First principles calculation of shift current in chalcopyrite semiconductor ZnSnP$_2$

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The bulk photovoltaic effect generates intrinsic photocurrents in materials without inversion symmetry. Shift current is one of the bulk photovoltaic phenomena related to the Berry phase of the constituting electronic bands: photo-excited carriers coherently shift in real space due to the difference in the Berry connection between the valence and conduction bands. Ferroelectric semiconductors and Weyl semimetals are known to exhibit such nonlinear optical phenomena. Here we consider the chalcopyrite semiconductor ZnSnP$_2$ which lacks inversion symmetry and calculate the shift current conductivity. We find that the magnitude of the shift current is comparable to recently measured values on other ferroelectric semiconductors and an order of magnitude larger than bismuth ferrite. The peak response for both optical and shift current conductivity, which mainly comes from P-3$p$ and Sn-5$p$ orbitals, is several eV above the band gap.

INTRODUCTION

Ternary compounds $A^{II}B^{IV}C^{VI}_2$ and $A'B^{IV}C^{VI}_2$ (where, $A, B = $ metals, $C = $ sulfur/pnictogen family) having chalcopyrite structure are of considerable interest because of their structural, mechanical, thermoelectric and nonlinear optical properties [1]. They are also promising materials for spintronics application because of the ability to host ferromagnetism at room temperature [2, 3]. The chalcopyrite structures are derived from the binary analogs $A^{II}B^{IV}$ and $A'B^{IV}$ in cubic zinc-blende structures and doubling of the unit cell along $c$, leading to a body-centered tetragonal unit cell. Each cation (anion) is surrounded by four nearest-neighbor anions (cations) as in the zinc-blende structure. The A and B cations alternatively occupy the Zn-positions and form a tetrahedral bonding of the two cation sublattice. The reduced symmetry lowers the band gap significantly in ternary compounds compared to their binary analogs [4]. This spatial symmetry reduction also plays an important role to realize the topological insulating and Weyl semimetallic phases in some ternary chalcopyrites [5–13].

Of particular interest is the ternary compound ZnSnP$_2$ (ZSP), type $A^{II}B^{IV}C^{VI}_2$, which is now recognized as an alternative photoabsorber material in solar cell applications [14, 15]. It undergoes a structural transition from the ordered chalcopyrite ZnSnP$_2$ (CH-ZSP) structure to a disordered sphalerite structure (SP-ZSP) at 990 K [16]. In SP-ZSP, the Sn and Zn atoms are randomly distributed over the cation sublattice. In comparison, in the ordered CH-ZSP, the P$^{5-}$ anions are surrounded by two Zn$^{2+}$ (A-type) and two Sn$^{4+}$ (B-type) cations while each cation are surrounded by four anions. Due to the possibility of bandgap engineering and tunability of the electronic and optical properties, the electronic structure and properties of ZSP is being investigated both theoretically and experimentally [14, 17–23]. In comparison to other well known chalcopyrite ternary compounds, an important feature of CH-ZSP is the that the ground state is a trivial insulator, but lacks inversion symmetry due to anion-shift. It is also anisotropic due to the presence of two types of cationic bonding which also gives rise to high birefringence.

An interesting and potentially useful property of noncentrosymmetric crystals is that in such materials symmetry allows incident photons to induce a photocurrent. This is a bulk photovoltaic phenomenon and the induced current is referred to as the shift current [24–29]. In contrast to a conventional drift photocurrent under an electric field, the shift current originates from the charge center shifts in real space due to difference in the Berry connection between the valence and conduction bands involved in the optical excitation process [25, 29]. Recently, Weyl semimetals (WSMs) have been theoretically investigated for such nonlinear optical phenomena [28, 30–36].

The shift current with a less dissipative character has remarkable advantages over the conventional drift photocurrent driven by a built-in potential or external electric field [37–39]. For example, it depends on the polarization direction of the incident photon field, is insensitive to the sample resistivity or barrier formation near the electrodes [40] and is also independent of the external bias voltage [41, 42]. Moreover photocurrents induced by optical transitions obeying dipole and polarization selection rules naturally permit ultrafast manipulation. In particular shift currents induced by a properly tuned external pulsed photon sources can create coherent electromagnetic wave emission in the terahertz frequency regime, where control of the ellipticity and chirality over a broad spectral range is notoriously difficult [43, 44].

Here we show, using a recently developed multi-band approach [28, 45, 46], that the shift current conductivity in CH-ZSP is comparable to the SbSI [47] and an order of magnitude larger than the famous multiferroic
BiFeO$_3$ [48]. The multi-band approach involves the full set of Bloch states and a sum over all intermediate states participating in three-band transitions is considered. The three-band virtual transitions make the dominant contributions and are distributed uniformly in the momentum space. Naturally, in comparison to the widely used two-band effective models, estimates based on the multi-band approach are accurate and highly desirable for materials application.

