{k_x} \right)^{\dagger},
\]

(23)
Taking into account of both the edge- and bulk-state contributions, the total transport coefficients are then given by

\[ L_j = L_j^{\text{edge}} + L_j^{\text{bulk}} \quad (j = 0, 1, 2). \]  

(24)

III. RESULTS AND DISCUSSION

In this section, we present the numerical results and discussions on the band structure and thermoelectric properties of 2DTIs at relatively low temperatures (i.e., \( T \leq 70 \) K). For band structure calculation, the parameters such as \( E_{p}, \Delta_{p}, \gamma_{1}, \gamma_{2}, \) and \( \gamma_{3} \) are taken from Ref. 41. These parameters are frequently used and well documented in the literature. The valence band offset between HgTe and CdTe is taken to be 570 meV at \( T = 0 \) K (Ref. 41) and the temperature dependence of band-gap for HgI–CdTe alloys can be obtained in the previous work. 42

For the thermoelectric calculation, the transport parameters such as \( l, s, W, \tau, \) and \( \kappa_{p} \) are needed. We take the sample length as \( l = 1 \) \( \mu \)m.30,33 The cross-section area of the sample is taken as \( s = 100 \) nm \( \times 10 \) nm. The electron relaxation time \( \tau \) is taken as variable to study the nonmagnetic-impurity effect on the thermoelectric properties of 2DTIs. This is based on the fact that in doped semiconductor systems \( \tau \) is inversely proportional to the impurity density at relatively low temperatures where electron-impurity scattering determines mainly the electron mobility. The Hall-bar width \( W \) is also varied to investigate the finite-size effect on the thermoelectric properties of 2DTIs. Since the phonon conduction is also inversely proportional to the impurity density at relatively low temperatures due to dominant impurity scattering, we simply assume \( \kappa_{p}/\kappa_{0} = \tau/\tau_{0} \), where we take \( \kappa_{0} = 10 \) Wm\(^{-1}\)K\(^{-1}\) for \( \tau_{0} = 10^{-11} \) s.

In Fig. 2(a), we show the typical band structure of a CdTe/HgTe 2DTI with QW thickness \( L = 8 \) nm and Hall-bar width \( W = 400 \) nm at a fixed temperature \( T = 60 \) K. It is clear that in the 2DTI system, there indeed exist the gapless edge states lying inside the gapped bulk states. The characteristic features for edge and bulk states can be more clearly demonstrated by their probability densities \( \left| \Phi_{\text{edge}}(x, y) \right|^{2} \) and \( \left| \Phi_{\text{bulk}}(x, y) \right|^{2} \). As can be seen from Figs. 2(b) and 2(c), the edge (bulk) states are nearly located at the boundary (interior) of 2DTI system. Therefore, one can imagine that when a 2DTI sample is doped with a high density of nonmagnetic impurities, the bulk-state and phonon conductivities would be largely suppressed due to the strong impurity scattering.

In Figs. 3(a) and 3(b), we show the 2DTI band structures and edge-state wavefunctions for two different Hall-bar widths \( W = 400 \) and 100 nm at fixed QW thickness \( L = 8 \) nm and temperature \( T = 60 \) K. As can be seen, when the Hall-bar width is decreased, the edge states at the two boundaries of the 2DTI system can substantially overlap to produce a sub-gap of about several meV in the energy spectrum. In addition, the bulk energy-gap is enlarged and the number of bulk bands is reduced due to the quantum size effect. These interesting features can affect strongly the thermoelectric transports for the edge and bulk states, which can be seen clearly in the later part of the discussion.

Now we discuss the effect of nonmagnetic-impurity on the thermoelectric properties of CdTe/HgTe 2DTIs. For numerical calculations, the QW thickness, the temperature and

FIG. 4. Figure of merit as a function of the chemical potential for various 2DTIs doped with different impurity densities characterized by different electron relaxation times \( \tau \) as indicated. Here, the red and green solid curves represent the bulk- and edge-state contributions to the total \( ZT \) denoted by the blue solid curve.
the Hall-bar width are fixed at $L = 8 \text{ nm}$, $T = 60 \text{ K}$, and $W = 400 \text{ nm}$, respectively. The thermoelectric figure of merit $ZT$ is calculated for various 2DTIs doped with different impurity densities characterized by different electron relaxation times. The calculated results are shown in Fig. 4. As can be seen from Eqs. (16a)–(16c), the contributions from the edge and bulk states to the electronic conductivity are simply additive, but to the Seebeck coefficient and electron thermal conductivity are not simply additive. Therefore, from Eq. (1) one can see that the contributions from the edge and bulk states to $ZT$ are not simply additive but exhibit the following interesting behaviors. (1) In the case of a large $\tau$ (i.e., $\tau = 10^{-15} \text{ s}$) corresponding to a low impurity concentration, the bulk states dominate in the thermoelectric transport and the total $ZT$ exhibits the bulk-state behavior. (2) With reducing $\tau$ (i.e., $\tau = 10^{-13} \text{ s}$) or increasing the impurity concentration, the bulk-states compete with the edge states in the thermoelectric transport and their contributions to the transport tend to cancel each other, leading to a very small $ZT$. (3) In the case of a small $\tau$ (i.e., $\tau = 10^{-15} \text{ s}$) corresponding to a high impurity concentration, the edge-state transport becomes dominant while the bulk-state transport and the phonon conduction are largely suppressed. The total $ZT$ exhibits the edge-state behavior and can reach up to 6, which is much larger than that for conventional thermoelectric materials (usually smaller than 1). This implies that to realize the edge-state dominant transport and suppressed phonon conduction that can lead to a large $ZT$, the 2DTIs should be doped with nonmagnetic impurities of a high concentration.

