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The viability of Si-Ge alloys in thermoelectric applications lies in its high figure-of-merit, non-toxicity and earth-abundance. However, what restricts its wider acceptance is its operation temperature (above 1000 K) which is primarily due to its electronic band gap. By means of density functional theory calculations, we propose that iso-electronic Sn substitutions in Si-Ge can not only lower its operation to mid-temperature range but also deliver a high thermoelectric performance. While calculations find a near invariance in the magnitude of thermopower, empirical models indicate that the materials thermal conductivity would also reduce, thereby substantiating that Si-Ge-Sn alloys are promising mid-temperature thermoelectrics. © *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/10.1063/1.4916918]

Thermoelectric devices, which convert heat to electricity are solid state heat engines, the application of which on a commercial scale can render a solution to the increasing energy crisis. Since dissipation from various heat sources occurs over a wide temperature range, thermoelectric based technology therefore becomes a ubiquitous choice not only for energy generation but also to improve the over-all efficiency. For near room temperature applications (T < 450 K), Bi_2Te_3 based materials prove to be the choice,[1–9] while for high temperature (T > 900 K) applications it is the Si-Ge based alloys. For thermoelectric applications in the mid-temperature range (400 - 900 K) the search for an ideal material is being intensely pursued by scientists and engineers. The current promise which centers around PbTe based alloys[10–14] is less commercially acceptable due to its toxicity. Other materials of choice for mid temperature applications are the skutterudites, however, the presence of rare-earth ions pose serious limitations to the cost-optimized routine applications. Alternatively, it has been proposed that engineering the materials properties of low temperature thermoelectrics could elevate the operating temperatures.[15–17] The proposed methods are, however, not only expensive but are also being overlooked in terms of its scalability, reproducibility and durability. In this work, we propose band structure engineering of Si-Ge thermoelectrics, which by iso-electronic Sn substitutions can lower its operating temperature to the mid-temperature range. Devoid of toxicity and, that there exists a number of processing techniques of these earth abundant constituents, synthesis and optimization of these alloys if accomplished in experiments could resolve thermoelectrics as a green solution to the increasing energy demands.[18–21]

Si-Ge alloys display high thermoelectric performance at high temperatures and have played an integral role in power generation in extra-terrestrial space missions. Since Si and Ge have a relatively large electronic band gap, their binary alloys are quite suitable for high temperature operations, since problems with bipolar conduction are inhibited. Besides, the large phonon scattering associated with the underlying lattice also ensures a low thermal conductivity, with little effects on the materials electron mobility, thereby preserving the overall thermoelectric performance.[22]

To maximize power generation efficiency of a thermoelectric device, it is in the prerequisites that the temperature differential between the hot and cold sides of the thermoelectric generator must be as large as possible. Taking full advantage of the high temperature capabilities and mechanical properties of Si-Ge, the temperature of the hot end could be alleviated to $1000 - 1200$ K which is attained

by means of radiation based heat source. However, this largely limits the materials applications for terrestrial purposes. Noting that the operating temperature (T_O) of such a device is empirically governed by the $E_G = 10K_BT_C$ rule, where E_G and K_B are the band gap energy and Boltzmann's constant respectively, a work around to bring the Si-Ge alloys to operate in the mid-temperature range would prescribe to a reduction in the electronic band gap of the material, for which band gap engineering techniques would become useful.

The ab-initio calculations were performed using the full-potential linear augmented plane wave (FP-LAPW) method as implemented in the WIEN2K package.[23] Chemical disorder was modeled using the special quasi-random structure (SQS).[24] In SQS formalism, chemical disorder is incorporated by mimicking the correlation functions of a random alloy within that of a finite super-cell. In the present study, the structure for $Si_{0.75}Ge_{0.25}$ and $Si_{0.50}Ge_{0.125}Sn_{0.375}$ were adapted from Ref. 25. The equation of state parameters were computed by means of force and total energy minimization using the generalized gradient approximation (GGA),[26] while the electronic structure and transport properties were calculated following the prescription of Engel and Vosko[27] for the exchange-correlation effects. The transport properties were calculated within the constant relaxation-time approximation of the Boltzmann transport equation, as implemented in the BoltzTraP code.[28] Up to 4900 k-points in the Brillouin zone (BZ) were used to perform the averaging.

