

## Supplementary Information: Investigating charge carrier scattering processes in anisotropic semiconductors through first-principles calculations: The case of p-type SnSe

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### Fourier Interpolation

In order to introduce the main ideas behind Fourier interpolation within BoltzTraP, let us consider  $N_{KS}$  KS eigenvalues for a given band  $n$  of a three-dimensional (3D) periodic solid. The symmetry of the crystal's reciprocal space is incorporated in the energy bands. Therefore, it is natural to use star functions,  $Y_m(\mathbf{k})$ , as basis set to Fourier expand the quasi-particles energies

$$\tilde{\epsilon}_{\mathbf{k}} = \sum_{m=1}^M a_m Y_m(\mathbf{k}), \quad (1)$$

where

$$Y_m(\mathbf{k}) = \frac{1}{n_s} \sum_{\{v\}} \exp[i(v\mathbf{R}_m) \cdot \mathbf{k}], \quad (2)$$

with the sum running over all  $n_s$  point group operations  $\{v\}$  on the direct lattice translations,  $\mathbf{R}_m$ . The first derivatives are straightforwardly given by

$$\mathbf{v}_{\mathbf{k}} = \frac{\partial \tilde{\epsilon}_{\mathbf{k}}}{\partial \mathbf{k}} = \frac{i}{n_s} \sum_{m=1}^M a_m \sum_{\{v\}} (v\mathbf{R}_m) \exp[i(v\mathbf{R}_m) \cdot \mathbf{k}], \quad (3)$$

in which the main problem is the determination of Fourier coefficients,  $a_m$ .

BoltzTraP relies on the proposal by Shankland [1], according to which one should choose a set of basis functions for interpolation larger than the number of data points ( $M > N_{KS}$ ) and constrain the interpolation function to pass exactly through such points. In order to obtain a smooth interpolation, the extra basis functions are used to minimize a roughness function suitably defined by Pickett, Krakauer and Allen [2]

$$\mathbf{Re} = \sum_{m=2}^M |a_m|^2 \rho(R_m) \quad (4)$$

with

$$\rho(R_m) = \left(1 - c_1 \left(\frac{R_m}{R_{min}}\right)^2\right)^2 + c_2 \left(\frac{R_m}{R_{min}}\right)^6, \quad (5)$$

where  $R_m = |\mathbf{R}_m|$ ,  $R_{min}$  is the magnitude of the smallest nonzero lattice vector, and  $c_1 = c_2 = 3/4$ . Thus, the Lagrange multiplier method can now be used since the formulated problem is to minimize  $\mathbf{Re}$  subject to the constraints,  $\tilde{\epsilon}_{\mathbf{k}_l} = \epsilon_{\mathbf{k}_l}$ , with respect to the Fourier coefficients. From such minimization one obtains

$$a_m = \begin{cases} \rho(R_m)^{-1} \sum_{l=1}^{N_{KS}-1} \lambda_l^* [Y_m^*(\mathbf{k}_l) - Y_m^*(\mathbf{k}_{N_{KS}})] , & m > 1, \\ \epsilon_{\mathbf{k}_{N_{KS}}} - \sum_{m=2}^M a_m Y_m(\mathbf{k}_{N_{KS}}), & m = 1, \end{cases} \quad (6)$$

in which the Lagrange multipliers,  $\lambda_l^*$ , can be evaluated from

$$\epsilon_{\mathbf{k}_p} - \epsilon_{\mathbf{k}_{N_{KS}}} = \sum_{l=1}^{N_{KS}-1} \mathbf{H}_{pl} \lambda_l^*, \quad (7)$$

with

$$\mathbf{H}_{pl} = \sum_{m=2}^M \frac{[Y_m(\mathbf{k}_p) - Y_m(\mathbf{k}_{N_{KS}})] [Y_m^*(\mathbf{k}_l) - Y_m^*(\mathbf{k}_{N_{KS}})]}{\rho(R_m)}. \quad (8)$$

