Defect properties of Sn- and Ge-doped ZnTe: suitability for intermediate-band solar cells

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Abstract

We investigate the electronic structure and defect properties of Sn- and Ge-doped ZnTe by first-principles calculations within the DFT+GW formalism. We find that (SnZn) and (GeZn) introduce isolated energy levels deep in the band gap of ZnTe, derived from Sn-s̄ and Ge-4s̄ states, respectively. Moreover, the incorporation of Sn and Ge on the Zn site is favored in p-type ZnTe, in both Zn-rich and Te-rich environments. The optical absorption spectra obtained by solving the Bethe–Salpeter equation reveals that sub-bandgap absorptance is greatly enhanced due to the formation of the intermediate band. Our results suggest that Sn- and Ge-doped ZnTe would be a suitable material for the development of intermediate-band solar cells, which have the potential to achieve efficiencies beyond the single-junction limit.

Keywords: ZnTe, DFT+GW, solar cells, intermediate-band

(Some figures may appear in colour only in the online journal)

1. Introduction

Zinc telluride (ZnTe) is a wide-gap II–VI semiconductor with a direct band gap of ∼2.26 eV at room-temperature. It is a potential candidate for solid-state applications such as green light emitting diodes [1, 2], terahertz (THz) imaging applications [3], detectors [4, 5], transparent conductors [6], and solar cells [7, 8]. Moreover, ZnTe can be doped both p- and n-type, but the latter is difficult to achieve in practice due to the high concentration of native acceptors, such as (Te²⁻) and (VZn), that shift the position of the Fermi level toward the valence band (VB), favoring p-type conduction [9].

In semiconductor-based solar cells, one of the major limiting factor on the conversion efficiency is the incomplete utilization of the photon energy. Only photons whose energies are higher than to the energy difference between the bottom of the conduction band (CB) and the top of the VB, i.e., the energy gap, can be absorbed to generate electron–hole pairs. Furthermore, photo-generated carriers with energies in excess of the band gap are lost to heat as they rapidly thermalize; thus, the smaller the energy gap, more of the Sun energy can be utilized. However, the largest recoverable voltage, i.e., the open-circuit voltage, is limited by the energy gap potential difference and decreases with decreasing the band gap of the semiconductor. In 1961, Shockley and Queisser [10, 11] found that the maximum efficiency for an ideal device with an energy gap of 1.1 eV (in which all recombination is assumed to be radiative) illuminated by black body radiation at 6000 K is 30.0%. Later, this result was extended to any absorption spectrum by Mathers [12], who found a limit of 31% for the conversion efficiency of an ideal solar cell under AM1 spectrum.

Several strategies for increase the efficiencies beyond the Shockley–Queisser limit have been proposed in the last years [13]. Improved photovoltaic conversion efficiency can be achieved by using a sequence of materials of decreasing band gap such that each material absorbs in one part of the solar spectrum [14]. However, this approach is currently limited to concentrator [15] and space systems due to its high manufacturing costs. Another suggestion [16], consists in the introduction of an isolated metallic band in the forbidden gap of a wide-gap semiconductor. This intermediate band (IB) allows additional optical transitions, thereby enabling sub-band gap energy photons to contribute to the photocurrent by pumping electrons from the VB to the IB and from the IB to the CB [17, 18]. In this regard, different approaches have been explored to implement the intermediate-band solar cell (IBSC) concept: (1) the use of highly mismatched alloys.
(HMA)\textsuperscript{s} [19, 20], a class of materials in which an isolated band is formed as a result of a band anti-crossing mechanism between the localized states of an isolating dopant and the extended states of the host [21, 22]; (2) the development of quantum dots solar cells, in which a periodic array of quantum dots introduce an IB in the fundamental gap of a suitable host [23–25]; (3) the use of heavily doped semiconductors [26–30], in which a suitable dopant introduces its \( d \) or \( s \) orbitals deep in the band gap, giving rise to a delocalized impurity band [17, 31].