We note that binary $Si_{1-x}Sn_x$ has been extensively studied in the past, both experimentally and theoretically.[29–34] To study the effects of Sn substitutions in Si-Ge alloys ($Si_{0.50}Ge_{0.125}Sn_{0.375}$), we compute the properties of $Si_{0.75}Ge_{0.25}$ - a near composition that had been extensively used in thermoelectric applications, with its thermoelectric figure-of-merit (ZT) being 1.3 and 0.95 for n and p type, respectively.[35,36] For the fully relaxed structure, the equilibrium lattice constant (bulk modulus) were determined as 5.536 Å (80.5 GPa) and 5.899 Å (52.1 GPa) for $Si_{0.75}Ge_{0.25}$ and $Si_{0.50}Ge_{0.125}Sn_{0.375}$, respectively. The estimated bulk modulus, for $Si_{0.75}Ge_{0.25}$ is in good agreement with the phenomenological expression given as $(97.9 - 22.8\,x)$ GPa with x being the Ge $at.\%$ in $Si_{1-x}Ge_x$ alloys.[37] The notable reduction in the bulk modulus with Sn substitutions indicate to a soft underlying lattice, which is quite preferential to thermoelectric materials design. Note that bulk modulus is correlated with the velocity of sound and thus its low values infer to soft underlying phonon modes.

The electronic density of states (DOS) of $Si_{0.75}Ge_{0.25}$ is shown in Fig. 1(a). As like that for FCC Si, three energy regions are identified in the valence band region : In the energy range $-12 \le E$ (eV) ≤ -8, the states are primarily "s" in character, followed by an amalgam of s and p states over the energy range $-8 \le E$ (eV) ≤ -4. The near vicinity of the Fermi energy ($E_F \equiv 0$ eV) which extends from $-4 \le E$ (eV) $\le E_F$ constitute the p bands. The band gap of $Si_{0.75}Ge_{0.25}$, in the Engel-Vosko parameterization of the exchange correlation, is estimated as 1.14 eV and is consistent with the earlier reports.[38–40]

