

Phonon-limited carrier transport in the Weyl semimetal TaAs

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Topological Weyl semimetals represent a novel class of quantum materials that exhibit remarkable properties arising from their unique electronic structure. In this work, we employ state-of-the-art *ab initio* methods to investigate the role of the electron-phonon interactions on the charge transport properties of TaAs. Our calculations of the temperature-dependent electrical conductivity with the iterative Boltzmann transport equation show excellent agreement with experimental measurements above 100 K. Extending the analysis to doped systems, we demonstrate that even small shifts in the Fermi level can lead to substantial changes in conductivity, driven by the complex topology of the Fermi surface. In particular, modifications in Fermi surface nesting emerge as a key factor influencing scattering processes and carrier lifetimes. These findings offer critical insights into the microscopic mechanisms that govern transport in TaAs and highlight the sensitivity of Weyl semimetals to doping and carrier dynamics.

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I. INTRODUCTION

Topological Weyl semimetals (WSMs) are attracting tremendous interest because of their exotic electronic, optical, and magnetic properties [1–4], as well as their potential applications in quantum technologies [5–9]. These materials feature nontrivial topological band structures, hosting pairs of Weyl points with opposite chirality where the conduction and valence bands cross linearly, forming a three-dimensional (3D) analog of graphene [10]. Additionally, akin to the surface states in topological insulators, WSMs exhibit Fermi arc surface states, which connect the surface projections of the Weyl points. These surface states are a direct consequence of the fact that the Weyl nodes act as topological monopoles, serving as either “sources” or “sinks” of Berry curvature [11]. Taken together, the interplay between bulk Weyl fermions and surface Fermi arcs gives rise to a range of novel physical phenomena, including the chiral anomaly [12–14], negative magnetoresistance [13,15–17], the anomalous quantum Hall effect [18,19], and topological superconductivity [20–24].

Despite extensive experimental efforts, the first Weyl semimetal was only realized in 2015 [25–30], following the prediction of a topological Weyl semimetal state in the TaAs materials class [31,32]. Angle-resolved photoemission spectroscopy (ARPES) and microwave transmission measurements [9,25,26,30,33] confirmed the existence of 12 pairs of Weyl nodes near the Fermi level in the bulk, along with Fermi arc states on the surface. Subsequent experimental studies revealed exceptional transport properties in these materials,

including ultrahigh carrier mobility [34,35], extremely large linear magnetoresistance [32,36], and chiral-anomaly-induced negative longitudinal magnetoresistance [13–15,37]. Notably, TaAs, the prototypical compound of this family, has been reported to exhibit ultrahigh electron mobility of approximately $1.8 \times 10^5 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$ at 10 K [13] and $4.8 \times 10^5 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$ at 2 K [38]. The electron mobility changes rapidly with increasing temperature, dropping by two orders of magnitude above 80 K [13]. Electron-phonon (e-ph) interactions play a crucial role in determining electronic conductivity in TaAs, but theoretical studies have so far focused on their effects on the phonon linewidth [39], linear optical conductivity [40], and thermal transport [41]. The study of carrier transport is further complicated by the material’s band topology, where linear band dispersion at the Weyl pockets requires extremely dense Brillouin zone sampling to accurately capture contributions from these localized hot spots, making the computations very challenging.

In this work, we present a first-principles investigation of the temperature-dependent conductivity of TaAs, focusing on the effect of electron-phonon interactions. Our computational results, based on the iterative solution of the Boltzmann transport equation (BTE), show excellent agreement with experimental measurements. By analyzing electron-phonon scattering rates, we identify phonon wave vectors associated with pronounced Fermi surface nesting as the dominant contributors to scattering, whereas the electron-phonon matrix elements remain of the same order of magnitude across the entire Brillouin zone. Furthermore, we demonstrate that while the conductivity decreases with electron doping, it is enhanced by hole doping. This behavior is attributed to the evolution of the Fermi surface rather than changes in the electron-phonon coupling strength. Finally, calculations using the

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constant relaxation time approximation (CRTA) exhibit large discrepancies with experiments, highlighting the importance of accounting for the temperature and doping dependence of scattering rates. These findings provide valuable insights into the microscopic mechanisms governing transport in TaAs.

II. METHODS

We use the QUANTUM ESPRESSO (QE) package [42] with optimized norm-conserving Vanderbilt pseudopotentials (ONCVSP) [43] from the Pseudo Dojo library [44] generated with the fully relativistic Perdew-Burke-Ernzerhof (PBE) parametrization [45]. We use a plane-wave cutoff of 80 Ry, a Methfessel-Paxton smearing [46] value of 0.01 Ry, and a Γ -centered 12^3 $\mathbf{k}$ -grid. The lattice parameters and atomic positions are relaxed until the total energy is converged within 10^{-6} Ry and the maximum force on each atom is less than 10^{-4} Ry/Å. Spin-orbit coupling (SOC) is included in the electronic structure calculations. The dynamical matrices and the linear variation of the self-consistent potential arising from atomic displacements are calculated within density-functional perturbation theory [47] on a 4^3 $\mathbf{q}$ -grid.

To investigate electron-phonon interactions and transport properties, we use the EPW code [48–50]. The electronic wavefunctions required for the Wannier interpolation [51,52] are obtained on a uniform Γ -centered 8^3 $\mathbf{k}$ -grid. We use 32 atom-centered orbitals to describe the electronic structure of TaAs, with five d and three p orbitals on each Ta and As atom as initial guesses for the Wannier functions, respectively. The Weyl node positions are determined using the Nelder-Mead algorithm as implemented in WannierTools [53].

To converge the Fermi level within 0.1 meV, Brillouin zone $\mathbf{k}$ -grids with at least 80^3 points are required, as shown in Fig. S1 within the Supplemental Material (SM) [54]. This level of accuracy is essential in TaAs because the relative energy positions of the Weyl nodes with respect to the Fermi level are in the order of just a few meV. Accordingly, we obtain a converged Fermi level, $\varepsilon_F^0 = 17.0633$ eV, using the Wannier-interpolated electronic structure within the EPW code [49,50], with $\mathbf{k}$ -grids ranging from 80^3 to 120^3 and a Fermi-Dirac smearing of 26 meV (corresponding to 300 K). The resulting ε_F^0 is used both to locate the Weyl points and in the transport calculations for the undoped system.

The semimetallic nature of TaAs, combined with its complex Fermi surface featuring multiple electron- and hole-like pockets arising from both Weyl node crossings and trivial states, makes transport calculations particularly sensitive to the Fermi level position and the sampling density of the $\mathbf{k}$ - and $\mathbf{q}$ -point grids. The Boltzmann transport equations are solved on fine uniform 140^3 $\mathbf{k}$ - and 70^3 $\mathbf{q}$ -point grids, with an energy window of ± 0.2 eV around the Fermi level. These grids yield well-converged results, as demonstrated by our convergence tests in Fig. S2 within the SM [54]. All Dirac δ functions appearing in the expressions for the iterative BTE, scattering rate, phonon linewidth, and nesting function are approximated by Gaussians with a broadening of 2 meV. To assess the sensitivity of our results to this parameter, we performed transport calculations using both 1 meV and 2 meV broadening values. As shown in Table S1 within the SM [54], the resulting conductivities are converged within the numerical accuracy of

our calculations, demonstrating the robustness of our results with respect to the chosen broadening. We also note that while transport properties in semiconductors are more sensitive to the choice of broadening [55,56], this is generally not the case for metals and semimetals, as demonstrated here.