The key challenge in an accurate density functional theory (DFT) description of insulating materials is the well known problem of bandgap underestimation by the local and semi-local functionals. These problems can be cured by employing schemes which take into account the self-energy of a many-body electronic system, such as the GW approximation [49], and the hybrid exchange correlation (HSE) functional [50]. However, they are computationally very expensive. Traditionally, such a deficiency is addressed by using “scissors” operation on the standard DFT (GGA/LDA) bands where the conduction bands are rigidly shifted such that the resulting electronic bandgap matches the experimental value. As an alternative, a semi-empirical DFT+$U$ approximation might be used to improve the corrected gap values. Very recently, an empirical Tran-Blaha modified Becke-Johnson (TB-mBJ) potential was shown to be lead to an accuracy comparable to the much expensive hybrid functional and GW approximation at a computational cost comparable to standard DFT calculations. Here, we thus, consider the latter three approaches, viz., the scissors operation (GGA+$\Delta$), DFT+$U$ and TB-mBJ methods and discuss their implications for the electronic and optical properties on ZSP.

**COMPUTATIONAL DETAILS**

We performed density functional theory (DFT) calculations within the Perdew-Burke-Ernzerhof PBE implementation [51] of the generalized gradient approximation (GGA) using the full-potential local-orbital (FPLO) code [52, 53]. Self-consistent calculations employing the default scalar relativistic approximation were performed on a $k$-mesh with $18 \times 18 \times 18$ subdivisions. Starting from the experimental structure [54, 55], several crystal structures with different unit cell volumes were considered: $0.90V_{\text{exp}} \leq V \leq 1.10V_{\text{exp}}$, where $V_{\text{exp}}$ is the unit cell volume of the experimental crystal structure. For each case, the internal parameters (atomic positions) were optimized such that net force on all atoms was less than 1 meV/Å and the ground state energy was evaluated. The optimized structure was considered for further detailed study of electronic and optical properties.

To overcome the issue of bandgap underestimation, both DFT+$U$ and TB-mBJ calculations were carried out. The on-site orbital dependent electron electron correlations ($U$) were applied to Zn-3$d$ as well as P-3$p$ states and the evolution of the bandgap was studied.

The TB-mBJ calculations [56] were carried out using the full-potential Augmented Plane Waves + local orbital (APW+lo) method as implemented in the WIEN2k code [57]. A good quantitative agreement between the two codes were obtained within the scalar relativistic GGA calculations. For the mBJ potential, the self-consistent parametrization for $c$ was used [56]. The energy convergence of the obtained solutions is better than $10^{-5}$ Ryd per unit cell and the charge convergence is better than $10^{-4}$ e/a.u.3.

The optical properties within the linear response theory were obtained using the well-known relations implemented in the FPLO code: the imaginary part of the dielectric function is given by

$$
\epsilon_2^{ij}(\omega) = \text{Im}[\epsilon_{ij}(\omega)] = \frac{-4\pi^2e^2}{\hbar^2m_0^2\omega^2}\int \frac{dk}{(2\pi)^3}\sum_{n,l,m}\left(\frac{n_f - n_l}{f(E_{kn} - E_{kl} - \hbar\omega - i\delta)}\right).
$$

where, $i, j = (x, y, z)$ are the Cartesian coordinates, $\delta = \hbar/\tau$ is the particle lifetime and the quasi-particle lifetime $\tau$. The real part can be obtained via the Kramers-Kronig relation:

$$
\epsilon_1^{ij}(\omega) = \text{Re}[\epsilon_{ij}(\omega)] = \frac{\omega\epsilon_2^{ij}(\omega)}{4\pi}.
$$

All optical response functions can now be derived from these. In particular, the optical conductivity is

$$
\sigma_{ij}(\omega) = \frac{\omega\epsilon_2^{ij}(\omega)}{4\pi}.
$$

To calculate the shift current response, we used the general relation for the photoconductivity in quadratic response theory [28, 45, 46]:

$$
\sigma_{ij}^{\text{sh}} = \frac{|e|^{3}}{8\pi^{3}\omega^{2}}\text{Re}\left\{ \phi_{ij} \sum_{\Omega=-\pm l,m,n} \sum_{BZ} dk (f_l - f_n) \times \frac{(kn|\hat{v}_{i}|kl)(kl|\hat{v}_{j}|kn)(kn|\hat{v}_{j}|k)}{(E_{kn} - E_{kl} - \hbar\Omega - i\delta)(E_{kn} - E_{kl} + \hbar\Omega - i\delta)} \right\}.
$$