The density of states for $Si_{0.50}Ge_{0.125}Sn_{0.375}$ (Fig. 1(b)), preserves most of the valence band features, in particular the three energy regions of the valence band. The distribution of states appears quite similar to an otherwise ordered system. Since in these alloys, disorder is associated with iso-electronic chemical substitutions and that their electro-negativities being more or less similar (Si : 1.90, Ge : 2.01 and Sn : 1.96), it is least expected that the alloy density of states would display any additional feature in the spectra. However, it may be expected that the effects of disorder may be manifested in the near Fermi energy density of states as a gradually decreasing function, rather than being abrupt. On the contrary, we find that the energy derivative of the density of states at the upper valence band and lower conduction bands of $Si_{0.50}Ge_{0.125}Sn_{0.375}$ alloys is higher than the $Si_{0.75}Ge_{0.25}$ alloys. This is partly associated with the expansion of the unit cell volume where the volume of $Si_{0.50}Ge_{0.125}Sn_{0.375}$ is determined to be $\simeq 6.5\%$ larger than $Si_{0.75}Ge_{0.25}$. Increasing volume proportionate with increasing inter-atomic distances thereby decreasing the wave-function overlap. Such an effect leads to narrowing of bands, and hence a reduction in the energy dispersion. Within the electronic structure perspectives, less energy dispersed bands in the vicinity of Fermi energy is expected to enhance thermopower (α), according to the Mott relation $\alpha \propto dN(E_F)/dE$, where $N(E_F)$ is the density of state at the Fermi energy. Besides, we also find a dramatic reduction in the electronic gap (0.61 eV) in $Si_{0.50}Ge_{0.125}Sn_{0.375}$. As mentioned above, the $10K_BT_C$ hypothesis therefore suggests that the operating temperature of the disordered $Si_{0.50}Ge_{0.125}Sn_{0.375}$ would be scaled to lower temperatures in comparison to the $Si_{0.75}Ge_{0.25}$ alloys.
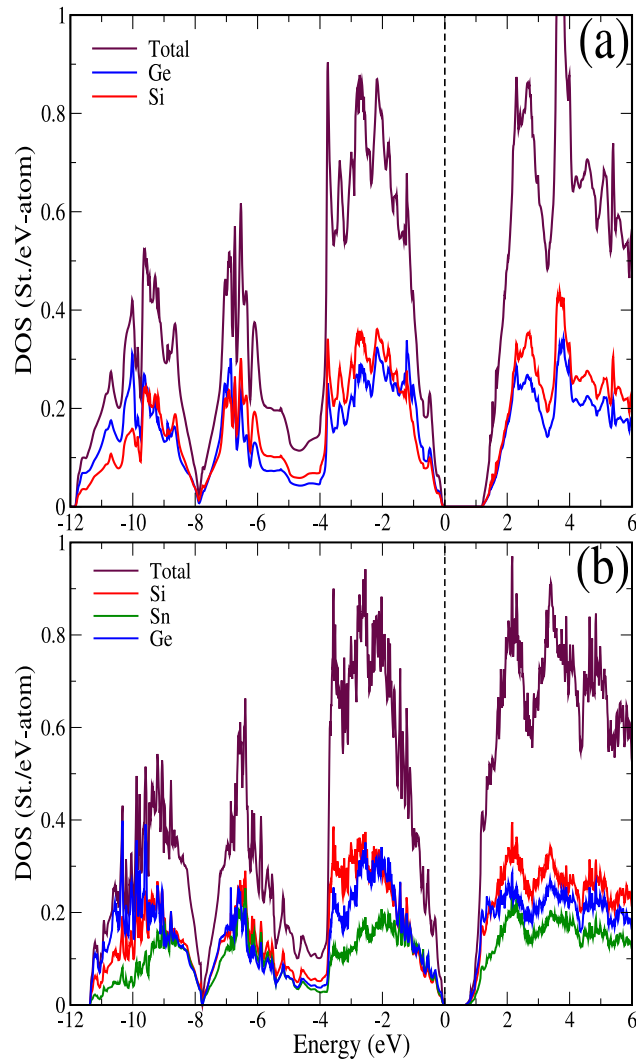
FIG. 1. The EV-GGA generated total and atom resolved partial density of states of SQS based (a) $Si_{0.75}Ge_{0.25}$ alloys and (b) $Si_{0.50}Sn_{0.375}Ge_{0.125}$ alloys, expressed in units of States/eV-atom. The vertical line through energy zero represents the reference alloy Fermi energy.

To look into the finer details of the electronic structure of $Si_{0.75}Ge_{0.25}$ and $Si_{0.50}Ge_{0.125}Sn_{0.375}$ alloys, we show in Fig. 2 the distribution of electronic states along various high symmetry directions of the BZ, i.e., the E(k) diagram. On comparison of the band structure of $Si_{0.75}Ge_{0.25}$ and $Si_{0.50}Ge_{0.125}Sn_{0.375}$, one finds that the sp^3 hybridized bands undergo severe modulation with the substitution of Sn in the semi-conducting Si-Ge matrix. Of importance is the dispersion of states around the center of the BZ (Γ-point). For $Si_{0.75}Ge_{0.25}$, we find a three band degeneracy at the Γ-point which are dispersed quite differently along different BZ directions. For example, while two of these remain degenerate in the Γ-X and Γ-Z directions, they all appear split along the Γ-R, Γ-A and Γ-M high symmetry directions of the BZ. Beyond, these valence band dispersion along the Γ-R and Γ-Z directions are more linear in comparison to that of the Γ-A and Γ-M directions. On the other hand, the lower conduction band regime of $Si_{0.75}Ge_{0.25}$ show multiple valleys for a small energy range of 0.2 eV. Apart from the two bands at Γ-point, we also find valley structures along the Γ-X and at the Z points of the BZ.