To evaluate the variation in electron-phonon coupling among different phonon modes, we define the modulus of the mode-resolved e-ph coupling strength as

$$|g_{\mathbf{qv}}| = \left[\sum_{m\mathbf{k}} |g_{m\mathbf{nv}}(\mathbf{k}, \mathbf{q})|^2 / (N_{\mathbf{k}} N_b^2) \right]^{1/2}, \quad (1)$$

where $g_{m\mathbf{nv}}(\mathbf{k}, \mathbf{q})$ is the e-ph coupling matrix element for the scattering between the electronic states $|n\mathbf{k}\rangle$ and $|m\mathbf{k} + \mathbf{q}\rangle$ through a phonon of frequency $\omega_{\mathbf{qv}}$. Here, $N_{\mathbf{k}}$ is the number of $\mathbf{k}$ -points and $N_b = 8$ is the number of bands near the Fermi level included in the summation.

To elucidate the role of e-ph interactions, we also compute the phonon linewidth

$$\gamma_{\mathbf{qv}} = \pi \sum_{mn} \int \frac{d\mathbf{k}}{\Omega_{\text{BZ}}} |g_{m\mathbf{nv}}(\mathbf{k}, \mathbf{q})|^2 \times (f_{n\mathbf{k}}^0 - f_{m\mathbf{k}+\mathbf{q}}^0) \delta(\varepsilon_{m\mathbf{k}+\mathbf{q}} - \varepsilon_{n\mathbf{k}} - \hbar\omega_{\mathbf{qv}}), \quad (2)$$

and the Fermi surface nesting function

$$\zeta_{\mathbf{q}} = \sum_{mnv} \int \frac{d\mathbf{k}}{\Omega_{\text{BZ}}} \frac{1}{\hbar\omega_{\mathbf{qv}}} (f_{n\mathbf{k}}^0 - f_{m\mathbf{k}+\mathbf{q}}^0) \delta(\varepsilon_{m\mathbf{k}+\mathbf{q}} - \varepsilon_{n\mathbf{k}} - \hbar\omega_{\mathbf{qv}}). \quad (3)$$

At low temperatures, the Fermi factors restrict the $\mathbf{k}$ integration to a narrow region about the Fermi surface of width $\omega_{\mathbf{qv}}$, reducing the phonon linewidth and the nesting function to the following expressions [57]:

$$\gamma_{\mathbf{qv}} = \pi \hbar\omega_{\mathbf{qv}} \sum_{mn} \int \frac{d\mathbf{k}}{\Omega_{\text{BZ}}} |g_{m\mathbf{nv}}(\mathbf{k}, \mathbf{q})|^2 \times \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_F) \delta(\varepsilon_{m\mathbf{k}+\mathbf{q}} - \varepsilon_F), \quad (4)$$

$$\zeta_{\mathbf{q}} = \sum_{mnv} \int \frac{d\mathbf{k}}{\Omega_{\text{BZ}}} \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_F) \delta(\varepsilon_{m\mathbf{k}+\mathbf{q}} - \varepsilon_F). \quad (5)$$

The electrical conductivity is calculated by solving the linearized Boltzmann transport equation [58]

$$\sigma_{\alpha\beta} = -\frac{e}{(2\pi)^3} \sum_n \int d\mathbf{k} v_{n\mathbf{k},\alpha} \partial_{E_\beta} f_{n\mathbf{k}}, \quad (6)$$

where e is the electronic charge, and $v_{n\mathbf{k},\alpha}$ is the band velocity of an electron with momentum $\mathbf{k}$ at band n along the Cartesian direction α . The function $f_{n\mathbf{k}}$ represents the electronic occupation factor, and its derivative with respect to the electric field $\partial_{E_\beta} f_{n\mathbf{k}}$ is obtained by iteratively solving the following equation:

$$\begin{aligned} \tau_{n\mathbf{k}}^{-1} \partial_{E_\beta} f_{n\mathbf{k}} = & e \frac{\partial f_{n\mathbf{k}}^0}{\partial \varepsilon_{n\mathbf{k}}} v_{n\mathbf{k},\beta} + \frac{2\pi}{\hbar} \sum_{mv} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} |g_{m\mathbf{nv}}(\mathbf{k}, \mathbf{q})|^2 \\ & \times [(n_{\mathbf{qv}} + 1 - f_{n\mathbf{k}}^0) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{qv}}) \\ & + (n_{\mathbf{qv}} + f_{n\mathbf{k}}^0) \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{qv}})] \partial_{E_\beta} f_{m\mathbf{k}+\mathbf{q}}. \end{aligned} \quad (7)$$

Here, $\varepsilon_{n\mathbf{k}}$ is the energy eigenvalue of the electronic state $|n\mathbf{k}\rangle$, Ω^{BZ} is the volume of the Brillouin zone, $f_{n\mathbf{k}}^0$ is the Fermi-Dirac distribution function, and $n_{\mathbf{q}\nu}$ is the bosonic occupation factor. The scattering rate $\tau_{n\mathbf{k}}^{-1}$ is defined as

$$\tau_{n\mathbf{k}}^{-1} = \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{d\mathbf{q}}{\Omega^{\text{BZ}}} |g_{mn\nu}(\mathbf{k}, \mathbf{q})|^2 \times \left[(n_{\mathbf{q}\nu} + 1 - f_{m\mathbf{k}+\mathbf{q}}^0) \delta(\varepsilon_{m\mathbf{k}+\mathbf{q}} - \varepsilon_{n\mathbf{k}} + \hbar\omega_{\mathbf{q}\nu}) + (n_{\mathbf{q}\nu} + f_{m\mathbf{k}+\mathbf{q}}^0) \delta(\varepsilon_{m\mathbf{k}+\mathbf{q}} - \varepsilon_{n\mathbf{k}} - \hbar\omega_{\mathbf{q}\nu}) \right]. \quad (8)$$

Omitting the second term on the right-hand side of Eq. (7) reduces the expression for $\sigma_{\alpha\beta}$ to the self-energy relaxation time approximation (SERTA) form of the conductivity [59],

$$\sigma_{\alpha\beta}^{\text{SERTA}} = -\frac{e^2}{(2\pi)^3} \sum_n \int d\mathbf{k} \frac{\partial f_{n\mathbf{k}}^0}{\partial \varepsilon_{n\mathbf{k}}} v_{n\mathbf{k},\alpha} v_{n\mathbf{k},\beta} \tau_{n\mathbf{k}}. \quad (9)$$

Furthermore, if the relaxation time in Eq. (9) is approximated as a constant, $\tau_{n\mathbf{k}} = \tau$, the expression takes the form used in the CRTA.

