Enhanced Shift Currents in Monolayer 2D GeS and SnS by Strain-Induced Band Gap Engineering

Ngewo Tolbert Kaner, Yadong Wei, Yingjie Jiang, Weiqi Li,* Xiaodong Xu, Kaijuan Pang, Xingji Li, Jianqun Yang, YongYuan Jiang,* Guiling Zhang, and Wei Quan Tian*

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ABSTRACT: Group IV monochalcogenides exhibit spontaneous polarization and ferroelectricity, which are important in photovoltaic materials. Since strain engineering plays an important role in ferroelectricity, in the present work, the effect of equibiaxial strain on the band structure and shift currents in monolayer two-dimensional (2D) GeS and SnS has systematically been investigated using the first-principles calculations. The conduction bands of those materials are more responsive to strain than the valence bands. Increased equibiaxial compressive strain leads to a drastic reduction in the band gap and finally the occurrence of phase transition from semiconductor to metal at strains of −15 and −14% for GeS and SnS, respectively. On the other hand, tensile equibiaxial strain increases the band gap slightly. Similarly, increased equibiaxial compressive strain leads to a steady almost four times increase in the shift currents at a strain of −12% with direction change occurring at −8% strain. However, at phase transition from semiconductor to metal, the shift currents of the two materials completely vanish. Equibiaxial tensile strain also leads to increased shift currents. For SnS, shift currents do not change direction, just as the case of GeS at low strain; however, at a strain of +8% and beyond, direction reversal of shift currents beyond the band gap in GeS occur.

INTRODUCTION

Under uniform steady illumination on homogeneous crystals lacking inversion symmetries, a steady-state direct current (DC) is generated as a result of a second-order nonlinear optical response of the crystal, leading to phenomenon such as the bulk photovoltaic effect (BPVE).1−6 The direction of these direct currents has been found to depend on the light polarization, movement of electrons upon excitation, and photon energies.7 Arising from this light-matter interaction, two components of bulk photovoltaic effect (BPVE) arise, whose evolution mechanisms are distinct physical processes.8 Injection currents (also known as circular currents, CCs) arise from the nonsymmetric transport of electrons and holes and the self-rotation of the wave packet, while shift currents (SCs), which form the core of this study, stem from the displacement of the wave packet upon photon absorption, i.e., it is second-order bulk photovoltaic effect arising from the difference in the real space positions of Bloch electrons between the valence band (VB) and the conduction band (CB).9,10 SCs can be described to occur as a result of a charge transfer associated with a shift in the coordinate accompanying the photo-excitation of electrons from the valence band to the conduction band and originate from interband velocity matrix elements, which depend both on their magnitudes and phases.11−14 This actually describes the change of the intracell position of the Bloch wavefunction between VB and CB involved in the optical transition. Photocurrent generation involves two steps: creation of electron−hole pairs by light irradiation and then spatial separation of the electrons and holes. The electrons are excited to coherent superpositions, which allows for the net current flow ascribed to the asymmetry of the potential, in a process where it has firmly been verified that only symmetry inversion must be broken but there is no requirement for polarization.15,16 Although SCs were studied way back in the early 1960s, they have recently gained greater attention in part due to their potential application in efficient solar cells design and their recent observations in Weyl semimetals and topological insulators.17−20 Both first-principle calculations and experimental studies have helped reveal substantial information, leading to a considerably good understanding of the
occurrence of SCs in materials. As a matter of fact, findings of many studies on SCs have led their current status, where they are strongly being considered as an alternative to the photocurrents generated by traditional semiconductor p–n junctions for photovoltaic applications. It is now well established that SCs are generated in homogeneous materials in contrast to standard semiconductor solar cells whose active region is a heterogeneous pn junction. It has also been established that SCs are generated in homogeneous materials with the band dispersion of materials, which is in the order of the bandwidth, thus the strength of the shift currents is related to the e−e− minus the earlier findings of many studies on SCs have led their current status, where they are strongly being considered as an alternative to the photocurrents generated by traditional semiconductor p–n junctions for photovoltaic applications. It is now well established that SCs are generated in homogeneous materials in contrast to standard semiconductor solar cells whose active region is a heterogeneous pn junction. It has also been demonstrated that in SCs, charge carriers rapidly propagate to electrodes as a result of the coherent evolution of electron and hole wavefunctions, thus minimizing the probabilities of energy losses. This arises from the fact that it is a bulk phenomenon, i.e., not dependent on the internal electric fields. Consequently, much larger above band gap voltages can be generated since the limitations of Shockley–Queisser are feasibly overcome. Recent studies have also revealed that the photocarriers in SCs can travel long distances, compared to drift transport mechanism in traditional solar cells; hence, SCs can offer efficient solar energy conversion. From the first-principle calculations, Tan and co-workers reported that electronic states with delocalized covalent bonding highly asymmetric along the polarization direction are required for strong SC enhancements, which affirms the earlier findings on BaTiO3 by Young and Rappe. SCs are also associated with the band dispersion of materials, which is in the order of bandwidth, thus the strength of the shift currents is related to the “shift” of the intracell coordinates of the generated electrons and holes.