Conventional thermoelectrics with a single valley band structure represent a single optimum point in the power factor[41] versus carrier concentration profile. In these perspectives, multiple valleys in the band structure serve better for the enhancement of thermoelectric performance as they introduce
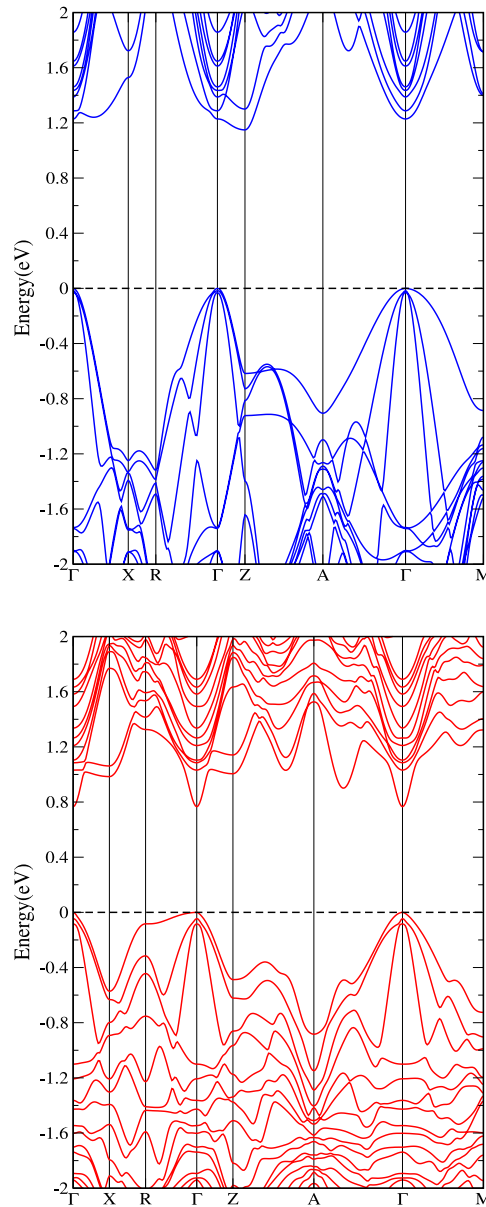
FIG. 2. The EV-GGA generated band structure of SQS modeled $Si_{0.75}Ge_{0.25}$ (upper panel) and $Si_{0.50}Ge_{0.125}Sn_{0.375}$ (lower panel) over the energy range $-2 \leq E$ (eV) ≤ 2, with the horizontal line through energy zero representing the alloy Fermi energy, E_F.

more peaks which can effectively increase the energy derivative of the density of states and therefore the Seebeck coefficient. At the same time, each valley also portray to a small effective mass and therefore large carrier mobility. Such multiple valleys are thought to be associated with the enhanced thermoelectric properties in Bi_2Te_3[42] and PbTe based systems.[43]