### Anisotropic $\mathbf{k}$ -mesh

In practice, a finer and anisotropic  $\mathbf{k}$ -mesh can be generated for the interpolation. To accomplish this, lattice points and their respective star functions are generated in real space following point the group operations of the crystal symmetry. The corresponding translation vector can be given as  $\mathbf{R} = u_1 \mathbf{a}_1 + u_2 \mathbf{a}_2 + u_3 \mathbf{a}_3$ , in which  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ ,  $\mathbf{a}_3$  are related to the crystal primitive vectors. Such points are generated inside a sphere of a radius  $R' = \sqrt[3]{3 \cdot n_{kpt} \cdot (M/N_{KS}) \cdot \Omega / 4\pi}$ , where  $n_{kpt}$  is the number of  $\mathbf{k}$ -points of the original  $\mathbf{k}$ -mesh in the

entire BZ,  $(M/N_{KS})$  is the required number of star functions per  $\mathbf{k}$ -point and  $\Omega$  is the volume of the unit cell. Consequently,  $R'$  determines the full extension of the real space and can be properly changed, for example, by increasing the number of star functions per  $\mathbf{k}$ -point. The corresponding reciprocal lattice, with a translation vector,  $\mathbf{k} = k_1\mathbf{b}_1 + k_2\mathbf{b}_2 + k_3\mathbf{b}_3$  can be determined by generating its three primitive vectors from the direct ones from  $[\mathbf{b}_1\mathbf{b}_2\mathbf{b}_3]^T = [\mathbf{a}_1\mathbf{a}_2\mathbf{a}_3]^{-1}$ , in which the  $2\pi$  factor was omitted following the crystallographic definition of reciprocal space. In order to capture the crystal anisotropy, the extension of the real space can be determined for each crystal direction, defining spheres for each crystallographic axis with the maximum radius given by  $R_{max}(t) = INT(R' \cdot \sqrt{\mathbf{b}_t \cdot \mathbf{b}_t}) + 1$ , with  $t = \{1, 2, 3\}$  and  $INT(x)$  gives the largest integer number that does not exceed the magnitude of  $x$ . Hence, lattice points fill all the spheres space inside the  $\{-R_{max}(t), R_{max}(t)\}$  range. Within BoltzTraP, a 3D array containing all vectors are sorted considering their concentric radius,  $r$ , from the sphere center, and providing that all vectors,  $\mathbf{R}$ , have different star functions,  $m$ . In practice, to determine all  $\mathbf{k}$  vectors from  $\mathbf{R}_m$ , a 3D Fast Fourier Transform (FFT) is performed, being possible to redefine a finer and anisotropic  $\mathbf{k}$ -mesh.

The magnitude of each  $\mathbf{R}_m$  vector,  $r$ , is defined through the metric tensor formalism. Let us consider the scalar product of two arbitrary vectors in the coordinate system of the real space,  $\mathbf{r}_1 \cdot \mathbf{r}_2 = (x_1\mathbf{a}_1 + y_1\mathbf{a}_2 + z_1\mathbf{a}_3) \cdot (x_2\mathbf{a}_1 + y_2\mathbf{a}_2 + z_2\mathbf{a}_3)$ . In the matrix notation this is written as

$$\mathbf{r}_1 \cdot \mathbf{r}_2 = \begin{bmatrix} x_1 & y_1 & z_1 \end{bmatrix} \begin{bmatrix} \mathbf{a}_1 \cdot \mathbf{a}_1 & \mathbf{a}_1 \cdot \mathbf{a}_2 & \mathbf{a}_1 \cdot \mathbf{a}_3 \\ \mathbf{a}_2 \cdot \mathbf{a}_1 & \mathbf{a}_2 \cdot \mathbf{a}_2 & \mathbf{a}_2 \cdot \mathbf{a}_3 \\ \mathbf{a}_3 \cdot \mathbf{a}_1 & \mathbf{a}_3 \cdot \mathbf{a}_2 & \mathbf{a}_3 \cdot \mathbf{a}_3 \end{bmatrix} \begin{bmatrix} x_2 \\ y_2 \\ z_2 \end{bmatrix} = \bar{\mathbf{X}}_1 \mathbf{G} \mathbf{X}_2. \quad (9)$$