To analyze the scattering rates in detail, we also define the energy-averaged scattering rate

$$\tau^{-1}(\varepsilon) = \frac{\sum_{n\mathbf{k}} \tau_{n\mathbf{k}}^{-1} \delta(\varepsilon_{n\mathbf{k}} - \varepsilon)}{\sum_{n\mathbf{k}} \delta(\varepsilon_{n\mathbf{k}} - \varepsilon)}. \quad (10)$$

and the mode-resolved scattering rate [60]

$$\frac{\partial \tau_{n\mathbf{k}}^{-1}}{\partial \omega} = \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{d\mathbf{q}}{\Omega^{\text{BZ}}} |g_{mn\nu}(\mathbf{k}, \mathbf{q})|^2 \delta(\omega_{\mathbf{q}\nu} - \omega) \times \left[(n_{\mathbf{q}\nu} + 1 - f_{m\mathbf{k}+\mathbf{q}}^0) \delta(\varepsilon_{m\mathbf{k}+\mathbf{q}} - \varepsilon_{n\mathbf{k}} + \hbar\omega_{\mathbf{q}\nu}) + (n_{\mathbf{q}\nu} + f_{m\mathbf{k}+\mathbf{q}}^0) \delta(\varepsilon_{m\mathbf{k}+\mathbf{q}} - \varepsilon_{n\mathbf{k}} - \hbar\omega_{\mathbf{q}\nu}) \right]. \quad (11)$$

Note that the difference between Eqs. (11) and (8) is the $\delta(\omega_{\mathbf{q}\nu} - \omega)$ term in the former, such that

$$\tau_{n\mathbf{k}}^{-1} = \int d\omega \frac{\partial \tau_{n\mathbf{k}}^{-1}}{\partial \omega}. \quad (12)$$

We can also define the mode-resolved energy-averaged scattering rate as

$$\frac{\partial \tau^{-1}(\varepsilon)}{\partial \omega} = \frac{\sum_{n\mathbf{k}} \frac{\partial \tau_{n\mathbf{k}}^{-1}}{\partial \omega} \delta(\varepsilon_{n\mathbf{k}} - \varepsilon)}{\sum_{n\mathbf{k}} \delta(\varepsilon_{n\mathbf{k}} - \varepsilon)}. \quad (13)$$

Similar to Eq. (12), we have

$$\tau^{-1}(\varepsilon) = \int d\omega \frac{\partial \tau^{-1}(\varepsilon)}{\partial \omega}. \quad (14)$$

Finally, we derive a simplified expression for the conductivity that relates it to the density of states (DOS), the average squared velocity, and the scattering rate at the Fermi level. At low temperatures, the derivative of the Fermi-Dirac distribution $-\frac{\partial f_{n\mathbf{k}}^0}{\partial \varepsilon_{n\mathbf{k}}}$ can be approximated by a delta function $\delta(\varepsilon_{n\mathbf{k}} - \varepsilon_F)$. Under this approximation, and assuming $\beta = \alpha$, we replace the state-dependent quantities $v_{n\mathbf{k},\alpha}$, $v_{n\mathbf{k},\alpha}$ and $\tau_{n\mathbf{k}}$ with their averages near the Fermi level, denoted as $\langle v_\alpha^2 \rangle$ and $\tau(\varepsilon_F)$. The average squared velocity is defined as

$$\langle v_\alpha^2 \rangle = \frac{\sum_{n\mathbf{k}} v_{n\mathbf{k},\alpha}^2 \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_F)}{\sum_{n\mathbf{k}} \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_F)}. \quad (15)$$

With this substitution, the summation and energy integration in Eq. (9) reduce to the electronic density of states at the Fermi level, $N(\varepsilon_F)$. The resulting simplified conductivity expression is

$$\sigma_{\alpha\alpha}^{\text{SIMPLE}} = \frac{e^2}{(2\pi)^3} N(\varepsilon_F) \langle v_\alpha^2 \rangle \tau(\varepsilon_F). \quad (16)$$

III. RESULTS AND DISCUSSION

TaAs crystallizes in the body-centered tetragonal lattice (space group $I4_1md$, no. 109) with broken spatial inversion symmetry [31,32], a key condition for the realization of Weyl fermions. The structure comprises interpenetrating Ta and As sublattices, shifted relative to each other by $(a/2, a/2, c/12)$, as illustrated in Fig. 1(a). The optimized lattice parameters are $a = 3.456 \text{ \AA}$ and $c = 11.719 \text{ \AA}$, 0.7% larger than the experimentally measured values [13,26,33], and in good agreement with previous theoretical studies [26,32,41].

The electronic and topological structure of TaAs has been extensively studied in previous works [31,32,63], so we summarize only the key aspects here. In the presence of SOC, the band structure becomes fully gapped along all high-symmetry directions. However, the valence band maximum and conduction band minimum lie at the Fermi level (ε_F^0), resulting in a semimetallic system, as shown in Fig. 1(b) (see Fig. S1 within the SM [54] for a zoomed-in view near ε_F^0). Orbital decomposition reveals that Ta-5d states dominate both sets of bands in this energy region, while As-4p states contribute only minimally. Because of the semimetallic character, the DOS remains low at ε_F^0 but increases rapidly with energy into both the valence and conduction bands.

As shown in Fig. 1(c), 12 pairs of Weyl nodes emerge in the bulk Brillouin zone because of the broken inversion symmetry [31,32]. In the absence of SOC, gapless crossings of the valence and conduction bands along some high-symmetry lines form two closed nodal lines in both the $k_x = 0$ and $k_y = 0$ mirror planes [32]. Inclusion of SOC gaps the four nodal lines, each of them evolving into three pairs of gapless points slightly displaced from the mirror planes (one pair in the $k_z = 0$ plane, labeled as W1, and two pairs in the $k_z = \pm\pi/c$ planes, labeled as W2, following the convention in Refs. [4,13]). Figure 1(d) presents a zoomed-in view of the band structure, highlighting the two distinct types of Weyl nodes. The W1 nodes are located 8.5 meV below the Fermi level, while the W2 nodes remain much closer, 2.5 meV above it, consistent with ARPES measurements [14]. Moreover, the 11 meV energy offset between the two sets of Weyl nodes is in excellent agreement with prior first-principles calculations (14 meV) [25,63] and ARPES measurements (13 meV) [14]. This consistency indicates that the PBE functional provides a reliable description of the electronic structure of TaAs. For comparison, a previous study using the PBEsol functional [39] reported an energy difference of only 4 meV between the Weyl nodes. More importantly, both sets of nodes were located below the Fermi level, and their energy ordering was inverted, features that deviate significantly from the experimental observations. Figure 2(a) illustrates the phonon dispersion of TaAs, color-coded by the e-ph coupling strength, along with the projected phonon density of states