With Sn substitutions, the noticeable changes in the band structure are of those along the Γ-R, where one of the sp^3 hybridized bands deviate considerably from being simple parabolic. Such bands in the vicinity of Fermi energy significantly contribute to the energy derivative of the density of states, thereby increasing the thermopower. Besides, the dispersion of states in the conduction bands also show certain desirable features that would enhance thermopower with electron doping. For example, one observes an increased number in the valley structures of $Si_{0.50}Ge_{0.125}Sn_{0.375}$ electronic structure in comparison to their Si-Ge counterparts. Thus, based on the electronic structure it may be well anticipated that the Sn substitutions in Si-Ge alloys would render better thermoelectric properties.
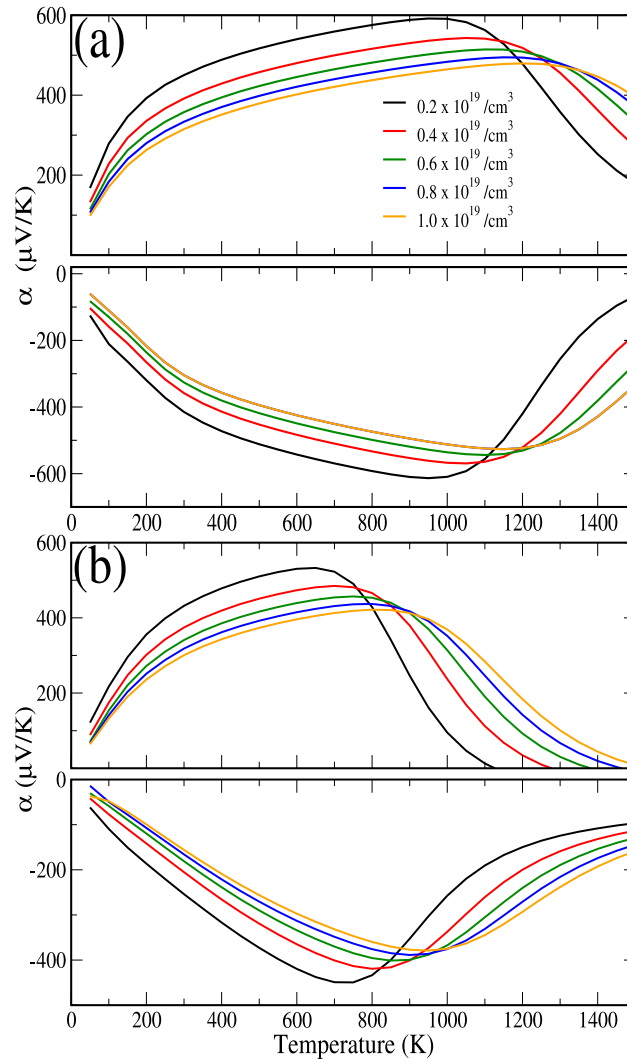
FIG. 3. The temperature dependence of thermopower (α) as a function of carrier concentration as indicated by the legends, for p-type (upper panel) and n-type (lower panel) in (a) $Si_{0.75}Ge_{0.25}$ and (b) $Si_{0.50}Ge_{0.125}Sn_{0.375}$, calculated using the Boltzmann Transport equation in the constant scattering time approximation.

In Fig. 3(a) and 3(b), we show the temperature and carrier concentration dependence of thermopower in $Si_{0.75}Ge_{0.25}$ and $Si_{0.50}Ge_{0.125}Sn_{0.375}$, respectively, calculated using the Boltzmann transport equation in the constant scattering time approximation. In $Si_{0.75}Ge_{0.25}$, the variation in $\alpha(T)$ is consistent with the experiments showing the optimum value at higher temperatures $T \simeq 1000$ K. The features in $\alpha(T)$ also reflect the multiple valley structures of the band structure by its display of a broad maximum over the temperature range 800 - 1100K. With increased carrier concentration, one observes not only an shift in the peak of $\alpha(T)$ to higher temperature but to an overall reduction in its magnitude, as well. For example, while for a carrier concentration of 0.2×10^{19}/cm^3 the thermopower of the electron (hole) doped system peaks to $\simeq 610$ (590) $\mu V/K$ at 950 K, an increase to 1.0×10^{19}/cm^3 results in a decrease, i.e., 512 (480) $\mu V/K$, respectively, at 1200 K. This suggests that for optimum performance of the device based on Si-Ge, the carrier concentration plays an important role. The wide range of figure-of-merit (ZT) reported for these alloys may be, therefore, mostly associated with the materials electronic structure properties. Note the symmetric variation in $\alpha(T)$ for both n and p- type doping, which is extremely important from the device engineering point of view.

In Fig. 3(b), we show the variation of $\alpha(T)$ for a set of carrier concentrations of $Si_{0.50}Ge_{0.125}Sn_{0.375}$ alloys. The overall features of $\alpha(T)$ is similar to that of $Si_{0.75}Ge_{0.25}$ with thermopower initially increas-

ing with temperature and then decreases beyond an optimal temperature. Consistent with the predictions that follows from the materials band structure, the optimum temperature at which thermopower peaks maximum, decreases in comparison with the $Si_{0.75}Ge_{0.25}$ alloys. We also observe that with increasing carrier concentration, the peak maximum is shifted to higher temperatures with a concomitant decrease in its magnitude, as well. The sharp decrease in $\alpha(T)$ above the optimum temperature is due to the bipolar conduction which results from the reduction of the materials electronic band gap. We also note that symmetric variation of thermopower for the electron and hole doping in the temperature profile as calculated for $Si_{0.75}Ge_{0.25}$ is not very true with Sn substitutions. For example, a carrier concentration of 0.2×10^{19} /cm^3 in $Si_{0.50}Ge_{0.125}Sn_{0.375}$ shows that for electron doping the peak maximum in $\alpha(T)$ ($\simeq 450 \ \mu V/K$) is at $T \simeq 750$ K, while for hole counterparts ($\alpha \simeq 530 \ \mu V/K$) is observed at $T \simeq 650$ K. Moreover, from the technological application point of view, what matters the most is the decrease in the operating temperature range which from the high temperatures (T > 1000 K in $Si_{0.75}Ge_{0.25}$) is scaled down to the mid-temperature range with Sn substitutions.