Considering that  $\mathbf{r}_1 = \mathbf{r}_2 = \mathbf{R}_m$ , the magnitude of the real space vector is given by  $r = \sqrt{\bar{\mathbf{X}}\mathbf{G}\mathbf{X}}$ , with  $\bar{\mathbf{X}} = [u_1 u_2 u_3]$ . For all  $\mathbf{R}_m$  in the Bravais lattice, the reciprocal lattice is characterized by a set of wavevectors  $\mathbf{k}$ , such that,  $e^{2\pi i \mathbf{k} \cdot \mathbf{R}_m} = 1$ . Given  $\mathbf{R}_m$  and  $\mathbf{k}$  in the same direction, the magnitude of the vector  $\mathbf{k}$  in the reciprocal space is given by  $|\mathbf{k}| = (k_1 u_1 + k_2 u_2 + k_3 u_3) / r = (n_{int}(1) + n_{int}(2) + n_{int}(3)) / r$ , where  $n_{int}(t) = 1, 2, \dots, k_{max}(t)$  are integer numbers with  $k_{max}(t) = 2R_{max}(t) + 1$  defining the  $\mathbf{k}$ -mesh grid. In practice,  $k_{max}(t)$  should be carefully taken as the product of small primes in order to improve the efficiency of FFT. If we consider just one specific crystallographic axis, the magnitude of the  $\mathbf{k}$  vector can be determined for each axis by  $|\mathbf{k}|_t = k_t = n_{int}(t) / r$ . Hence, through the definition of anisotropic  $\mathbf{k}$ -mesh the anisotropy of materials TE properties can be captured.

## Scattering Mechanisms and the RTA

Within the Born approximation in the scattering theory, the magnitude of the Hamiltonian of the charge carrier interaction,  $H'$ , is considered to deviate only slightly from the magnitude of the non-perturbed Hamiltonian,  $H$ , that is,  $H' - H \ll H$ . The transition probability per-unit-time between Bloch states  $\Psi_{j,\mathbf{k}'}$  and  $\Psi_{n,\mathbf{k}}$  can be obtained from the first order perturbation theory (Fermi's golden rule)

$$W(n, \mathbf{k} | j, \mathbf{k}') = \frac{2\pi}{\hbar} |\langle \Psi_{j,\mathbf{k}'} | H' | \Psi_{n,\mathbf{k}} \rangle|^2 \delta(\epsilon_{j,\mathbf{k}'} - \epsilon_{n,\mathbf{k}}), \quad (10)$$

which is valid in the so-called weak coupling regime [3]. Integrating out such probability over the BZ, the total scattering rate is obtained. Specifically, in the presence of a phonon field, an electron in the Bloch state  $\Psi_{n,\mathbf{k}}$  will experience a perturbation  $H'$ , inducing a transition to the state  $\Psi_{j,\mathbf{k}'}$ . In such a process, momentum and energy are conserved so that  $\mathbf{k}' = \mathbf{k} \pm \mathbf{q}$  and  $\epsilon_{j,\mathbf{k}'} = \epsilon_{n,\mathbf{k}} \pm \hbar\omega_{\mathbf{q}}^\lambda$ , where  $\omega_{\mathbf{q}}^\lambda$  is the phonon frequency with wave vector  $\mathbf{q}$  and mode number  $\lambda$ . The plus-minus sign refers to phonon absorption or emission, respectively. The respective per-unit-time transition probability is calculated from Eq. (10) as

$$W(n, \mathbf{k} | j, \mathbf{k} \pm \mathbf{q}) = \frac{2\pi}{\hbar} |\langle \Psi_{j,\mathbf{k} \pm \mathbf{q}} | H' | \Psi_{n,\mathbf{k}} \rangle|^2 \delta(\epsilon_{j,\mathbf{k} \pm \mathbf{q}} - \epsilon_{n,\mathbf{k}} \mp \hbar\omega_{\mathbf{q}}^\lambda). \quad (11)$$

By using the above equations along with Eq. (10) of the main text, expressions for the different scattering mechanisms RTs can be derived, mostly following Ref. [4], as will be discussed below.