Group IV monochalcogenides with a general formula MX (where M = Ge, Sn, X = S, Se, Te) have recently emerged as promising materials in the fields of renewable energy, nanotechnology, and nanodevices. With reduced crystal symmetries, they possess distinct electrical, optical, and thermal properties along different in-plane crystal directions. As a result of their unique features, these materials provide possibilities of unexplored tunable characteristics for optical, electrical, thermal, and mechanical devices for applications in semiconductors with striking attributes. Since these materials show polar characteristics and have promising band gaps within the visible range, SCs in group IV–VI single-layer monochalcogenides have been studied most recently, with GeS being a good benchmark material. Using first-principles calculations, Rangel and co-workers have reported much larger shift currents in the monolayer two-dimensional (2D) GeS, GeSe, SnS, and SnSe than any other material reported so far. Applying the Wannier interpolation scheme, Sousa and co-workers have produced results that match perfectly with those of the previous work on GeS, confirming the observed large SCs. Most recently, Chan and co-workers, employing first-principles interacting Green’s function approach on the Keldysh contour, predicted strong SCs at sub-band gap excitation frequencies in the monolayer GeS, which they attributed to strongly bound excitons as well as giant enhancement in the SCs coefficients at the above band gap photon frequencies.

It is well known that strain on 2D materials can be readily induced via lattice mismatch between substrates and 2D layers, significantly changing the properties of 2D ferroelectric materials. Nguyen and co-workers have reported the effect of strain on the electronic properties of both monolayer 2D GeS and SnS from the first-principles calculations. Similarly, Xu and co-workers have predicted angular and strain dependence of charge carrier effective masses of the monolayers of GeS, GeSe, SnS, and SnSe from the first-principles calculations. In addition, F rogoso and co-workers have suggested exploring different chemical compositions, alloying, and strain engineering as approaches to improve photovoltaics through large SCs. However, currently, there is no known reported work on the effect of strain on the SCs in the monolayer 2D GeS and SnS. Therefore, by employing the first-principles calculations, we will study the photocurrents generated by nonlinear optical processes in the monolayer 2D GeS and SnS under an external equibiaxial strain in this work. We find a correlation between the band gap evolution and the observed shift currents as a result of strain.

### COMPUTATIONAL DETAILS

All of the calculations reported in this work were carried out based on the density functional theory (DFT). Quantum ESPRESSO (QE) computer code was used for structural optimization and obtaining ground states of the two materials. Generalized gradient approximation-Perdew–Burke–Ernzerhof (GGA-PBE) functionals was chosen for the electron exchange and correlation energy calculations, while norm-conserving pseudopotentials (PPs) with a nonlinear correction form were used to model the core–valence interactions for Ge/Sn and S atoms. A k-mesh grid of 18 × 18 × 1 was used to sample the Brillouin zone (BZ) of the two materials. The kinetic energy cutoffs set at 80 and 90 Ry were applied in the expansion of the Kohn–Sham wavefunction with all of the geometry fully relaxed for GeS and SnS, respectively. Energy convergence was set to be less than 10−8 Ry. All of the electronic properties calculations for both materials were performed using Wannier90, a code that calculates maximally localized Wannier functions (MLWFs) from a set of Bloch energy bands that may or may not be attached to or mixed with other bands. Since DFT-PBE is known to underestimate the band gap of materials, calculations based on hybrid functional (HSE) were done and the results were compared. To obtain well-converged shift-current spectra, Wannier functions were constructed from a dense 1000 × 1000 × 1 regular k-mesh grid. The maximally localized Wannier functions were constructed in a standard way by projecting into hydrogenic s-like and p-like orbitals on both Ge/Sn and S atoms along with two s-like orbitals in the vacuum region that are needed to represent the vacuum states. The frozen window for the disentanglement procedure spans up to 6.2 eV above the Fermi level. Equibiaxial strain (εxy), i.e., acting along the x- and y-directions concurrently for both compressive and tensile strain, was considered. An active single layer with a thickness of 2.57 Å for GeS and 2.60 Å for SnS and a vacuum of 17.11 Å in the z-direction to prevent spurious interactions between periodic images was set for the two materials. Equibiaxial strain in a range of −15 to +15% is considered in GeS, while that in the range of −14 to +14% is considered for SnS, where the negative sign implies a compressive strain, while the positive sign implies a tensile strain.