Due to its wide band gap, ZnTe has been proposed as a good candidate for the development of IB photovoltaic devices. For instance, ZnTe:O [32–35] has been extensively investigated as a HMA, with promising results reported in [36–38]. However, \( n \)-type doping may be required in order to partially fill the IB so that two-photon photocurrent would be maximized. Heavily doping [39, 40] and co-alloying [41] were also proposed as a means to introduce an IB in ZnTe. In this context, Xiao-Juan \textit{et al} [42] have recently studied the \( \text{Sn}_{1-x} \text{Zn}_x \text{Te} \) ternary alloy using the Heyd–Scuseria–Ernzerhof hybrid functional [43], and suggested the existence of an IB in Sn-doped ZnTe systems.

In this work, we investigate the role of Sn and Ge as impurities in ZnTe. We calculate their formation energies and charge transition levels within the density functional theory (DFT) + GW method [44–47], which combines quasiparticle energies obtained within the GW approximation with total energy calculations based on the DFT. We find that under Zn-rich growth conditions the compensation mechanisms in both Sn- and Ge-doped ZnTe are favorable for the formation of an isolated and half-filled IB; thereby, greatly enhancing the solar energy conversion efficiency by enabling the absorption of sub-bandgap photons in a two-step excitation process.

2. Methods

2.1. Computational details

We performed total energy DFT calculations using the gradient-corrected exchange and correlation functional of Perdew, Burke, and Ernzerhof [48], as implemented in the Quantum-ESPRESSO package [49]. The electron–ion interactions were described by the ultrasoft pseudopotentials generated by Garrity \textit{et al} [50]. We used a 36 Ry energy cutoff for the plane-wave basis set expansion and a 200 Ry cutoff to represent the charge density. Moreover, our calculations were performed using large 512-atom supercells, in which all the atoms were allowed to relax until the forces acting on each ion were smaller than 0.001 Ry/Bohr. The Brillouin zone is sampled by the \( \Gamma \) point only.

Many-body \( G_0W_0 \) calculations of defect-containing supercells were performed using the WEST code [51, 52], which implements the formalism proposed in [51, 53] that avoids the explicit summation over empty electronic states by using a technique called projective eigendecomposition of the dielectric screening. In our calculations, we used 512 projective dielectric eigenpotential basis vectors to represent the dielectric matrix and norm-conserving Vanderbilt pseudopotentials [54] including 20 and 16 valence electrons for Zn and Te atoms, respectively, with a plane-wave energy cutoff of 70 Ry. For the absolute position of the valence band maximum (VBM), we used \( \Delta E_{\text{VBM}} = -0.81 \text{ eV} \), as obtained in [55] employing the self-consistent GW approximation, which includes a first-order vertex correction in the self-energy and the effect of the spin–orbit coupling as \textit{a posteriori} correction.

The optical properties of Sn- and Ge-doped ZnTe were investigated within the GW-BSE formalism using the ABL-NIT code [56–58]. We used a \( 3 \times 3 \times 2 \) supercell containing a single substitutional impurity occupying the Zn site. The matrix elements of the Bethe–Salpeter (BSE) Hamiltonian were first calculated on a \( 3 \times 3 \times 4 \) k-grid shifted along the (0.11, 0.12, 0.13) direction and subsequently interpolated onto a much finer 6 \( 	imes \) 6 \( 	imes \) 8 k-grid, by using the technique proposed in [59]. We used the Tamm–Dancoff approximation [60] in which only the resonant part of the BSE Hamiltonian is considered.

2.2. Defect formation energies and chemical potentials

The formation energy of a defect in charge state \( q \) can be expressed as [46, 61, 62]

\[
E_q^f([\textbf{R}]) = E_q^f(\textbf{R}) - E_{\text{ref}} + qE_F,
\]

where \( E_q^f([\textbf{R}]) \) is the total energy of the system in charge state \( q \) and ionic configuration \( \textbf{R} \); \( E_{\text{ref}} \) is the energy of a reference system, i.e., the defect-free supercell; and \( E_F \) is the Fermi energy.