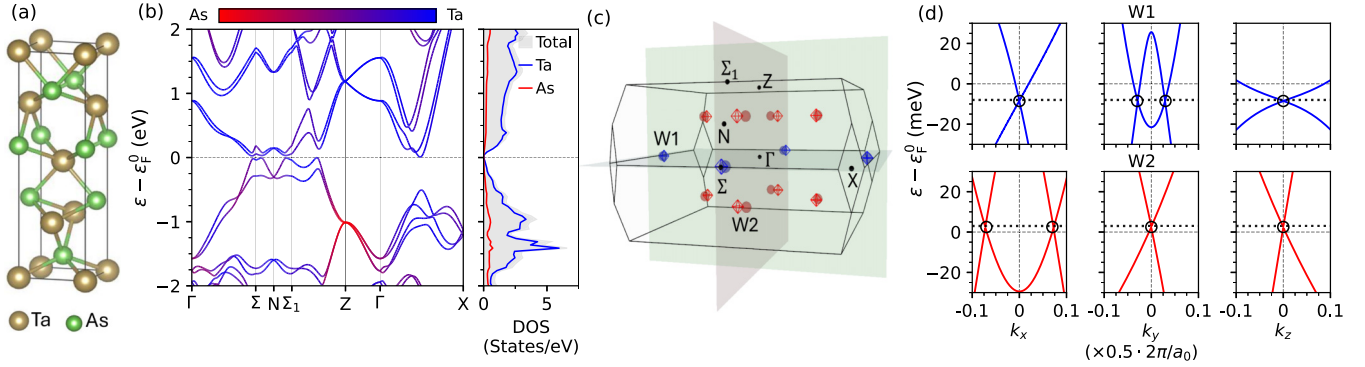


FIG. 1. (a) Crystal structure of TaAs, with Ta and As atoms shown as brown and green spheres, respectively. (b) Electronic band structure with orbital-resolved (fat band) character, along with total and partial density of states (DOS). (c) Brillouin zone with the $k_x = 0$ and $k_y = 0$ mirror planes showing the 12 pairs of Weyl nodes. The two distinct types of Weyl nodes, W1 and W2, are indicated by blue and red, respectively. Solid spheres and open diamonds represent the opposite chirality of the Weyl points. (d) Zoomed-in view of the band structure highlighting the Weyl nodes W1 located approximately 8.5 meV below the Fermi level and the Weyl nodes W2 located approximately 2.5 meV above it. The a_0 in the x -axis label denotes the unit cell edge length, given by $\sqrt{2a^2 + c^2}/2$.

(PhDOS). The acoustic modes (0–15 meV) are smoothly dispersive and primarily involve Ta contributions, as evidenced by the overlapping blue (Ta) and red (As) PhDOS projections. As previously noted [41,65], the optical phonon spectrum is clearly split into two distinct regions by a gap of approximately 4 meV, indicating weak hybridization between vibrations of the heavier Ta atoms and the lighter As atoms. Consistent with their mass difference, the lower-frequency vibrations (15–20 meV) are mainly associated with Ta atoms, while higher-frequency modes (24–35 meV) are dominated by As vibrations. Raman measurements confirm all optical phonon modes at the Brillouin zone center, identifying one A_1 , two B_1 , and three E modes [61]. Their distinct symmetries and energies are consistent with our first-principles results.

To shed light on the role of the e-ph interactions in TaAs, we evaluate the modulus of the mode-resolved e-ph coupling strength $|g_{qv}|$, as defined in Eq. (1) (see Sec. II). Analysis of Fig. 2(a) shows that the coupling strength is relatively uniform across most modes, with an average of around 10 meV. The strongest coupling comes from the low-energy optical modes within the 11–20 meV range, reaching values up to 15 meV, as indicated by the bright yellow coloring at the Γ and Z points and along the Σ -N- Σ_1 and Γ -Z directions. In contrast, the phonon linewidths γ_{qv} , defined in Eq. (2) and shown in Fig. 2(b), span a much broader range, over three orders of magnitude, from 10^{-2} down to 10^{-5} meV. The largest values are again associated with the same low-energy optical modes, though now primarily near the Γ point and along the Γ -Z path, consistent with previous findings [39]. This wide variation

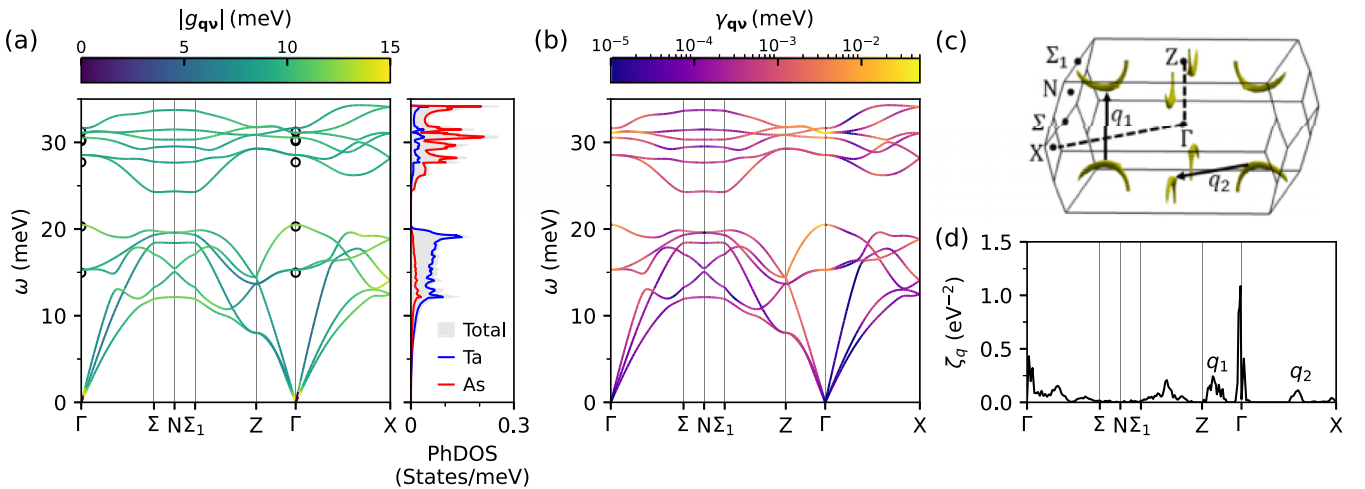


FIG. 2. Phonon dispersion of TaAs with (a) mode-resolved electron-phonon coupling strength $|g_{qv}|$ and (b) phonon linewidths γ_{qv} indicated by a color scale. The total and atom-projected phonon density of states (PhDOS) are shown alongside (a). Hollow black circles in the phonon dispersion in (a) correspond to Raman data from Ref. [61]. (c) Fermi surface generated using a 10-meV energy window around the Fermi level with the XCrySDen package [62]. The surface reveals eight banana-shaped hole pockets, each containing a pair of W2 nodes. The black solid arrows indicate possible inter-pocket scatterings with $\mathbf{q}_1$ and $\mathbf{q}_2$ wave vectors along the Γ -Z and Γ -X directions (dashed lines), respectively. (d) Nesting function shown along the same high-symmetry path as in (a) and (b). The two peaks along the Γ -Z and Γ -X directions are labeled by wave vectors $\mathbf{q}_1$ and $\mathbf{q}_2$.

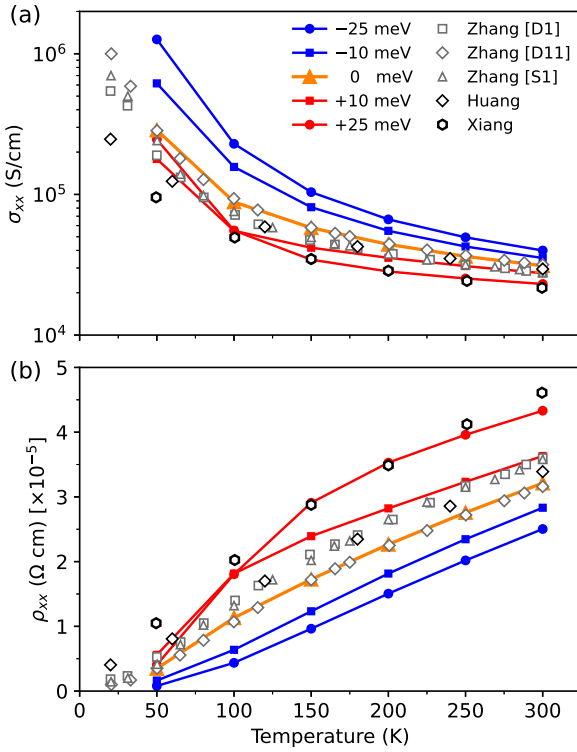


FIG. 3. (a) Electrical conductivity and (b) resistivity of TaAs for the undoped system ($\varepsilon_F = \varepsilon_F^0$) and for two levels of electron and hole doping ($\varepsilon_F = \varepsilon_F^0 \pm 25$ meV and $\varepsilon_F = \varepsilon_F^0 \pm 10$ meV). Experimental data from Refs. [13,38,64] are shown as hollow symbols for comparison. The three highest-quality samples, labeled as S1, D11, and D1, from Ref. [38] are used.

suggests that the linewidths are more strongly influenced by the structure of the Fermi surface than by the strength of the e-ph coupling.