### RESULTS AND DISCUSSION

**Structural and Electronic Properties.** At the equilibrium state, monolayer 2D GeS and SnS have a space group symmetry Pmn21, with an anisotropic geometric structure in which a Ge(S)/Sn(S) atom is covalently bonded to three S(Ge)/S(Sn) atoms. The anisotropy in the structure of the...
monolayer 2D GeS and SnS leads to different electronic, optical, and mechanical properties along the armchair or the zigzag directions. Both the two 2D materials contain two layers of $M$ (Ge or Sn) and S stacked in the z-direction, forming a puckered honeycomblike structure similar to that of black phosphorous, as shown in Figure 1. The optimized cell parameters for GeS are $a = 3.6628$ and $b = 4.4591$ Å, whereas SnS has $a = 4.0298$ and $b = 4.2651$ Å, in agreement with previous reports. The optimized structural parameters used in this work for GeS and SnS are tabulated in Table 1.

Table 1. Bond Length and Bond Angles of Relaxed 2D GeS and SnS Cell

| Material | $d_1$ (Å) | $d_2$ (Å) | $\theta_1$ (deg) | $\theta_2$ (deg) |
|----------|------------|------------|------------------|------------------|
| GeS      | 2.4042     | 2.4675     | 94.14            | 104.62           |
| SnS      | 2.4105     | 2.5144     | 89.37            | 101.82           |

The bond length and bond angles correspond with those shown in Figure 1b.

In this work, both monolayer 2D GeS and SnS are indirect band gap materials of 1.90 and 1.45 eV, respectively, and this agrees well with the previous first-principles predictions and are close to experimental results. It is a well-understood limitation that DFT-PBE underestimates the band gap. To overcome this limitation, we applied hybrid functional (HSE) calculations whose results are presented in Figure 2. The predicted HSE band gap of the monolayer 2D GeS and SnS are 2.36 and 1.92 eV, respectively. The valence band maximum (VBM) is located at the $\Gamma$-point in GeS and at Y in SnS, while the conduction band minimum (CBM) is located at the X-point (see Figures 2, 3a, and 4a). The difference between $\Gamma$- and Y-points in SnS was about 0.03 eV. Two valleys are observed in the direction of S high-symmetry point from both X- and Y-directions, which is an indication of the high orientation dependency of the electronic band structure of the monolayer 2D GeS and SnS.

The total density of states and the projected density of states were plotted (see Figures S1 and S2). The projected density of states suggests that both the frontier VBs and the CBs have the contributions from both Ge/Sn-p and S-p states to the bonding in the 2D GeS and SnS. The VBs primarily consist of the S-p states and with a small amount of hybridization by the Ge/Sn-p states, while the CBs are dominated by the Ge/Sn-p states and with a small amount of hybridization by the S-p states, clearly indicating that the excitation across the band gap involved majorly the Ge/Sn-p and S-p states. The contributions of the S-s states to the VBs are also significant; however, the Ge/Sn-s states have insignificant contributions to the CBs. The CBM of GeS is dominated by the Ge-4p, orbital, while the VBM is dominated by the S-3p, orbitals, with some contributions by the Ge-4s orbitals. The VBM of the monolayer SnS has similar compositions as those of GeS, while the CBM is dominated...
by the Sn-Sp, orbital. An s-atomic orbital is known to be nondispersive and shows homogeneities in chemical bonding with other atoms.