To ensure the stability of the ZnTe crystal, the chemical potentials must be thermodynamically limited by the following equation:

\[
\Delta \mu_{Zn}^f + \Delta \mu_{Te}^f = E^f(ZnTe),
\]

where \( E^f(ZnTe) = -0.92 \text{ eV} \) is the calculated formation enthalpy of bulk ZnTe. Moreover, since \( \Delta \mu_i^f = 0 \) means that the \( i \)-th element is rich enough to form a pure solid phase, \( \Delta \mu_{Zn} < 0 \), \( \Delta \mu_{Te} < 0 \), \( \Delta \mu_{Ge} < 0 \), and \( \Delta \mu_{Sn} < 0 \) are also required. In addition, to avoid the formation of secondary phases of Ge or Sn with the host atoms, the chemical potentials are also bounded by the following relations:

\[
\Delta \mu_{Ge} + \Delta \mu_{Te} \leq E^f(\text{GeTe}) = -0.15 \text{ eV},
\]

\[
\Delta \mu_{Sn} + \Delta \mu_{Te} \leq E^f(\text{SnTe}) = -0.58 \text{ eV},
\]

where \( E^f(\text{GeTe}) \) and \( E^f(\text{SnTe}) \) are the calculated formation enthalpies of GeTe and SnTe, respectively. In the case of ZnTe:Ge, considering equation (4) and the need of avoid the
formation of pure phases of germanium, the chemical potential of tin is restricted by

\[
\Delta \mu_{\text{Ge}} \leq \min(0, E'_{[\text{GeTe}]} - \Delta \mu_{\text{Te}}),
\]

(6)

Hence, under Te-rich conditions, we have \(\Delta \mu_{\text{Te}} = 0\) and \(\Delta \mu_{\text{Zn}} = -0.92\), then

\[
\Delta \mu_{\text{Ge}}^{\text{Te-rich}} \leq -0.15 \text{ eV}.
\]

(7)

For Zn-rich conditions, \(\Delta \mu_{\text{Te}} = -0.92\) and \(\Delta \mu_{\text{Zn}} = 0\), then

\[
\Delta \mu_{\text{Ge}}^{\text{Zn-rich}} \leq 0 \text{ eV}.
\]

(8)

Similarly, for the case of ZnTe:Sn, the chemical potential of tin is bounded by

\[
\Delta \mu_{\text{Sn}} \leq \min(0, E'_{[\text{SnTe}]} - \Delta \mu_{\text{Te}}).
\]

(9)

Under Te-rich conditions, \(\Delta \mu_{\text{Te}} = 0\) and \(\Delta \mu_{\text{Sn}} = -0.92\), then

\[
\Delta \mu_{\text{Sn}}^{\text{Te-rich}} \leq -0.58 \text{ eV}
\]

(10)

and, for Zn-rich conditions, \(\Delta \mu_{\text{Te}} = -0.92\) and \(\Delta \mu_{\text{Sn}} = 0\), then

\[
\Delta \mu_{\text{Sn}}^{\text{Zn-rich}} \leq 0 \text{ eV}.
\]

(11)

### 2.3. DFT + GW formalism

According to equation (1), the formation energy of a defect in charge state \(q - 1\) is given by

\[
E_{q-1}^f[\mathbf{R}_q] = E_{q-1}[\mathbf{R}_q] - E_{\text{ref}} + (q - 1)E_F.
\]

(12)

Adding and subtracting first \(E_{q-1}[\mathbf{R}_q]\) and then \(E_q[\mathbf{R}_q]\), we have

\[
E_{q-1}^f[\mathbf{R}_q] = \{E_{q-1}[\mathbf{R}_q] - E_q[\mathbf{R}_q]\} + \{E_{q-1}[\mathbf{R}_q] - E_{q-1}[\mathbf{R}_q]\} + E_q[\mathbf{R}_q] - E_q
\]

\[
\equiv E_{\text{QP}} + E_{\text{relax}} + E_q[\mathbf{R}_q] - E_F.
\]

(13)

The first term in the last equation, \(E_{\text{QP}} = \{E_{q-1}[\mathbf{R}_q] - E_q[\mathbf{R}_q]\}\), is a charged excitation, i.e., an electron addition energy. This quantity is usually not well described within DFT, but it may be evaluated using the GW approximation that can provide an accurate description of excited states [63]. The second term, \(E_{\text{relax}} = \{E_{q-1}[\mathbf{R}_q] - E_{q-1}[\mathbf{R}_q]\}\), corresponds to a structural relaxation energy that could be evaluated at DFT-level, since we avoid the computation of energy differences between configurations with distinct number of electrons.