## Carrier-Acoustic Phonons Non-polar Scattering

The deformation potential technique, as introduced by Bardeen and Shockley [5] and extended by Herring and Vogt [6] has been used to derive an expression for the RT for the non-polar scattering of charge carrier by acoustic phonons. When an acoustic wave with vanishing  $\mathbf{q}$  vector travels through a finite crystal it may induce shifts in the spacing between neighboring atoms, resulting in local fluctuations of the energy band gap. These are known as acoustic deformation potentials (ADPs), which can be measured by quantifying the energy variation of the valence and conduction band edges per unit of strain. The former variation represents the interaction energy of holes with lattice oscillations. The magnitude

of the shifts,  $\mathbf{u}_s$ , are given in terms of plane waves as

$$\mathbf{u}_s(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} \sum_{\lambda=1}^3 \mathbf{e}_\lambda(\mathbf{q}) \cdot \left[ b_{\lambda,\mathbf{q}} \exp\{i\mathbf{q} \cdot \mathbf{r}\} + b_{\lambda,\mathbf{q}}^* \exp\{-i\mathbf{q} \cdot \mathbf{r}\} \right], \quad (12)$$

where  $\mathbf{r}$  are the atomic coordinates in real space,  $N$  is the number of atoms in the periodic crystal,  $\mathbf{e}_\lambda(\mathbf{q})$  is the polarization unit vector and  $b_{\lambda,\mathbf{q}}$  are the complex normal coordinates. In Eq. (12), all atoms in the elementary unit cell oscillate in phase and the interaction energy must be proportional to the first derivative of the  $\mathbf{u}_s(\mathbf{r})$  with respect to  $\mathbf{r}$

$$H'_{ac} = E_1 \nabla \mathbf{u}_s(\mathbf{r}), \quad (13)$$

where  $E_1$  is the effective deformation potential.

Going back to Eq. (10), it is possible to obtain the per-unit-time transition probability, and, along with Eq. (10) of the main text, the RT for a given electronic band  $n$  can be written as

$$\frac{1}{\tau_{\mathbf{k}}} = \frac{2\pi}{MN} \frac{E_1^2}{\hbar v_0^2} k_B T \sum_{\mathbf{k}'} \left( 1 - \frac{\mathbf{k} \cdot \mathbf{k}'}{kk'} \right) \delta(\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}}), \quad (14)$$

where  $M$  is the atomic mass and  $v_0$  is the sound velocity. In Eq. (14), it was considered that the scattering is elastic, and hence, the phonon energy has been neglected. Such approximation, is valid for  $T \gg 1\text{K}$  [4], which meets the conditions usually found in TE applications. Finally, considering that the electronic dispersion is arbitrary but spherically symmetric, the summation over  $\mathbf{k}'$  can be turned into an integral that can be solved by using spherical coordinates and properties of  $\delta$ -functions. Hence, one finds the following expression for the RT for non-polar scattering of charge carriers by acoustic phonons in a single band  $n$

$$\tau_{ac}(k) = \frac{\pi \hbar \rho}{E_1^2} \frac{v_0^2}{k_B T} \frac{1}{k^2} \left| \frac{\partial \epsilon_k}{\partial k} \right|, \quad (15)$$

where,  $\rho = MN/V$  is the mass density of the material and  $V$  is the crystal volume.