Strain in materials is due to the lattice mismatch between the substrate and the 2D materials or mechanical misloading, and its effects on the electronic properties of 2D materials have been extensively reported.\(^{14,43}\) Compressive strain leads to massive defects formation in 2D materials, thus significantly influencing their band structure. Apart from being ferroelectric, monolayer 2D GeS and SnS are also known to be ferroelastic. It has been predicted that the elastic stiffnesses (C\(_{ij}\)) of group IV monochalcogenides are about 4–6 times smaller than that of MoS\(_2\) and GaSe.\(^{49}\) Monolayer SnS has been predicted to have a negative Poisson’s ratio similar to that of phosphorene and remains stable even under a strain of up to 27%.\(^{50}\) It is therefore expected that the two 2D materials under consideration can withstand considerable strain. It is also known that the in-plane pressure in 2D materials is difficult to quantify. In this study, therefore, the lattice parameters \(a\) and \(b\) of the two materials were varied and the energies of the unit cells with such lattice parameters were predicted. As can be seen in Figure 5, changes in the compressive equibiaxial strain have a very small yet significant change in energy as compared to the corresponding tensile equibiaxial strain with similar trends observed for both materials. The change in energies was established to have a direct correlation with the changes in the electronic band gap and shift-current variations of the two materials under strain conditions.

The band gaps of the two materials vary more rapidly when a compressive equibiaxial strain is due to the lattice mismatch between the substrate and the 2D materials or mechanical misloading, and its effects on the electronic properties of 2D materials have been extensively reported.\(^{14,43}\) Compressive strain leads to massive defects formation in 2D materials, thus significantly influencing their band structure. Apart from being ferroelectric, monolayer 2D GeS and SnS are also known to be ferroelastic. It has been predicted that the elastic stiffnesses (C\(_{ij}\)) of group IV monochalcogenides are about 4–6 times smaller than that of MoS\(_2\) and GaSe.\(^{49}\) Monolayer SnS has been predicted to have a negative Poisson’s ratio similar to that of phosphorene and remains stable even under a strain of up to 27%.\(^{50}\) It is therefore expected that the two 2D materials under consideration can withstand considerable strain. It is also known that the in-plane pressure in 2D materials is difficult to quantify. In this study, therefore, the lattice parameters \(a\) and \(b\) of the two materials were varied and the energies of the unit cells with such lattice parameters were predicted. As can be seen in Figure 5, changes in the compressive equibiaxial strain have a very small yet significant change in energy as compared to the corresponding tensile equibiaxial strain with similar trends observed for both materials. The change in energies was established to have a direct correlation with the changes in the electronic band gap and shift-current variations of the two materials under strain conditions.

The band gaps of the two materials vary more rapidly when a compressive equibiaxial strain is applied as compared to the case with the tensile strain (see Figures 3b,c,f and 4b,c,f). The compressive strain causes a change in the transition of the material from an indirect band gap to a direct band gap at a certain level (~8% strain). The Ge/Sn-p-Sp to Ge/Sn-p-Sp in the CBM and the S-p-Sp to S-p in the VBM are responsible for the transformation from the indirect band gap to the direct band gap. Finally, the materials change into metal-like behavior at a certain level (~15% for GeS and ~14% for SnS, the lowest CB in the \(\Gamma-Y\)-direction moves down more rapidly and the CBM finally goes below the Fermi level and overlaps with the highest VB at this site; thus, the monolayer 2D GeS and SnS transform to metal-like behavior. On the other hand, the highest VB changes gradually with the changes in strain. According to the variation of the lowest CB and the highest VB with strain, the lowest CB is more sensitive to equibiaxial strain than the highest VB. With an increase in the equibiaxial tensile strain, the CBM shifts upward slightly, resulting in a small increase in the energy gap. The shift of the highest VB is very small. An important feature is that the Fermi level gradually shifts upward with an increase in equibiaxial strain. The projected density of states (PDOS) (see Figure S2) follows a similar trend with the variation of strain. Specifically, the relative contributions of the p orbitals for Ge and Sn atoms at energies close to the VBM increases with increasing strain.

**Shift Currents.** A monochromatic electric field is in the form, \(E(t) = E(\omega)e^{i\omega t} + E(-\omega)e^{-i\omega t}\), and the shift current can be expressed in terms of a third rank tensor, \(\sigma^{abc}(0; \omega, -\omega)\) as

\[
J_{\text{shift}}^{\text{a}}(\omega) = 2 \sum_{bc} \sigma^{abc}(0; \omega, -\omega) E^b
\]