In order to disentangle the two contributions, we further examine the nesting function depicted in Fig. 2(d). For consistency with the phonon linewidth analysis, we focus on the results obtained with Eq. (3). However, similar trends were found using the commonly adopted double-delta approximation given in Eq. (5) (see Fig. S3 within the SM [54]). The nesting function exhibits its highest peak near the Γ point, with pronounced features along the Γ - Σ , Z - Σ_1 , and Γ - Z directions, as well as a smaller peak along Γ - X . To interpret these features, we show the Fermi surface in Fig. 2(c), which reveals eight banana-shaped hole pockets, each containing a pair of W2 nodes. The strong peak in $\zeta_{\mathbf{q}}$ at Γ can be attributed to intrapocket scattering, while the other peaks are associated with the inter-pocket scattering. In particular, the black arrows in Fig. 2(c) indicate possible inter-pocket transitions mediated by phonons with wave vectors $\mathbf{q}_1$ and $\mathbf{q}_2$ along the Γ - Z and Γ - X directions, respectively. These observations highlight the key role of Fermi surface nesting in governing e-ph scattering processes in TaAs.

We now turn to the transport properties of TaAs and compute the temperature-dependent electrical conductivity using the iterative BTE [58], as described in Sec. II. Figure 3(a) displays the calculated conductivity for the undoped system ($\varepsilon_F = \varepsilon_F^0$) and for two levels of electron and

hole doping ($\varepsilon_F = \varepsilon_F^0 \pm 25$ meV and $\varepsilon_F = \varepsilon_F^0 \pm 10$ meV). In all cases, the transport behavior is metallic, with the conductivity decreasing as temperature increases. We find that the computed conductivity for the undoped and electron-doped systems closely matches experimental data [13,38,64]. Notably, to minimize the effect of charge-impurity scattering, in Fig. 3(a) we compare our results with measurements for the three highest-quality samples among the nine reported in Ref. [38]. These samples, labeled D1, D11, and S1 in Fig. 1(c) of Ref. [38], exhibit the largest residual resistance ratios. As pointed out in that study, sample quality is highly sensitive to the growth conditions, which in turn strongly influence the position of the Fermi level and the impurity concentration, key factors affecting electrical conductivity. Our results also reveal a strong sensitivity to the position of ε_F . Specifically, hole doping yields higher conductivity values than electron doping across the entire temperature range. For completeness, we also present the resistivity in Fig. 3(b), which shows that the slope of the temperature dependence of resistivity for the undoped case is close to that observed in experimental samples from Refs. [13,38]. These results confirm that the transport in high-quality TaAs samples is phonon-limited. To illustrate the variation in sample quality, in Fig. S4 within the SM [54], we include data for additional, lower-quality samples [35,38]. These samples exhibit significantly reduced conductivity (or increased resistivity), likely because of charge-impurity scattering, and therefore are not directly comparable to our phonon-limited computational results.

A comparison with results from the SERTA shows that it produces conductivities that differ from the iterative BTE by less than 5% [see Fig. S5(a) within the SM [54]]. This behavior can be understood by examining the expressions for SERTA and BTE. The iterative BTE [Eqs. (6) and (7)] couples the nonequilibrium occupations $\partial_{E_{\beta}} f_{n\mathbf{k}}$ across different states via e-ph scattering. This term captures scattering-in contributions from other $\mathbf{k}$ -points and thus accounts for the redistribution of carriers under the applied electric field. While in SERTA [Eq. (9)], the conductivity depends only on the state-dependent scattering rates $\tau_{n\mathbf{k}}$. When the results from BTE and SERTA agree closely, it indicates that the e-ph coupling and Fermi surfaces are isotropic, such that forward and backward scattering processes are similar, a typical behavior in metals.

Given the small variation in e-ph matrix elements across the Brillouin zone, we also computed the conductivity using the CRTA, adopting a fixed relaxation time of $\tau = 0.216$ ps at 300 K to reproduce the iterative BTE result in the undoped case. As shown in Figs. S5(a) and S5(b) within the SM [54], the significant discrepancies between CRTA and iterative BTE at different temperatures or under electron doping indicate that CRTA is inadequate for describing transport in TaAs.

Insight into the conductivity behavior is obtained by examining the impact of electron and hole doping on the Fermi surface and nesting function. Compared to the undoped system, hole doping preserves the eight original large hole pockets and introduces several additional small hole pockets around the k_z plane, where the W1 Weyl nodes are located [see Fig. 4(a)]. In contrast, electron doping markedly alters

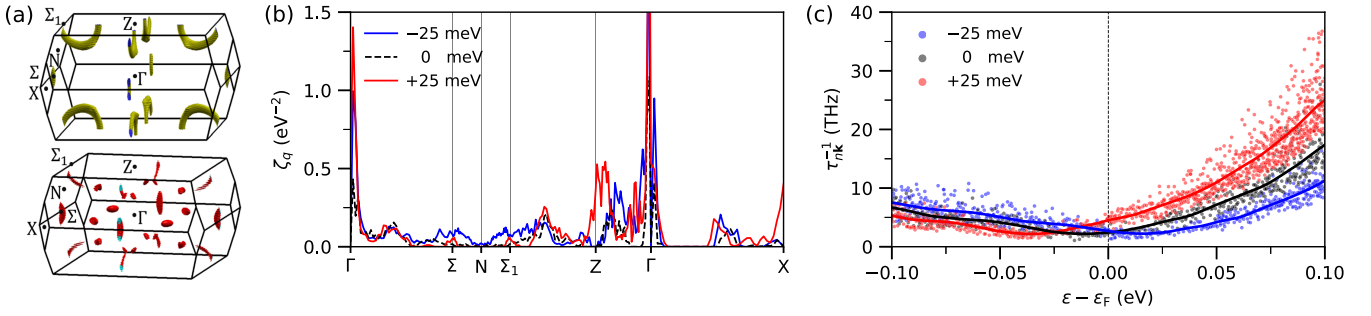


FIG. 4. (a) Three-dimensional Fermi surface, (b) nesting function, and (c) scattering rates for hole-doped ($\varepsilon_F = \varepsilon_F^0 - 25$ meV) and electron-doped ($\varepsilon_F = \varepsilon_F^0 + 25$ meV) TaAs. Panels (b) and (c) show quantities evaluated at 300 K, with results for the undoped system ($\varepsilon_F = \varepsilon_F^0$) included for comparison. In (c), the energy-averaged scattering rates are shown as solid lines.

the Fermi surface topology, leading to the disappearance of hole pockets and the emergence of multiple smaller electron pockets. As a result, the nesting function undergoes more pronounced changes in the electron-doped case, with additional peaks near the Z and X points and an enhanced peak at Γ , as shown in Fig. 4(b).