The conductivity $\sigma_{ij}^{\text{sh}}(i,j,k = x,y,z)$ is a third rank tensor representing the photocurrent $J_{E_i}$ generated by an electrical field via $J_{k} = \sigma_{ij}^{\text{sh}}(E_i)\hat{E}_j$. $\phi_{ij}$ is the phase difference between the driving field $\hat{E}_i$ and $\hat{E}_j$. The integral in Eq. (4) describes the shift current response under linearly polarized light.
The starting point for the shift current calculation is a bandstructure and the corresponding eigenstates and energies in the Brillouin zone. To this end, a tight binding model was obtained using maximally projected Wannier functions (WFs) for the Zn-3d, Sn-4d, 5s, 5p and P-3p orbitals in the energy range of -7.0 eV to 5.0 eV. For the integral in Eq. (4), the Brillouin zone (BZ) was sampled by a $200 \times 200 \times 200$ k-grids with satisfactory convergence. The value of the conductivity changes only by $\leq 4\%$ above that k-mesh. The broadening parameter was set to $\delta = 0.1$ eV for both linear and non-linear response.

ZnSnP$_2$ belongs to the $D_{4d}$ (4m2) point group in the ferroelectric phase. Therefore, with the 2nd-order photoconductivity ($\sigma_{ij}$) tensor of the form

$$\sigma^{k}_{ij} = \begin{pmatrix} 0 & 0 & \sigma^{x}_{yz} & 0 & 0 \\ 0 & 0 & 0 & \sigma^{y}_{zx} & 0 \\ 0 & 0 & 0 & 0 & \sigma^{x}_{xy} \end{pmatrix}$$

The second-harmonic susceptibility $\chi_{ij}^k (\chi_{ij}^k = \sigma_{ij}^k/2i\omega)$ has the same symmetry. The crystal has a mirror reflection $M_{xy}$ in the x-y plane, which exchanges x and y indexes. In addition, the 4$_2$ screw rotation symmetry about the z axis gives $\sigma^{x}_{yz} = \sigma^{y}_{zx}$, leaving only two independent nonlinear optical photoconductivity tensor elements $\sigma^{x}_{yz}$ and $\sigma^{x}_{xy}$.

### RESULTS AND DISCUSSION

![FIG. 1. (a) Unit cell of ZnSnP$_2$ chalcopyrite lattice (b) The top view of the ZnSnP$_2$ structure. It has two twofold glide rotational and mirror symmetries $C_2(x), C_2(y)$, $M_{xy}$ and $M_{x-y}$. (C) Brillouin zone (BZ) along with the high symmetric points.](image)

Termary ZSP crystallize in the body-centered tetragonal structure which in the chalcopyrite phase has a space group I42d (No. 122). It has eight atoms per primitive unit cell. Basically, it is a superlattice of zinc-blende structure doubling the zinc-blende unit cell along the z direction. The unit cell of ZnSnP$_2$ is shown in Fig. 1(a).

In an ideal zinc-blende structure of binary compound, each anion has four similar cations as nearest neighbors. So, all the four bond lengths are equal and the charge distribution is identical around each bond. Consequently, in binary compounds with zinc blende structure, $u$ is 0.25 and $\eta = c/a = 1$. Therefore, the ideal case for the doubled unit cell, such as in CH-ZSP, corresponds to $u = 0.25$ and $\eta = c/a = 2$.

In CH-ZSP, each anion has two Zn and two Sn cations as nearest neighbors. Due to dissimilar atoms as neighbors the anion acquires an equilibrium position closer to one pair of cation than to other. The displacement of the position of anion is due to such bond alternation. In the most general case, $u \neq 0.25$ and $\eta \neq 2$. In contrast to other chalcopyrite compounds, ZSP does not exhibit a tetragonal distortion ($\eta = 2$) but exhibits an anion shift (displacement toward the smaller cation). The positions of the different types of atoms in the tetragonal unit cell are: Zn atom at $(0, 0, 0)$; Sn atom at $(0, 0, 0.5)$ and P atom at $(u, 0.25, 0.125)$, where $u$ is the anion displacement parameter. The equilibrium lattice parameters and the optimal internal parameters for ZSP are presented in Table I. Compared to the binary compounds, the cubic symmetry is broken and the non-centrosymmetric ZSP crystal has two twofold glide rotational symmetries $C_2(x), C_2(y)$ and two glide mirror symmetries $M_{xy}$ and $M_{x-y}$. It has also a twofold rotational symmetry along z [see Fig. 1(a)].