The shift-current tensor is given by

\[
\sigma^{abc}(0; \omega, -\omega) = -\frac{i\varepsilon^3}{2\hbar^2} \int \frac{dk}{8\pi^3} \sum_{nm} f_{nm} \left( r_{mn}^{a'} r_{mn}^{a} + r_{mn}^{a} r_{mn}^{a'} \right) \delta(\omega_{mn} - \omega)
\]

where \(r_{mn}^{a}\) is the velocity matrix element and \(r_{mn}^{a} \) is the generalized derivative, defined as

\[
r_{mn}^{a,b} = \frac{\partial r_{mn}^{a}}{\partial k^b} - i(A_{mn}^{b} - A_{mn}^{a}) r_{mn}^{a}, \quad A_{mn}^{a} = \begin{cases} 1, & \text{the Berry connection, with } a = b, \text{ thus, } \text{eq } 2 \text{ is proportional to the shift “vector” } R_{mn}^{a}, \text{ defined as} \\ \frac{1}{2} [\text{Im}][r_{mn}^{b} r_{mn}^{b} - \overline{r_{mn}^{b}} r_{mn}^{b}] \\
\end{cases}
\]

The point group mm2 to which the monolayer 2D GeS and SnS belong allows for seven tensorial components of \(\sigma^{abc}(0; \omega, -\omega)\) to be nonzero. If the spontaneous polarization is chosen along \(z\), the nonzero components are \(zzz, zyy, zxx, yyz = yzy, \) and \(xzx = xzx.\) Figure 6a,b represents the \(zzz, zyy, \) and \(zzz\) components of the shift-current spectrum as a function of photon energies for the strain-free cells of the 2D GeS and SnS, respectively. These results were obtained from the calculations without the inclusion of the spin–orbit coupling. Clearly, both the \(zyy\) and \(zzz\), which are in-plane components, are much larger than the out-of-plane component \(zxx.\) Similarly, the components \(zyy\) and \(zzz\) show slight differences especially in the height of peaks as a result of separate valley pumping of the BZ with linearly polarized light, resulting in different amounts of SCs. These results agree reasonably with the previous work (ref 21). The slight deviations are due to the differences in the algorithms and parameters used. A
comparison of the two components $zyy$ and $zzz$ for the pristine, monolayer 2D GeS and SnS indicates a difference, i.e., $zyy$ is slightly larger than $zzz$ in SnS, whereas they are almost the same in GeS.

For the $zzz$ component in the two materials, several peaks occur at the frequency below 3.0 eV. In GeS, three peaks appear for the $zzz$ component, with the first one appearing at a frequency of 1.95 eV just slightly above the band edge. The second peak is located at a frequency of 2.20 eV, while the third peak is located at a frequency of 2.80 eV. The first peak has contributions from the $K$-point around the BZ center ($\Gamma$-point), while the second peak above the band gap edge is attributed to the transition around the BZ boundary (at $\Gamma$-points). The third peak is the largest and result from the contribution of the excitonic effect in the valley along the $Y\rightarrow S$-direction. SnS has more peaks than GeS below 3.0 eV. The first peak with contributions from the $K$-point around the BZ center ($\Gamma$-point) is located at 1.57 eV, followed by the other eight very weak peaks with transitions around the BZ boundary (at $Y$-points). The peaks at frequencies 2.33 and 2.40 eV are the largest and are attributed to the exciton in the valley along the $Y\rightarrow S$-direction. The sharp peaks at the band edges highlight the significance of these features on the behavior of the SCs. The band edges induce a Van Hove in the density of states resulting from strong singularities provided by 2D materials, leading to magnified sharpness of the peaks of photoresponse spectra. The large SCs are related to the composition of the highest VB and the lowest CB of the two materials with major contributions from the $p$ orbitals and minor contributions from the $s$ orbitals, which are highly delocalized. Strong covalent bonding plays a fundamental role in the large SCs. In this study, the presence of $s$ and $p$ orbitals in the two materials, leading to the presence of sp-$\sigma$ bonds, which have hopping integrals of alternating signs, result to increased SCs. The large SCs could also be attributed to strong anisotropy and one-dimensional (1D) conducting channels. The occurrence of the maximum SCs in the visible range is an important feature since it highlights the potential applications of these materials for optoelectronics. The sub-band gap SCs in both materials are due to the exciton in the valley along the $\Gamma\rightarrow Y$-direction.

As shown in Figures 6c–f and 7, upon the introduction of equibiaxial strain on the two materials, the SC tensors change significantly compared with those without strain. These present in a manner similar to the case of electronic band structure evolution. The changes of the SCs spectra depend on the level and type of strain applied. Compression strain leads to increased onset photon energies culminating in increased SCs. Direction change of SCs due to compressive strain is also observed. At a compressive strain of $−12\%$, the SCs peak is almost 4 times that of the SCs in the pristine GeS and SnS. At the phase change from semiconductor to metal (strains of $−15$ and $−14\%$ for GeS and SnS, respectively), the SCs spectra vanish. Tensile strain also leads to increased SCs; however, no reversal of the SC directions for the two materials occurs (Figure 6e, f, c, d). Another notable difference in the SCs as a result of compressive and tensile strains is the shift of the peaks toward lower frequencies as a result of compressive strain and opposite occurrence due to tensile strain. This is attributed to the level of localization of the ground hole state, where at large atomic separation distances very weak localization is observed, whereas at close spacing and overlap no localization is seen.