One of key parameters in optimizing the thermoelectric figure-of-merit is thermal conductivity (κ). While a low value of κ is desired, its dependence with the electronic conductivity through Wiedemann-Franz law pose limitations to the optimization. Many alternatives have been adopted such as nanostructuring, forming super-lattice structures, alloying and others. Among these, alloying which is an cost-effective strategy can render quite strong scattering effects and thus can be engineered to control thermal conductivity. In case the scattering is elastic, one may also expect a weak temperature dependence for the materials thermal conductivity. Apart from simple chemical disorder scattering which effects both electronic and phonon conduction on equal footing, substitution of iso-electronic Sn ions in Si-Ge introduce mass-difference scattering. We note that in case of Si-Ge alloys mass-difference scattering had been quite effective in reducing the thermal conductivity. One may note that the thermal conductivity of $\simeq 1.3$ Wcm^{-1}K^{-1} in Si at room temperature is almost reduced by an order of magnitude ($\simeq 0.1$ Wcm^{-1}K^{-1}) with alloying with Ge in Si-Ge alloys.[37,44] Thus with Sn being more massive, one may expect further reduction in the thermal conductivity in Si-Ge-Sn ternary alloys.

The phenomenology of thermal conductivity reduction also emphasize on large unit-cells, presence of massive ions, high coordination number and existence of voids. Diamond type lattices have low packing fraction due to large interstitial voids. It is interesting to note that all these criteria are met in the case of Si-Ge-Sn alloys. Besides, we also note that the underlying lattice is preserved in Si-Ge-Sn alloys and that the coordination number is little being changed in comparison to the Si-Ge binary alloys. However, what is further observed from the structural relaxation of these alloys is that the effective bond distances between the alloy constituents have a higher degree of variance. For example, in $Si_{0.75}Ge_{0.25}$ analysis of the fully relaxed structure shows that the average Si-Si, Si-Ge and Ge-Ge bond distances are 2.378 ± 0.007 Å, 2.4151 ± 0.006 Å and 2.4556 ± 0.001 Å, respectively. However, for the ternary $Si_{0.50}Ge_{0.125}Sn_{0.375}$ alloy, the Si-Si, Si-Ge, Si-Sn, Ge-Ge, Ge-Sn and Sn-Sn bond distances are estimated as 2.430 ± 0.033 Å, 2.494 ± 0.024 Å, 2.607 ± 0.039 Å, 2.521 ± 0.001 Å, 2.628 ± 0.043 Å and 2.748 ± 0.029 Å, respectively. Such large variance in the distribution of bond distances among iso-electronic ions also are quite effective in scattering the phonons. If one adopts to the Einstein's model of specific heat where each scatterer in the system vibrates with same frequency, an distribution of bond-distances would map to different force constants in the system. Thus, soft lattice modes as inferred from the materials equation of state and a wide distribution of force constants in Si-Ge-Sn alloys suggest to a low thermal conductivity. Hence, finding that thermopower and electrical conductivity scales better than that of its corresponding binary Si-Ge counterparts, the figure-or merit of these ternary Si-Ge-Sn alloys are expected to scale high with an advantage of being a promising thermoelectric material in the mid-temperature applications.

In summary, the electronic structure and transport properties of Sn substituted Si-Ge alloys, computed by means of *ab-initio* density functional theory and Boltzmann transport equation, show that the ternary Si-Ge-Sn alloys are promising mid-temperature thermoelectrics with added advantage of them being earth-abundant and non-toxic. Apart from lowering the materials thermoelectric operation temperature to the 400 - 900 K range, one also finds a substantial increase in the thermopower.