The observed conductivity trend can be understood qualitatively using the simplified conductivity expression in Eq. (16), which relates the DOS, averaged squared velocity, and scattering rates at the Fermi level. This analysis is done for $\varepsilon_F = \varepsilon_F^0$ and $\varepsilon_F = \varepsilon_F^0 \pm 25$ meV, and the results shown in Table S2 within the SM [54]. The energy-averaged scattering rates $\tau^{-1}(\varepsilon)$, defined in Eq. (10), and shown as solid lines in Fig. 4(c), indicate that $\tau^{-1}(\varepsilon_F)$ remains comparable to the undoped case for hole doping, but increases by almost a factor of two for electron doping. This is because of the asymmetry in the electronic DOS, which provides more available states for scattering in the electron case. Similarly, the energy-averaged squared velocity at ε_F , $\langle v_\alpha^2 \rangle$, is approximately four times larger for hole doping compared to both the undoped and electron-doped systems, as shown in Fig. S6 within the SM [54]. Since the $N(\varepsilon_F)$ values for electron and hole doping are nearly identical, this leads to an enhanced conductivity in the hole-doped case, consistent with the full BTE results.

Additional insight into this asymmetric behavior can be gained by examining the difference in the phonon linewidths between the doped and undoped systems, as presented in Fig. S7 within the SM [54]. While $\gamma_{\mathbf{q}\nu}$ is largely unchanged throughout the Brillouin zone, notable variations appear along the Γ -Z and Γ -X directions. In the hole-doped case, a strong suppression is observed along Γ -Z, consistent with the small changes in Fermi surface topology and nesting. Conversely, electron doping leads to a pronounced enhancement along Γ -Z and a moderate increase along Γ -X, indicative of stronger e-ph scattering in these momentum regions. These enhancements can be further understood by analyzing the contribution of each phonon mode to the scattering rate.

To this end, we evaluate the electron-energy-averaged, phonon-frequency-resolved scattering rate $\partial\tau^{-1}(\varepsilon)/\partial\omega$, defined in Eq. (13). Figure 5 presents both $\partial\tau^{-1}(\varepsilon)/\partial\omega$ and its cumulative integral $\int_0^\omega d\omega' \partial\tau^{-1}(\varepsilon)/\partial\omega'$, which represents the electron-energy-averaged scattering rate. These quantities are evaluated at the Fermi level for three cases, correspond-

ing to $\varepsilon_F = \varepsilon_F^0$ and $\varepsilon_F = \varepsilon_F^0 \pm 25$ meV. All three spectral profiles exhibit similar features, with a broad peak in the mid-frequency region (10–20 meV) and a narrower peak in the high-frequency region (30–35 meV), both attributed primarily to the optical phonon modes connecting states on the Fermi surface, such as those along the Γ -Z direction (see Fig. 2). However, the cumulative integral is markedly different in the electron-doped case, approaching 5 THz, nearly twice the value obtained for the undoped and hole-doped systems. In particular, the optical modes from the 14–21 meV region contribute around 1.80 THz of the total integrated scattering rate, $\tau^{-1}(\varepsilon_F) = 4.75$ THz, while modes above 30 meV contribute approximately 0.95 THz. This trend aligns with the pronounced phonon linewidths $\gamma_{\mathbf{q}\nu}$ of the optical phonons in these two energy regions along the Γ -Z direction (see Fig. S7 within the SM [54]), as well as with the increase in the nesting function around the Z point [see Fig. 4(b)]. Together, these dependencies correlate with the observed reduction in conductivity for electron doping. In contrast, hole doping leads to a reduced scattering rate, with the optical phonons from the two regions contributing 1.00 THz and 0.60 THz, respectively, to a total $\tau^{-1}(\varepsilon_F) = 2.75$ THz, consistent with the suppression of $\gamma_{\mathbf{q}\nu}$ along the Γ -Z direction. The spectral dependence in the hole-doped system remains close to that of the undoped case, indicating that the increase in conductivity with hole-doping

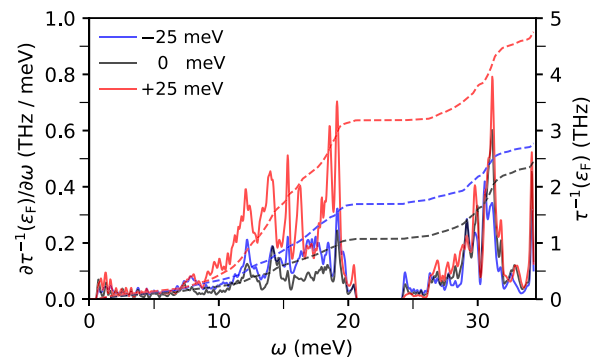


FIG. 5. Frequency-resolved scattering rate $\partial\tau^{-1}(\varepsilon)/\partial\omega$ (solid curves, left axis) and cumulative integral $\int_0^\omega d\omega' \partial\tau^{-1}(\varepsilon)/\partial\omega'$ (dashed curves, right axis) evaluated at the Fermi level for undoped ($\varepsilon_F = \varepsilon_F^0$), hole-doped ($\varepsilon_F = \varepsilon_F^0 - 25$ meV), and electron-doped ($\varepsilon_F = \varepsilon_F^0 + 25$ meV) systems at 300 K.

stems primarily from the enhanced DOS at the Fermi level relative to the undoped system.

IV. SUMMARY

In summary, using state-of-the-art *ab initio* transport calculations, we have shown that electrical conductivity in high-quality TaAs samples is well described by phonon-limited transport. Our results reveal that conductivity is highly sensitive to carrier doping because of the complex topology of the Fermi surface. In particular, electron doping leads to a reduction in conductivity relative to the undoped case, which can be attributed to the formation of additional electron pockets that enhance the nesting function and open new scattering channels. In contrast, hole doping results in increased conductivity, driven by an enhancement in the density of states at the Fermi level compared to the undoped system. Analysis of the phonon lifetimes and the spectral decomposition of scattering rates further demonstrates that optical phonons involved in the inter-pocket scatterings, such as those along the Γ -Z direction, play a dominant role in charge carrier relaxation. These findings provide a fundamental understanding of the electron-phonon coupling mechanisms in TaAs and pave the way for similar investigations in other Weyl semimetals.

Note added. Recently, we became aware of a related study on TaAs by another group [66], which independently reports results consistent with ours, including a similar agreement between SERTA and IBTE, further supporting our findings.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [67].