Similarly, we obtain

\[
E_{q+1}^f[\mathbf{R}_{q+1}] = \{E_{q+1}[\mathbf{R}_{q+1}] - E_q[\mathbf{R}_q]\} + \{E_{q+1}[\mathbf{R}_{q+1}] - E_{q+1}[\mathbf{R}_q]\} + E_q[\mathbf{R}_q] + E_F
\]

\[
\equiv E_{\text{QP}} + E_{\text{relax}} + E_q[\mathbf{R}_q] + E_F.
\]

(14)

### 2.4. Expected level of accuracy

In supercell calculations, when periodic boundary conditions are imposed, finite-size errors arise due to spurious interactions between the periodic images of defects. In addition, the structural distortions around the defects may result in long-range elastic forces that may affect the calculation of relaxation energies within the DFT+GW scheme. Furthermore, in the case of charged systems, the electrostatic error in the individual DFT eigenvalues needs to be accounted for [61].

To avoid the finite-size effects as much as possible, we calculated both the relaxation as well as the excitation energies by using 512-atom supercells. The elastic effects are expected to be negligible small. Moreover, due to the high dielectric constant of ZnTe, the position of the defect levels relative to the VBM are expected to be within the numerical accuracy of the \(G_0W_0\) calculations (about 0.10–0.15 eV).

Table 1 contains the calculated defect formation energies

| Reference system | \(E'_{\text{Te-rich}}\) | \(E'_{\text{Zn-rich}}\) |
|------------------|----------------------|----------------------|
| \((\text{SnCd})^2\) | -0.72                | -0.39                |
| \((\text{SnZn}-\text{VZn})^0\) | 1.55                | 2.77                |
| \((\text{Sn})^2\) | 0.64                | 0.05                |
| \((\text{SnTe})^0\) | 3.86                | 2.35                |
| \((\text{GeCd})^2\) | -0.79                | -0.02                |
| \((\text{GeZn}-\text{VZn})^0\) | 1.45                | 3.14                |
| \((\text{Ge})^2\) | 0.19                | 0.04                |
| \((\text{GeTe})^0\) | 3.42                | 2.35                |

Using Kohn–Sham (KS) eigenvalues \(\epsilon_{\epsilon n k}^{KS}\) and wave functions \(\psi_{\epsilon n k}^{KS}\) as mean-field starting point, the quasiparticle energy is calculated by adding the first-order perturbative correction

\[
E_{\epsilon n k}^{\text{QP}} = \epsilon_{\epsilon n k}^{KS} + \langle \psi_{\epsilon n k}^{KS}(E_{\text{QP}} - E_F)^{\epsilon n k} \rangle,
\]

(15)

which comes from replacing the KS exchange-correlation potential \(V_{xc}\) with the self-energy operator \(\Sigma\), which contains the effects of the exchange and correlation among the electrons.

Additionally, it is important to note that the quasiparticle corrections obtained within the \(G_0W_0\) approximation mainly reflect the difference between \(V_{xc}\) and the non-local electron self-energy operator \(\Sigma\), and thus are less dependent to the supercell size [64]. Therefore, considering the high computational demands, in the present work we calculated the quasiparticle \(G_0W_0\) corrections by using 64-atom defect-containing supercells at the \(\Gamma\) point only. These corrections were then used to correct the KS eigenvalues of 512-atom supercells by means of a scissors operator, and obtain the quasiparticle energies of interest with respect to the average electrostatic potential.
3. Results and discussion

3.1. Defect formation energies

We first calculate the formation energies of Sn impurities in ZnTe. We consider tin atoms occupying substitutional sites, i.e., (SnZn) and (SnTe); the interstitial site (Sn); and the possible formation of a defect complex of Sn with a Zn vacancy, i.e., the (SnZn–VZn) complex.

Figure 1 shows the calculated formation energies under Te-rich and Zn-rich growth conditions. In all cases, with the sole exception of Sn, we observe that the incorporation of Sn introduces deep charge transition levels in the band gap. Moreover, when the position of the Fermi energy is near to mid-gap or close to the VBM, we find that the most favorable is the substitutional site (SnZn) in which Sn acts as a donor. The (SnZn) introduces two charge transition levels $\epsilon (0/–)$ and $\epsilon (+2/ +)$, and $\epsilon (+0/ +)$ at VBM + 0.94 eV and VBM + 1.12 eV, respectively. This result differs from the analogous case of (SnCd) in CdTe. It was found that the latter exhibits a negative-U behavior, i.e., $\epsilon (0/–)$ is lower in energy than $\epsilon (+2/ +)$ [65, 66].