### Carrier-Optical Phonons Non-polar Scattering

In more complex crystal lattices with two or more atoms in the unit cell, alongside with the scattering by acoustic phonons, the polar and non-polar scattering by optical phonons are at play. The idea of deformation potentials has been extended to the interaction between charge carriers and long-wavelength ( $\mathbf{q} \rightarrow 0$ ) non-polar optical phonons, giving rise to the optical deformation potentials (ODP), corresponding to shifts of the elec-

tronic bands due to relative displacement between two sublattices of the crystal. Unlike the scattering by acoustic lattice oscillations, optical phonons oscillate out of phase, and the center of mass remains at rest. In the case of the scattering by non-polar optical phonons, the interaction energy related to the induced variation of the energy band gap should be proportional to the shift of any atom in the unit cell [4]

$$H'_{npol} = \sum_{\lambda=4}^{3s} \mathbf{A}_\lambda \mathbf{u}_s^\lambda, \quad (16)$$

where  $\mathbf{A}_\lambda$  is a constant vector related to the symmetry of the arrangement of the band edges,  $\mathbf{u}_s^\lambda$  is the atomic displacement (similar to Eq. (12)) associated with mode  $\lambda$ , and  $s$  is the number of atoms in the unit cell. Consequently, the energy operator in this case appears to be much more involving than the case of acoustic phonons. In order to proceed, an effective vector can be taken to represent all interactions in an average manner, and hence, all the complexity can be encompassed within such effective vector. Considering a specific optical phonon branch,  $\lambda$ , in which the scattering is occurring on its minimum,  $\mathbf{A}$  can be defined as

$$\mathbf{A} = E_0 \mathbf{b}_g, \quad (17)$$

where  $E_0$  is the effective ODP,  $\mathbf{b}_g = (\pi/a)\mathbf{g}$  is the reciprocal lattice vector with  $\mathbf{g}$  being a unit vector directed from the BZ center to the minimum, while  $a$  is the lattice constant.

Within the previous considerations, the per-unit-time transition probability for charge carriers, for a specific band  $n$ , can be obtained as

$$W_{npol}(\mathbf{k}|\mathbf{k}') = \frac{\pi E_0^2}{NM\omega_0} \left( \frac{\pi}{a} \right)^2 [N_0 \delta(\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}} - \hbar\omega_{\mathbf{q}}) + (N_0 + 1) \delta(\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}} + \hbar\omega_{\mathbf{q}})], \quad (18)$$

with  $\omega_0 = \omega_{(\mathbf{q} \rightarrow 0)}$  and  $N_0$  is the Bose-Einstein distribution. Additionally, we considered only coupling parallel to the unit polarization vector ( $\mathbf{e}_\lambda(\mathbf{q})$ ). The non-polar scattering of charge carriers by optical phonons is essentially non-elastic, due to the magnitude of optical phonon energy. However, the description of this scattering within the RT approximation may arise from the evenness of the transition probability function,  $W(\mathbf{k}|\mathbf{k}') = W(|\mathbf{k} - \mathbf{k}'|)$ , which is a condition satisfied by the scattering probability as given by Eq. (18). On the basis of such considerations, at high temperatures,  $k_B T \gg \hbar\omega_0$ , the following simple expression is obtained for the RT for the non-polar scattering by optical phonons at a specified band  $n$  [4]

$$\tau_{npol}(k) = \frac{1}{\pi \hbar} \beta^2 \frac{\rho a^2}{k_B T} \frac{1}{k^2} \left| \frac{\partial \epsilon_k}{\partial k} \right|, \quad (19)$$

in which  $\beta = \hbar\omega_0/E_0$  is the reciprocal ODP normalized by the energy of optical phonons. In particular,  $\tau_{n, pol}(k)$  presents the same temperature dependence as the scattering by acoustic phonons.