Similar to the case of the electronic band structure, the SCs of GeS and SnS show dependence on the localization magnitude of the initial and final states, which has been found to depend on atomic displacements. The increase of nonthermalized polaron hopping leads to increased SCs in bulk LiNbO$_3$ since the energy of phonons involved in the formation of polarons decreases under strain, and this is the same case in the 2D materials. The compressive strain causes the $p$-orbital-dominated conduction state to sharply shift downward in energy and overlap with the valence state. This rapid shift leads to the delocalized $p$ electronic orbitals moving much closer to the band edges, causing a large increase in the SCs since current-carrying excited states are more likely to be constructed from a superposition of delocalized orbitals rather than heavily localized orbitals. At a higher strain of $−12\%$, strong atomic interactions result in resonant excitation, consequently stronger absorption peaks, leading to even much larger SCs.

Figure 6. Shift-current tensors of monolayer 2D GeS and SnS. (a, b) Comparison of $zxx$, $zyy$, and $zzz$ tensor components for pristine structures (c, d) with compressive strain and (e, f) with tensile strain.

Figure 7. Photon energy dependence of shift current tensor $zyy$ of Group IV monochalcogenides GeS and SnS. (a) GeS under compressive strain, (b) SnS under compressive strain, (c) GeS under tensile strain, (d) SnS under tensile strain.
The direction change of the SCs becomes more pronounced at \(-8\%\) strain and is ascribed to the shift vector switching and rotation of the polarization of the two materials under compressive strain. From the “shift vector” term and the Berry curvatures of eq 2, the shift vector term and the Berry curvatures rotate \(90^{\circ}\) under strain, effectively switching the \(yz\) index.\(^1\) Thus, under the same condition, for linearly and polarized light, nonlinear SCs will rotate \(90^{\circ}\) upon ferroelectric polarization switching. Similarly, since SCs are polar vectors, their signs change upon ferroelectric polarization switching. Thus, under the same condition, for linearly polarized light, nonlinear SCs reverse their direction to \(180^{\circ}\) upon ferroelectric polarization following the flip by the SC susceptibility tensor, \(\sigma_{\alpha \beta}(0; \omega, -\omega)\). Despite the minimal effect of tensile strain on the band gap, the modification of the band edges of the two materials leads to a shift of the delocalized electron orbitals away from the band edges, resulting in increased SCs. This may be attributed to the coincidences of transition intensity and large shift vectors. It is also a result of the CB potential well becoming shallower, leading to increases in the energy splitting between bonding and antibonding sites, especially in the \(p\) states. In summary, the introduction of strain to the two materials brings about the correlation between shift currents and band gap evolution in these two materials.

# CONCLUSIONS
The effect of equibiaxial strain on the band structure and shift currents of the monolayer 2D GeS and SnS has been investigated with first-principles calculations in the present work. The increase of the equibiaxial compressive strain leads to a drastic downward shift of the conduction band significantly reducing the band gaps of the two materials. Consequently, the indirect band gap to direct band gap transition occurs. Finally, at \(\varepsilon_{xy} = -15\) and \(-14\%\) for GeS and SnS, respectively, phase transitions from semiconductor to metal occur. Similarly, equibiaxial compressive strain results in a large increase as well as direction reversal of the shift currents, which eventually vanishes at the semiconductor—metal phase transition. The SCs direction reversal occurs at all compressive strain levels but becomes more pronounced at \(\varepsilon_{xy} = -8\%\) and beyond. At the same time, equibiaxial tensile strain leads to a small upward shift of the conduction band and a slight increase in the band gap. Tensile strain also brings about an increase in the shift currents but with no direction reversal. However, for strong tensile strain, small direction change of SCs occurs in GeS with small peaks. In general, the conduction band is more responsive to strain than the valence band. Equibiaxial strain on the two materials brings about a correlation between shift currents and band gap evolution in these two materials.

# ASSOCIATED CONTENT

* Supporting Information
The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsomega.0c01319.

Total density of states and projected density of states of monolayer 2D GeS and SnS (PDF)

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