The absence of negative-U effect in (SnZn) may be due to the larger band gap of ZnTe that helps to stabilize the (SnZn)$^{+1}$ configuration, which has an unpaired electron occupying an isolated energy level in the band gap (mostly derived from Sn 5s states). The calculated band structure of (SnZn)$^{+2}$ and the charge density isosurface corresponding to the energy level in the gap are shown in figure 2.

When the Fermi level is close to the CB, we find that the most stable site depends on the chemical potential. Under Te-rich conditions, the formation of the (SnZn–VZn) complex is preferred. This complex is a deep acceptor that introduces an isolated energy level in the gap mainly derived from Sn 5s states. It creates two charge transition levels $\epsilon (0/–)$ and $\epsilon (–/–)$ at VBM + 1.20 eV and VBM + 1.36 eV, respectively. Under Zn-rich conditions, the substitutional (SnTe) is the dominant defect. It acts as deep acceptor introducing three charge transition levels at VBM + 0.1 eV for $\epsilon (2/+)$, VBM + 0.36 eV for $\epsilon (+0)$, and VBM + 0.48 eV for $\epsilon (0/–)$ in $T_d$ symmetry. The (SnTe) introduces a three-fold degenerate $t_2$ level deep in the band gap, and thus is subject to Jahn–Teller distortions [67, 68]. We found that the $T_d$ to $C_{3v}$ distortion splits the $t_2$ level into a two-fold degenerate $e$ level and a non-degenerate $a_1$ level that lies deep in the band gap. The latter level is likely to act as a non-radiative Shockley–Read–Hall recombination center [69] with a deleterious impact in carrier transport. However, for values of the Fermi level above $\epsilon (–/–)$ the $t_2$ level is fully occupied and the Jahn–Teller distortion will not occur.

The interstitial site (Sn) is a shallow donor, which does not introduce any charge transition level in the band gap. The Sn impurity occupies an octahedral coordinated position in which its four nearest neighbors are Zn atoms. Moreover, its formation energy is lower under the Zn-rich growth conditions.

Next, we focus on the Ge doping. The calculated formation energies are shown in figure 3; we can see that, overall, our results are qualitatively similar to those previously found for Sn. A major discrepancy occurs, however, in the case of (Ge$_n$) which is also a shallow donor, but the Ge impurity occupies an octahedral position surrounded by Te atoms instead of Zn atoms, as is the case of (Sn$_n$).

In Zn-rich and p-type ZnTe, the formation energies of (Ge$_n$)$^{+2}$ and (GeZn$_n$)$^{+2}$ are nearly degenerate, suggesting that the incorporation of Ge via interstitial diffusion is more favorable than Sn in this regime. Moreover, when the Fermi level is near the VBM, the substitutional (GeZn$_n$) is the most stable site for both Te-rich and Zn-rich conditions. The electronic structure of this defect is similar to that of (SnTe), exhibiting an isolated
level derived from Ge 4s states deep in the gap. It introduces two donor levels $\epsilon(+2/+) \text{ and } \epsilon(+/0)$ at 0.75 eV and 0.86 eV above the VBM, respectively. In the charge state +2, the Ge atom occupies the center of a Zn vacancy forming four equivalent Ge–Te bonds. The nearest-neighbor Te atoms relax slightly outwards by $\sim0.04\%$, resulting in Ge–Te bond lengths of 2.67 Å. On the other hand, the $(Sn_{Te})^{+2}$ configuration causes a more extend outward relaxation of $\sim5.64\%$, resulting in a Sn–Te bond length of 2.81 Å.

In addition, Ge impurities can form $(Ge_{Zn}-V_{Zn})$ complexes. As shown in figure 4, they introduce an isolated energy level in the band gap, which derives mainly from Ge 4s states. These complexes are easier to form under Te-rich growth conditions since a high concentration of Zn vacancies is expected. They act as deep acceptors introducing two charge transition levels at $\epsilon(0/-)$ and $\epsilon(-/-)$, at VBM + 0.95 eV and VBM + 1.16 eV, respectively. Finally, we find that the substitutional $(Ge_{Zn})$ configuration in the charge state $q = -2$ has $T_d$ symmetry. For the charge states $q = -1$, 0, +1, and +2, it undergoes a $T_d$ to $C_{3v}$ distortion, similarly to $(Sn_{Te})$. It introduces a double-donor level $\epsilon(+2/+)$ at 0.05 eV, a single-donor level $\epsilon(+/0)$ at 0.11 eV, and a double-acceptor level $\epsilon(0/-2)$ at 0.33 eV above the VBM.