### Carrier-Optical Phonons Polar Scattering

In semiconductor compounds with some degree of ionic bonding, there is an additional interaction with charge carriers known as polar mode scattering, in which the charge carriers are scattered by the electric polarization caused by longitudinal optical (LO) phonons. This was firstly discussed by Fröhlich [7] and Callen [8], while Howarth and Sondheimer [9] developed the theory of polar mode scattering, on the basis of electrons as charge carriers on a simple parabolic conduction band. Following the derivation by Fröhlich [10], the electric polarization due to ion displacement is given by

$$\mathbf{P}(\mathbf{r}) = \left( \frac{\hbar\omega^{LO}(q)}{8\pi V\zeta^*} \right)^{1/2} \sum_{\mathbf{q}} \sum_{\lambda=4}^{3s} \mathbf{e}_\lambda \cdot [b_\lambda(\mathbf{q}) \exp\{i\mathbf{q} \cdot \mathbf{r}\} + b_\lambda^*(\mathbf{q}) \exp\{-i\mathbf{q} \cdot \mathbf{r}\}] , \quad (20)$$

where  $\omega^{LO}(q)$  is the frequency of the LO phonons;  $1/\zeta^* = 1/\zeta_\infty - 1/\zeta_0$ , with  $\zeta_\infty$  and  $\zeta_0$  being the high-frequency and the static dielectric constants, respectively. From the Poisson's equation we can derive the scalar potential of the polarization vector,  $\nabla^2\phi = 4\pi\nabla \cdot \mathbf{P}(\mathbf{r})$ , which yields the following interaction energy of the polar mode scattering of charge carriers by optical phonons

$$H'_{pol} = \pm e\phi = \mp ie \left( \frac{4\pi\hbar\omega^{LO}(q)}{2V\zeta^*} \right)^{1/2} \sum_{\mathbf{q}} \sum_{\lambda=4}^{3s} \frac{1}{q^2} (\mathbf{e}_\lambda \cdot \mathbf{q}) [b_\lambda(\mathbf{q}) \exp\{i\mathbf{q} \cdot \mathbf{r}\} + b_\lambda^*(\mathbf{q}) \exp\{-i\mathbf{q} \cdot \mathbf{r}\}] , \quad (21)$$

with  $\mathbf{e}_\lambda \cdot \mathbf{q} = q$  in the case of LO phonons.

If the phonon dispersion is not considered,  $\omega^{LO}(q) = \omega_0^{LO}$ , then the following expression for the transition probability, at a specific band  $n$ , is obtained

$$W_{pol}(\mathbf{k}|\mathbf{k}') = \frac{4\pi^2 e^2}{V\zeta^*} \frac{\omega_0^{LO}}{(\mathbf{k}' - \mathbf{k})^2} \times [N_0\delta(\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}} + \hbar\omega_0^{LO}) + (N_0 + 1)\delta(\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}} + \hbar\omega_0^{LO})] . \quad (22)$$

Unlike non-polar mode scattering, from Eq. (22) it can be seen that  $W_{pol}(\mathbf{k}|\mathbf{k}')$  is dependent on the directions  $\mathbf{k}$  and  $\mathbf{k}'$  and, generally, it is impossible to introduce RT for polar mode scattering of optical phonons. However, at high temperatures,  $k_B T \gg \hbar\omega_0^{LO}$ , the non-elasticity can be neglected with  $\epsilon_{\mathbf{k}'} \sim \epsilon_{\mathbf{k}}$  and  $N_0 + 1 \sim N_0 \sim$

$k_B T / \hbar\omega_0^{LO}$ , which yields

$$W_{pol}(\mathbf{k}|\mathbf{k}') = \frac{8\pi^2 e^2 k_B T}{V\zeta^* \hbar} \frac{1}{(\mathbf{k}' - \mathbf{k})^2} \delta(\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}}) . \quad (23)$$

Thus, substituting Eq. 23 into Eq. (10) of the main text and transforming the summation over  $\mathbf{k}'$  into an integral that can be solved by using spherical coordinates and properties of  $\delta$ -functions, it results in the following closed expression for the RT of polar mode scattering of optical phonons, given a specific band  $n$ ,

$$\tau_{pol}(k) = \frac{\zeta^* \hbar}{2e^2 k_B T} \left| \frac{\partial \epsilon_k}{\partial k} \right| , \quad (24)$$

which does not depend on the phonon-frequency in the high temperature limit.