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- [1] M. Z. Hasan, G. Chang, I. Belopolski, G. Bian, S.-Y. Xu, and J.-X. Yin, Weyl, Dirac and high-fold chiral fermions in topological quantum matter, *Nat. Rev. Mater.* **6**, 784 (2021).
 - [2] B. Q. Lv, T. Qian, and H. Ding, Experimental perspective on three-dimensional topological semimetals, *Rev. Mod. Phys.* **93**, 025002 (2021).
 - [3] W. Witczak-Krempa and Y. B. Kim, Topological and magnetic phases of interacting electrons in the pyrochlore iridates, *Phys. Rev. B* **85**, 045124 (2012).
 - [4] B. Yan and C. Felser, Topological materials: Weyl semimetals, *Annu. Rev. Condens. Matter Phys.* **8**, 337 (2017).
 - [5] M. Z. Hasan, S.-Y. Xu, and G. Bian, Topological insulators, topological superconductors and Weyl fermion semimetals: Discoveries, perspectives and outlooks, *Phys. Scr.* **T164**, 014001 (2015).
 - [6] S. Jia, S.-Y. Xu, and M. Z. Hasan, Weyl semimetals, Fermi arcs and chiral anomalies, *Nat. Mater.* **15**, 1140 (2016).
 - [7] A. A. Burkov, Topological semimetals, *Nat. Mater.* **15**, 1145 (2016).
 - [8] J. Hu, S.-Y. Xu, N. Ni, and Z. Mao, Transport of topological semimetals, *Annu. Rev. Mater. Res.* **49**, 207 (2019).
 - [9] L. Lu, Z. Wang, D. Ye, L. Ran, L. Fu, J. D. Joannopoulos, and M. Soljačić, Experimental observation of Weyl points, *Science* **349**, 622 (2015).
 - [10] X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, Topological semimetal and Fermi-arc surface states in the electronic structure of pyrochlore iridates, *Phys. Rev. B* **83**, 205101 (2011).
 - [11] M. Z. Hasan, S.-Y. Xu, I. Belopolski, and S.-M. Huang, Discovery of Weyl fermion semimetals and topological Fermi arc states, *Annu. Rev. Condens. Matter Phys.* **8**, 289 (2017).
 - [12] S. A. Parameswaran, T. Grover, D. A. Abanin, D. A. Pesin, and A. Vishwanath, Probing the chiral anomaly with non-local transport in three-dimensional topological semimetals, *Phys. Rev. X* **4**, 031035 (2014).
 - [13] X. Huang, L. Zhao, Y. Long, P. Wang, D. Chen, Z. Yang, H. Liang, M. Xue, H. Weng, Z. Fang, X. Dai, and G. Chen, Observation of the chiral-anomaly-induced negative magnetoresistance in 3D Weyl semimetal TaAs, *Phys. Rev. X* **5**, 031023 (2015).
 - [14] C.-L. Zhang, S.-Y. Xu, I. Belopolski, Z. Yuan, Z. Lin, B. Tong, G. Bian, N. Alidoust, C.-C. Lee, S.-M. Huang *et al.*, Signatures of the Adler-Bell-Jackiw chiral anomaly in a Weyl fermion semimetal, *Nat. Commun.* **7**, 10735 (2016).
 - [15] F. Arnold, C. Shekhar, S.-C. Wu, Y. Sun, R. D. dos Reis, N. Kumar, M. Naumann, M. O. Ajeesh, M. Schmidt, A. G. Grushin *et al.*, Negative magnetoresistance without well-defined chirality in the Weyl semimetal TaP, *Nat. Commun.* **7**, 11615 (2016).
 - [16] Y. Li, Z. Wang, P. Li, X. Yang, Z. Shen, F. Sheng, X. Li, Y. Lu, Y. Zheng, and Z.-A. Xu, Negative magnetoresistance in

- Weyl semimetals NbAs and NbP: Intrinsic chiral anomaly and extrinsic effects, *Front. Phys.* **12**, 127205 (2017).
- [17] J. Du, H. Wang, Q. Chen, Q. Mao, R. Khan, B. Xu, Y. Zhou, Y. Zhang, J. Yang, B. Chen *et al.*, Large unsaturated positive and negative magnetoresistance in Weyl semimetal TaP, *Sci. China Phys. Mech. Astron.* **59**, 657406 (2016).
 - [18] I. Sodemann and L. Fu, Quantum nonlinear Hall effect induced by Berry curvature dipole in time-reversal invariant materials, *Phys. Rev. Lett.* **115**, 216806 (2015).
 - [19] K.-Y. Yang, Y.-M. Lu, and Y. Ran, Quantum Hall effects in a Weyl semimetal: Possible application in pyrochlore iridates, *Phys. Rev. B* **84**, 075129 (2011).
 - [20] T. Meng and L. Balents, Weyl superconductors, *Phys. Rev. B* **86**, 054504 (2012).
 - [21] P. Hosur, X. Dai, Z. Fang, and X.-L. Qi, Time-reversal-invariant topological superconductivity in doped Weyl semimetals, *Phys. Rev. B* **90**, 045130 (2014).
 - [22] G. Y. Cho, J. H. Bardarson, Y.-M. Lu, and J. E. Moore, Superconductivity of doped Weyl semimetals: Finite-momentum pairing and electronic analog of the $^3\text{He-A}$ phase, *Phys. Rev. B* **86**, 214514 (2012).
 - [23] G. Bednik, A. A. Zyuzin, and A. A. Burkov, Superconductivity in Weyl metals, *Phys. Rev. B* **92**, 035153 (2015).
 - [24] Y. Li and F. D. M. Haldane, Topological nodal Cooper pairing in doped Weyl metals, *Phys. Rev. Lett.* **120**, 067003 (2018).
 - [25] S.-Y. Xu, I. Belopolski, N. Alidoust, M. Neupane, G. Bian, C. Zhang, R. Sankar, G. Chang, Z. Yuan, C.-C. Lee *et al.*, Discovery of a Weyl fermion semimetal and topological Fermi arcs, *Science* **349**, 613 (2015).
 - [26] B. Q. Lv, N. Xu, H. M. Weng, J. Z. Ma, P. Richard, X. C. Huang, L. X. Zhao, G. F. Chen, C. E. Matt, F. Bisti *et al.*, Observation of Weyl nodes in TaAs, *Nat. Phys.* **11**, 724 (2015).
 - [27] S.-Y. Xu, I. Belopolski, N. Alidoust, M. Neupane, G. Bian, C. Zhang, R. Sankar, G. Chang, Z. Yuan, C.-C. Lee *et al.*, Discovery of a Weyl fermion state with Fermi arcs in niobium arsenide, *Nat. Phys.* **11**, 748 (2015).
 - [28] N. Xu, H. Weng, B. Lv, C. E. Matt, J. Park, F. Bisti, V. N. Strocov, D. Gawryluk, E. Pomjakushina, K. Conder *et al.*, Observation of Weyl nodes and Fermi arcs in tantalum phosphide, *Nat. Commun.* **7**, 11006 (2016).
 - [29] D.-F. Xu, Y.-P. Du, Z. Wang, Y.-P. Li, X.-H. Niu, Q. Yao, D. Pavel, Z.-A. Xu, X.-G. Wan, and D.-L. Feng, Observation of Fermi arcs in non-centrosymmetric Weyl semi-metal candidate NbP, *Chin. Phys. Lett.* **32**, 107101 (2015).
 - [30] L.-X. Yang, Z.-K. Liu, Y. Sun, H. Peng, H.-F. Yang, T. Zhang, B. Zhou, Y. Zhang, Y.-F. Guo, M. Rahn *et al.*, Weyl semimetal phase in the non-centrosymmetric compound TaAs, *Nat. Phys.* **11**, 728 (2015).
 - [31] H. Weng, C. Fang, Z. Fang, B. A. Bernevig, and X. Dai, Weyl semimetal phase in noncentrosymmetric transition-metal monophosphides, *Phys. Rev. X* **5**, 011029 (2015).
 - [32] S.-M. Huang, S.-Y. Xu, I. Belopolski, C.-C. Lee, G. Chang, B. Wang, N. Alidoust, G. Bian, M. Neupane, C. Zhang *et al.*, A Weyl Fermion semimetal with surface Fermi arcs in the transition metal monophosphide TaAs class, *Nat. Commun.* **6**, 7373 (2015).
 - [33] B. Q. Lv, H. M. Weng, B. B. Fu, X. P. Wang, H. Miao, J. Ma, P. Richard, X. C. Huang, L. X. Zhao, G. F. Chen *et al.*, Experimental discovery of Weyl semimetal TaAs, *Phys. Rev. X* **5**, 031013 (2015).
 - [34] C. Shekhar, A. K. Nayak, Y. Sun, M. Schmidt, M. Nicklas, I. Leermakers, U. Zeitler, Y. Skourski, J. Wosnitza, Z. Liu *et al.*, Extremely large magnetoresistance and ultrahigh mobility in the topological Weyl semimetal candidate NbP, *Nat. Phys.* **11**, 645 (2015).
 - [35] R. Sankar, G. Peramaiyan, I. P. Muthuselvan, S. Xu, M. Z. Hasan, and F. Chou, Crystal growth and transport properties of Weyl semimetal TaAs, *J. Phys.: Condens. Matter* **30**, 015803 (2018).
 - [36] C. Zhang, C. Guo, H. Lu, X. Zhang, Z. Yuan, Z. Lin, J. Wang, and S. Jia, Large magnetoresistance over an extended temperature regime in monophosphides of tantalum and niobium, *Phys. Rev. B* **92**, 041203(R) (2015).
 - [37] M. Naumann, F. Arnold, M. D. Bachmann, K. A. Modic, P. J. W. Moll, V. Süß, M. Schmidt, and E. Hassinger, Orbital effect and weak localization in the longitudinal magnetoresistance of Weyl semimetals NbP, NbAs, TaP, and TaAs, *Phys. Rev. Mater.* **4**, 034201 (2020).
 - [38] C.-L. Zhang, Z. Yuan, Q.-D. Jiang, B. Tong, C. Zhang, X. C. Xie, and S. Jia, Electron scattering in tantalum monoarsenide, *Phys. Rev. B* **95**, 085202 (2017).
 - [39] J. Coulter, G. B. Osterhoudt, C. A. C. Garcia, Y. Wang, V. M. Plisson, B. Shen, N. Ni, K. S. Burch, and P. Narang, Uncovering electron-phonon scattering and phonon dynamics in type-I Weyl semimetals, *Phys. Rev. B* **100**, 220301(R) (2019).
 - [40] C. A. C. Garcia, J. Coulter, and P. Narang, Optoelectronic response of the type-I Weyl semimetals TaAs and NbAs from first principles, *Phys. Rev. Res.* **2**, 013073 (2020).
 - [41] S. Han, Q. Tang, H. Yuan, Y. Luo, and H. Liu, Effects of electron-phonon coupling on the phonon transport properties of the Weyl semimetals NbAs and TaAs: A comparative study, *J. Materiomics* **9**, 520 (2023).
 - [42] P. Giannozzi, O. Andreussi, T. Brumme, O. Bunau, M. Buongiorno Nardelli, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, M. Cococcioni *et al.*, Advanced capabilities for materials modelling with QUANTUM ESPRESSO, *J. Phys.: Condens. Matter* **29**, 465901 (2017).
 - [43] D. R. Hamann, Optimized norm-conserving Vanderbilt pseudopotentials, *Phys. Rev. B* **88**, 085117 (2013).
 - [44] M. van Setten, M. Giantomassi, E. Bousquet, M. Verstraete, D. Hamann, X. Gonze, and G.-M. Rignanese, The PSEUDODOJO: Training and grading a 85 element optimized norm-conserving pseudopotential table, *Comput. Phys. Commun.* **226**, 39 (2018).
 - [45] J. P. Perdew, K. Burke, and M. Ernzerhof, Generalized gradient approximation made simple, *Phys. Rev. Lett.* **77**, 3865 (1996).
 - [46] M. Methfessel and A. T. Paxton, High-precision sampling for Brillouin-zone integration in metals, *Phys. Rev. B* **40**, 3616 (1989).
 - [47] S. Baroni, S. de Gironcoli, A. Dal Corso, and P. Giannozzi, Phonons and related crystal properties from density-functional perturbation theory, *Rev. Mod. Phys.* **73**, 515 (2001).
 - [48] F. Giustino, M. L. Cohen, and S. G. Louie, Electron-phonon interaction using Wannier functions, *Phys. Rev. B* **76**, 165108 (2007).
 - [49] S. Poncé, E. Margine, C. Verdi, and F. Giustino, EPW: Electron-phonon coupling, transport and superconducting properties using maximally localized Wannier functions, *Comput. Phys. Commun.* **209**, 116 (2016).
 - [50] H. Lee, S. Poncé, K. Bushick, S. Hajinazar, J. Lafuente-Bartolome, J. Leveillee, C. Lian, J.-M. Lihm, F. Macheda, H.