3.2. Suitability for IBSCs

In the previous section, we identified several defect configurations that introduce isolated energy levels in the fundamental gap of ZnTe, namely $(X_{Zn})$ and $(X_{Zn}-V_{Zn})$ $(X = Sn, Ge)$. In the dilute limit, they can be thought as isolated defects surrounded by millions of atoms of the host material; thus, quantum–mechanical interactions between them are expected to be negligible small. Moreover, if they are introduced at high concentrations, i.e., exceeding the Mott limit [70], the atomic wave functions localized at different sites would overlap forming a delocalized impurity band, which can suppress the non-radiative recombination associated with localized impurity states [18, 66, 71]. A delocalized impurity band avoids a strong electron–phonon coupling with the lattice (which facilitates non-radiative processes), as absorption and emission transitions do not involve delocalized-to-localized and localized-to-delocalized charge redistributions that could drive the system strongly out of equilibrium.

For an efficient operation of an IBSC, the IB must be half-filled and well isolated in the band gap. In this scenario, incoming photons are not only able to pump electrons from the VB to the CB, they also can pump electrons from the VB to the IB and from the IB to the CB, thereby allowing the absorption of low energy photons via a two-step excitation process [18, 72]. It is interesting to note that in the case of Sn- and Ge-doped ZnTe the half-filling of the IB can be naturally achieved under Zn growth conditions due to the amphoteric behavior of the dopants. At high concentrations, the compensation between donors, $(Sn_{Te})^{-2}$ and $(Ge_{Zn})^{+2}$, and acceptors, $(Sn_{Te})^{-2}$ and $(Ge_{Te})^{+2}$, will lead to the Fermi level pinning at the impurity band.

3.3. Optical properties

Finally, we investigate the optical spectra of pristine ZnTe and Sn- and Ge-doped ZnTe given by the imaginary part of the macroscopic dielectric function $\text{Im} \epsilon_M(\omega)$. We performed first-principles calculations based on the $GW+BSE$ approach, which proceeds in the following three steps: (1) a ground-state DFT calculation; (2) a $GW$ calculation to correct the KS eigenvalues; and (3) the solution of the BSE equation [73, 74] using the corrected eigenvalues to obtain the optical absorption spectra.

Figure 5 shows the calculated $\text{Im} \epsilon_M(\omega)$ for pristine and doped ZnTe. We can see that both Sn and Ge doping allow the absorption of photons in the sub-band gap region. The absorption peaks near 1.1 eV are due to transitions between

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**Figure 3.** Defect formation energies of Ge impurities in ZnTe as a function of the Fermi-level position within the band gap, under (a) Te-rich growth conditions and (b) Zn-rich growth conditions.

**Figure 4.** Electronic band structure of $(Ge_{Zn}-V_{Zn})^{0}$ and the charge density isosurface ($\rho = 0.0005e/\text{Bohr}^3$) corresponding to the isolated energy level in the band gap. The calculations were performed in a 250-atom supercells and $G_0W_0$ corrections were considered through the application of a scissors operator at the $\Gamma$ point. The empty circles indicate the occupation of the energy level in the band gap.
Figure 5. Imaginary part of the dielectric function for pristine ZnTe (dashed line) and ZnTe containing single substitutional Sn and Ge impurities occupying a Zn site (solid lines).

4. Summary

In summary, we report a comprehensive theoretical study on the defect properties of Sn- and Ge-doped ZnTe. We used the DFT+GW approximation and found that both (SnZn) and (GeZn) introduce well isolated IBs in the fundamental gap of ZnTe. Moreover, the calculated absorption spectra indicate that the optical excitation of sub-bandgap photons is greatly enhanced by the presence of the IB. Our results suggest that both ZnTe:Sn and ZnTe:Ge are suitable candidates for the development of high-efficiency IBSC devices.

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