Empirical considerations also infer to a reduction in materials thermal conductivity, and thus expected to yield much larger thermoelectric figure of merit than their binary Si-Ge counterparts.

[1] J. P. Fleurial, L. Gailliard, R. Triboulet, H. Scherrer, and S. Scherrer, J. Phys. Chem. Solids **49**, 1237 (1988).
[2] H. Scherrer and S. Scherrer, in *CRC Handbook of Thermoelectrics*, edited by D. M. Rowe (CRC Press, London, U.K., 1995), ch. 19.
[3] V. A. Kutasov, L. N. Lukyanova, and M. V. Vedernikov, in *Thermoelectrics Handbook Macro to Nano* (CRC, Boca Raton, 2006), Ch. 37.
[4] H. J. Goldsmid, J. Appl. Phys. **32**, 2198 (1961).
[5] Y. Ma, Q. Hao, B. Poudel, Y. C. Lan, B. Yu, D. Z. Wang, G. Chen, and Z. F. Ren, Nano Lett. **8**, 2580 (2008).
[6] N. K. Stark, T. E. Svechnikov, and S. N. Chizhevskaya, Inorg. Mater. **21**, 328 (1985).
[7] L. V. Prokofieva, D. A. Pshenay-Severin, P. P. Konstantinov, and A. A. Shabaldin, Semiconductors **43**, 937 (2009).
[8] L. D. Zhao, B. P. Zhang, W. S. Liu, H. L. Zhang, and J. F. Li, J. Solid State Chem. **181**, 3278 (2008).
[9] Z. H. Ge, B. P. Zhang, Y. Liu, and J. F. Li, Phys. Chem. Chem. Phys. **14**, 4475–4481 (2012).
[10] L. D. Zhao, S. H. Lo, J. Q. He, H. Li, K. Biswas, J. Androulakis, C. I. Wu, T. P. Hogan, D. Y. Chung, V. P. Dravid, and M. G. Kanatzidis, J. Am. Chem. Soc. **133**, 20476 (2011).
[11] Q. Y. Zhang, H. Wang, W. S. Liu, H. Z. Wang, B. Yu, Q. Zhang, Z. T. Tian, G. Ni, S. Lee, K. Esfarjani, G. Chen, and Z. F. Ren, Energy Environ. Sci. **5**, 5246 (2012).
[12] Y. Z. Pei, J. Lensch-Falk, E. S. Toberer, D. L. Medlin, and G. J. Snyder, Adv. Funct. Mater. **21**, 241 (2011).
[13] Q. Zhang, F. Cao, W. S. Liu, K. Lukas, B. Yu, S. Chen, C. Opeil, D. Broido, G. Chen, and Z. F. Ren, J. Am. Chem. Soc. 2012, **134**, 10031 (2012).
[14] X. Shi, J. Yang, J. R. Salvador, M. F. Chi, J. Y. Cho, H. Wang, S. Q. Bai, J. H. Yang, W. Q. Zhang, and L. D. Chen, J. Am. Chem. Soc. **133**, 7837 (2011).
[15] R. Venkatasubramanian, E. Siivola, T. Colpitts, and B. O'Quinn, Nature **413**, 597 (2001).
[16] P. Magri, C. Boulanger, and J. M. Lecuire, J. Mater. Chem. **6**, 773 (1996).
[17] W. Liu, K. C. Lukas, K. McEnaney, S. Lee, Q. Z., C. P. Opeil, G. Chen, and Z. Ren, Energy Environ. Sci. **6**, 552 (2013).
[18] M. Strasser, R. Aigner, M. Franosch, and G. Wachutka, Sens. Actuators A, Phys. **97**, 535 (2002).
[19] K. Itoigawa, H. Ueno, M. Shiozaki, T. Toriyama, and S. Sugiyama, J. Micromech. Microeng. **15**, S233 (2005).
[20] H. Bottner, J. Nurnus, A. Gavrikov, G. Kuhner, M. Jagle, C. Kunzel, D. Eberhard, G. Plescher, A. Schubert, and K. H. Schlereth, J. Microelectro- mech. Syst. **13**, 414 (2004).
[21] M. Kishi, H. Nemoto, T. Hamao, M. Yamamoto, S. Sudou, M. Mandai, and S. Yamamoto, in *Proc. 18th Int. Conf. Thermoelectrics* (1999) p. 301.