The generalization to include screening effects was subsequently developed by Ehrenreich [11]. Free carriers that are present in the sample screen out the electric field produced by optical vibrations, resulting twofold effects in the quasi-static approximation, namely, a change in the matrix element of charge carrier interaction with optical phonons and a shift in the frequency of longitudinal optical mode [11]. The former effect decreases the transition probability by a factor of  $1 - (r_\infty q)^{-2}$ , in which  $r_\infty$  is the screening radius given by

$$r_\infty^{-2}(k) = \frac{4\pi e^2}{\zeta_\infty} \int -\frac{\partial f^{(0)}(\epsilon)}{\partial \epsilon_k} g(\epsilon) d\epsilon , \quad (25)$$

where  $f^{(0)}(\epsilon)$  is the equilibrium electron distribution function and  $g(\epsilon)$  is the density of states (DOS), which is given explicitly in Eq. (29) of the main text. The latter effect leads to a frequency shift of the LO vibrations given by

$$(\omega^{LO})^2 = (\omega^{TO})^2 \left( \frac{\zeta_0/\zeta_\infty + (r_\infty q)^{-2}}{1 + (r_\infty q)^{-2}} \right) , \quad (26)$$

where  $\omega^{TO}$  is the transverse optical (TO) mode frequency. Therefore, the frequency of the LO phonon is strongly reduced, which also affects the transition probability [12]. The dynamical features of the screening were neglected here, since their effect is regarded to be quite small [12]. Hence, the consideration of quasi-static screening results in the following factor in the denominator of expression for the RT

$$F_{pol} = \left[ 1 - \frac{1}{2(r_\infty k)^2} \ln[1 + 4(r_\infty k)^2] + \frac{1}{1 + 4(r_\infty k)^2} \right]^{-1} . \quad (27)$$

It is important to note that the energy dependence of RT is also changed because of the energy dependence of the screening through  $r_\infty$  [12].

The necessary modifications when dealing with polar

mode scattering of p-like symmetry holes have also been addressed [13–16], beyond the polar mode scattering of s-like electrons. The work by Wiley [16] gave the first quantitative discussion of overlap effects on the polar mobility of holes, showing that, for carriers with p-like valence bands, the mobility is about twice the mobility for carriers with pure s-like wave functions. Conclusions, in the same line of reasoning, that the mobility increases due to the p-like symmetry of wave functions, were obtained by Kranzer [13] on the basis of a numerical solution of the BTE and by Costato *et al.* [14] by using a Monte Carlo technique for solving the coupled BTE. Consequently, besides screening effects, it is also necessary to include the correction factor,  $K_{pol}$ , in the RT given by Eq. (24), due to the p-like symmetry of the wave functions, which is important, for example, in the case of polar mode scattering of holes. The way the correction factor  $K_{pol}$  is determined in the actual calculations will be discussed later in the article.

### Carrier-Impurity Scattering

The consideration of extrinsic collision processes, beyond those involving the crystalline lattice, i.e., the intrinsic scattering by phonons, requires the presence of impurities in the crystal. Particularly, we will consider only the concentration of ionized impurities because the number of charged donors or acceptors is usually considerably larger than that of neutral imperfections. Ionized impurity scattering has been treated theoretically by Brooks and Herring (B-H) [17, 18], by considering a screened Coulomb potential, the Born approximation for the evaluation of transition probabilities, and neglecting the perturbation effects of the impurities on the electron energy levels and wave functions. In the B-H theory, the electron is scattered independently by dilute concentrations of ionized centers randomly distributed in semiconductors. It constitutes a good description without considering more complex effects, such as the contributions from coherent scattering from pairs of impurity centers, which requires a quantum transport theory [19].