Furthermore, we should point out that both of the edge-state contribution to $ZT$ in Fig. 4(a) and the bulk-state contribution to $ZT$ in Fig. 4(c) are not zero. They seem to be vanishing because of the scales used in the figure. Owing to the feature that the contributions from the edge and bulk states to $ZT$ are not simply additive, for the whole chemical potential region, i.e., $0 \leq \mu \leq 60 \text{ meV}$, the total $ZT$ may be larger than, equal to or smaller than the bulk- and edge-state contributions, depending on the position of chemical potential as well as the electron relaxation time used to characterize the doping level of nonmagnetic impurity.

Next we discuss the dependence of thermoelectric transport in 2DTIs on the Hall-bar width. The QW thickness, the temperature, and the relaxation time are fixed at $L = 8 \text{ nm}$, $T = 60 \text{ K}$, and $\tau = 10^{-15} \text{ s}$, respectively. As mentioned before, when the Hall-bar width is decreased, the edge states at the two boundaries of the 2DTI system can hybridize to form a subgap up to tens of meV (see Fig. 3), which can achieve an enhanced Seebeck coefficient. Moreover, since the number of bulk bands participating in the transport process is reduced, the edge states become dominant in the thermoelectric transport, leading to a dramatic increase of the electric conductivity. Therefore, the total $ZT$ increases with decreasing the Hall-bar width $W$, as shown in Fig. 5. In addition, we observe from this figure a shift in the maximum of $ZT$ as a function of $\mu$ when $W$ is reduced. As can be seen from Fig. 6, there are many subband minimums for the bulk states and $ZT$ has a maximum when $\mu$ is near one of the lowest subband minimums. The maximum of $ZT$ occurs due to the competition between the edge- and bulk-state transports around the bulk band minimum. With decreasing $W$, the energies at these minimum points increase due to the quantum size effect. As a result, a shift is induced in the maximum of $ZT$ as a function $\mu$ when $W$ is reduced.

![Fig. 5. Total figure of merit $ZT$ as a function of the chemical potential for different Hall-bar widths $W$ as indicated.](image)

![Fig. 6. (a) Band structure and (b) figure of merit for a 2DTI with $L = 8 \text{ nm}$, $W = 200 \text{ nm}$, $T = 60 \text{ K}$, and $\tau = 10^{-15} \text{ s}$. Here, in panel (a) the red solid lines and black solid curves represent the edge and bulk spectra, in panel (b) the blue solid curve represents the total figure of merit, and the black dotted line indicates the energy position of the third bulk subband minimum.](image)

$T = 60 \text{ K}$, and $\tau = 10^{-15} \text{ s}$, respectively.

### IV. CONCLUSION

In this paper, we have theoretically investigated the thermoelectric properties of 2DTIs realized from CdTe/HgTe QWs. We have started from a realistic band structure model...
and then calculated the corresponding thermoelectric transport properties on the basis of band structure results. The main advantage of present band-structure model is that no additional free parameters are required except for the well-known material parameters. It has been found that the thermoelectric transports for edge and bulk states in a 2DTI can be tuned effectively by adjusting the nonmagnetic impurity concentration which is characterized by the electron relaxation time. To realize the edge-state dominant transport that can lead to an enhanced ZT, the concentration of nonmagnetic impurity should be high. In such a case, the bulk-state conduction can be largely suppressed. For reasonable sample parameters, ZT can be much larger than 1, which is a great advance over conventional thermoelectric materials. Moreover, we have found that ZT can be considerably further improved by narrowing the Hall-bar width. These theoretical findings have demonstrated that the CdTe/HgTe 2DTIs doped with many nonmagnetic impurities can be potentially used to design high-efficiency thermoelectric materials and devices.

ACKNOWLEDGMENTS

This work was supported the National Natural Science Foundation of China (Grant No. 11304316), Ministry of Science and Technology of China (Grant No. 2011YQ130018), Department of Science and Technology of Yunnan Province, and by the Chinese Academy of Sciences.