[22] A. Bulusu and D. Walker, Superlattices and Microstructures **44**, 1 (2008).
[23] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, and J. Luitz, in *An Augmented Plane Wave Plus Local Orbitals Program for Calculating Crystal Properties*, edited by K. Schwarz (TU Wien, Austria, 2001).
[24] A. Zunger, S.-H. Wei, L. G. Ferreira, and J. E. Bernard, Phys. Rev. Lett. **65**, 353 (1990).
[25] A. Chroneos, C. Jiang, R. W. Grimes, and U. Schwingenschlögl, Chem. Phys. Lett. **493**, 97 (2010).
[26] J. P. Perdew, in *Electronic Structure of Solids 199I*, edited by P. Ziesche and H. Eschrig (Akademie Verlag, Berlin, 1991), Vol. 11.
[27] E. Engel and S. H. Vosko, Phys. Rev. B **47**, 13164 (1993).
[28] G. K. H. Madsen and D. J. Singh, Comput. Phys. Commun. **175**, 67 (2006).
[29] J. Tolle, A. V. G. Chizmeshya, Y.-Y. Fang, J. Kouvetakis, V. R. D'Costa, C.-W. Hu, J. Menendez, and I. S. T. Tsong, Appl. Phys. Lett. **89**, 231924 (2006).
[30] R. A. Soref and C. H. Perry, J. Appl. Phys. **69**, 539 (1990).
[31] V. R. D'Costa, C. S. Cook, J. Menendez, J. Kovetakis, J. Tolle, and S. Zollner, Solid State Commun. **138**, 309 (2006).
[32] J. L. Corkill and M. L. Cohen, Phys. Rev. B **47**, 10304 (1993).
[33] R. V. S. Jensen, T. G. Pedersen, and A. N Larsen, J. Phys.: Condens. Matter **23**, 345501 (2011).
[34] E. Simoen and C. Claeys, Electrochem. Soc. Proc. **17**, 223 (2000).
[35] G. Joshi, H. Lee, Y. C. Lan, X. W. Wang, G. H. Zhu, D. Z. Wang, R. W. Gould, D. C. Cuff, M. Y. Tang, M. S. Dresselhaus, G. Chen, and Z. F. Ren, Nano Lett. **8**, 4670 (2008).
[36] X. W. Wang, H. Lee, Y. C. Lan, G. H. Zhu, G. Joshi, D. Z. Wang, J. Yang, A. J. Muto, M. Y. Tang, J. Klatsky, S. Song, M. S. Dresselhaus, G. Chen, and Z. F. Ren, Appl. Phys. Lett. **93**, 193121 (2008).
[37] F. Schaffler, in *Properties of Advanced Semiconductor Materials GaN, AlN, InN, BN, SiC, SiGe*, edited by M.E. Levinshtein, S.L. Rumyantsev, and M.S. Shur (John Wiley & Sons, Inc., New York, 2001), p. 149.
[38] P. Moontragoon, Z. Ikonić, and P. Harrison, Semicond. Sci. Technol. **22**, 742 (2007).
[39] R. Braunstein, A. R. Moore, and F. Herman, Phys. Rev. **109**, 695 (1958).
[40] J. Weber and M. I. Alonso, Phys. Rev. B **40**, 5683 (1989).
[41] The power-factor ($P \equiv \alpha^2 \sigma$) is defined as the product of the square of thermopower (α) with electrical conductivity (σ).
[42] P. Konstantinov, L. Prokof'eva, M. Fedorov, D. Pshenai-Severin, Y. Ravich, V. Kompaniets, and V. Chistyakov, Semiconductors **39**, 1023 (2005).
[43] Y. Pei, X. Shi, A. LaLonde, H. Wang, L. Chen, G. J., and Snyder, Nature **473**, 66 (2011).
[44] H. Stohr and W. Klemm, Z. Anorg. Allgem. Chem. **241**, 305 (1954).