The per-unit-time transition probability for the scattering of charge carriers by ionized impurities can be written in the plane-wave approximation as

$$W(\mathbf{k}|\mathbf{k}') = \frac{2\pi}{\hbar} \frac{N_i}{V} \left| \int U(\mathbf{r}) \exp [i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}] d\mathbf{r} \right|^2 \delta(\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}}), \quad (28)$$

where  $U(\mathbf{r})$  is the scattering potential and  $N_i$  is the ionized impurity concentration.

The long-range Coulomb field,  $U(r) = e\phi(r) = \pm e^2/\zeta_0 r$ , where the potential  $\phi$  at a point  $r$  of the crystal

is due to the presence of positive (donor) or negative (acceptor) impurity ions. The straightforward application of this field in Eq. (28) leads to a logarithmic divergence, and hence, a screened Coulomb potential has to be considered. According to the B-H theory, the potential can be expressed in a more rigorous form as  $\phi(r) = \pm e/\zeta_0 r (\exp(-r/r_0))$ , where  $r_0$  is the radius of ion field screening defined by Eq. (31). From Eqs. (10) of the main text, (10), and (28), the RT for the scattering of charge carriers by ionized impurities can be expressed for each band  $n$  as

$$\tau_{imp}(k) = \frac{\hbar \zeta_0^2}{2\pi e^4 N_i F_{imp}(k)} k^2 \left| \frac{\partial \epsilon_k}{\partial k} \right| \quad (29)$$

where

$$F_{imp}(k) = \ln(1 + \eta) - \frac{\eta}{1 + \eta}, \quad (30)$$

is the screening function, with  $\eta = (2kr_0)^2$ , being

$$r_0^{-2}(k) = \frac{4\pi e^2}{\zeta_0} \int -\frac{\partial f^{(0)}(\epsilon)}{\partial \epsilon_k} g(\epsilon) d\epsilon. \quad (31)$$

### Anisotropy of Average hole velocity in SnSe

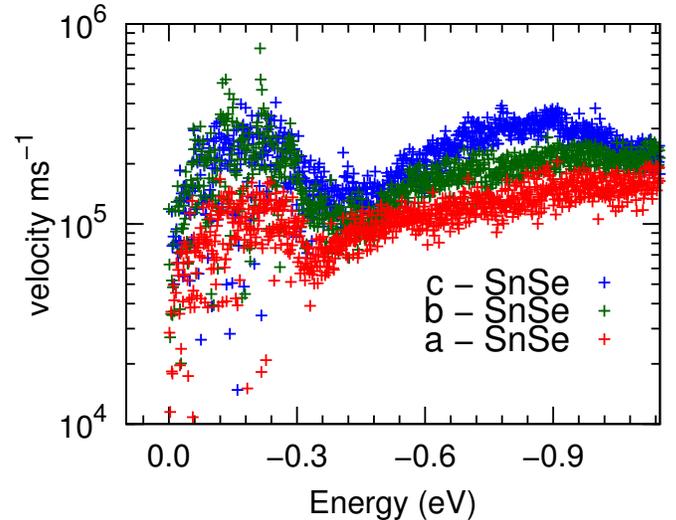


Figure 1. Average hole group velocity in function of hole energies in SnSe. The results are given along each crystalline axis  $\alpha$  ( $a$ ,  $b$ , and  $c$  axes) on the basis of the equation  $v_\alpha(\epsilon) = \sqrt{\sum_{n,\mathbf{k}} |v_{n,\mathbf{k}}^\alpha|^2 \delta(\epsilon - \epsilon_{n,\mathbf{k}}) / \sum_{n,\mathbf{k}} \delta(\epsilon - \epsilon_{n,\mathbf{k}})}$

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