The bandstructure along the high symmetry lines in the Brillouin zone and the density of states (DOS) is shown in Fig. 2. A direct bandgap is found at the $\Gamma$ point (2(a)). Within GGA, the bandgap is $\sim 0.69$ eV in good agreement with earlier calculations [23]. This is, however, merely $\sim 41\%$ of the experimental gap [20].

The valence band maximum are mainly contributed by P-3p, Sn-5p while the conduction band minimum are contributed by P-3p, Sn-5s,5p, reflecting the strong covalency effects in ZSP [see Fig. 2(b)]. There is strong hybridization between Sn-5s and P-3p states as well as between Zn-3d and P-3p states. Arguably, the Zn-3d states are over-hybridized with the Zn-p states similar to other strongly covalent systems involving Zn [58]. As a result, they are underbound and lie much higher in the energy, in the range of -5.1 eV to -7.6 eV, (just) below the P-3p states in the valence band. This, in turn, leads

| Material | $a$ (Å) | $c$ (Å) | $u$ | $u_{exp}$ |
|----------|--------|--------|-----|----------|
| ZnSnP$_2$| 5.7382 | 11.4764| 0.2272 | 0.239    |

|TABLE I. The equilibrium lattice parameters and optimized anion displacement parameter for CH-ZSP. |
FIG. 2. (a) The band structure from GGA and GGA+U, showing a direct bandgap at Γ. The GGA band gap is $\sim 0.69$ eV whereas the GGA+U band gap is $\sim 1.05$ eV, obtained with $U_d = 10$ eV and $U_p = 2$ eV. (b) The total and partial density of states from GGA+U. (c) Comparison of bandstructures obtained within GGA+Δ and TB-mBJ calculations. For comparison, the GGA conduction bands have been shifted by $\Delta = 0.71$ eV (bottom panel) to match the bandgap, and $\Delta = 0.45$ eV in an energy range of 1 eV and 5 eV (top panel), showing the qualitative agreement between the two methods in the description of the conduction band states.

FIG. 3. The real and imaginary parts of the dielectric constant as a function of the incident photon energy obtained within (a)-(b) GGA+U, and (c)-(d) TB-mBJ scheme, showing overall agreement.
Fig. 3 shows the real and imaginary part of dielectric function obtained within GGA+U and its comparison with the corresponding results from TB-mBJ. Tetragonal symmetry of the crystal structure implies that the in-plane (ij = xx, yy) and out of plane (ij = zz) components are distinct. The qualitative similarities in both the schemes is evident. The real part of the dielectric constant $\varepsilon_1$ has prominent peaks at approximately 2 eV, 3.54 eV and the zero energy crossings lie between 4.0 - 4.5 eV. An important quantity of $\varepsilon_1(\omega)$ is the zero frequency limit $\varepsilon_1(0)$, which is the electronic part of the static dielectric constant that depends strongly on the band gap. The static dielectric constant $\varepsilon_1(0)$ are found to be 10.8 [62]. The corresponding value in TB-mBJ calculations is 9.7. The imaginary part of the dielectric constant $\varepsilon_2$ qualitatively follows DOS and is characterized by two prominent peaks, at $\sim$ 2 eV and between 4.0-4.5 eV, similar to $\varepsilon_1$. These peak positions correspond to the interband transitions between the P-3p and Sn-5p bands. The dominant peak (at $\sim$ 4 eV) in $\varepsilon_2$ lies slightly lower than the corresponding peak in $\varepsilon_1$. These peak positions correspond to the interband transitions between the P-3p and Sn-5p bands.

In conclusion, we investigated the non-linear photocurrent in non-centrosymmetric chalcopyrite semiconductor ZnSnP$_2$ based on first principles calculations. We report that the shift current conductivity is around 6 $\mu$A/V$^2$ near the band gap and 12 $\mu$A/V$^2$ at photon energy (3.5-4) eV. This comes mainly from the large real space charge center shift between valence electrons and conduction electrons of P-3p and Sn-5p orbitals. Distinct from the diffusion mechanism in the p-n junction based photogalvanic effect, the generation of photocurrent under linear polarized electromagnetic radiation in ZnSnP$_2$ is dominated by Berry phase related shift current. Due to the underlying selection rules ultrafast photo-induced currents will strongly depend on the crystal orientation.
and laser polarization. This can offer a promising avenue to achieve efficient generation and control of secondary terahertz radiation, which in ZnSnP₂ will result from the intrinsic shift current mechanism [43]: the magnitude of the shift current is comparable to the recent experimental value on SbSI [47] and an order of magnitude larger than multi-ferroelectric compound bismuth ferrite (0.5 μA/V²) [48].

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