- Mori *et al.*, Electron-phonon physics from first principles using the EPW code, *npj Comput. Mater.* **9**, 2057 (2023).
- [51] N. Marzari, A. A. Mostofi, J. R. Yates, I. Souza, and D. Vanderbilt, Maximally localized Wannier functions: Theory and applications, *Rev. Mod. Phys.* **84**, 1419 (2012).
- [52] G. Pizzi, V. Vitale, R. Arita, S. Blügel, F. Freimuth, G. Géranton, M. Gibertini, D. Gresch, C. Johnson, T. Koretsune *et al.*, Wannier90 as a community code: new features and applications, *J. Phys.: Condens. Matter* **32**, 165902 (2020).
- [53] Q. Wu, S. Zhang, H.-F. Song, M. Troyer, and A. A. Soluyanov, WannierTools: An open-source software package for novel topological materials, *Comput. Phys. Commun.* **224**, 405 (2018).
- [54] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/x8zl-w5x3> for additional information. Figure S1 is a zoomed-in view of the TaAs band structure and presents convergence of the Fermi level with respect to **k**-point grids. Figure S2 shows the convergence of electrical conductivity with respect to **k/q**-point grids. Figure S3 compares the nesting function computed with and without the double-delta approximation. Figure S4 presents the conductivity and resistivity of several experimental results with our theoretical results. Figure S5 compares the conductivity obtained for undoped and one level of electron and hole doping using the iterative BTE, SERTA, and CRTA at different temperatures and a zoomed-in view of iterative BTE and CRTA at 300 K as a function of the Fermi level. Figure S6 shows the average squared velocity as a function of energy. Figure S7 presents the difference in phonon linewidths between doped and undoped cases. Table S1 compares the conductivity values obtained with two different broadening parameters, and Table S2 presents a conductivity analysis based on a simplified model.
- [55] S. Poncé, E. R. Margine, and F. Giustino, Towards predictive many-body calculations of phonon-limited carrier mobilities in semiconductors, *Phys. Rev. B* **97**, 121201(R) (2018).
- [56] J.-M. Lihm, S. Poncé, and C.-H. Park, Self-consistent electron lifetimes for electron-phonon scattering, *Phys. Rev. B* **110**, L121106 (2024).
- [57] P. B. Allen, Neutron spectroscopy of superconductors, *Phys. Rev. B* **6**, 2577 (1972).
- [58] S. Poncé, W. Li, S. Reichardt, and F. Giustino, First-principles calculations of charge carrier mobility and conductivity in bulk semiconductors and two-dimensional materials, *Rep. Prog. Phys.* **83**, 036501 (2020).
- [59] S. Poncé, F. Macheda, E. R. Margine, N. Marzari, N. Bonini, and F. Giustino, First-principles predictions of Hall and drift mobilities in semiconductors, *Phys. Rev. Res.* **3**, 043022 (2021).
- [60] S. Poncé, M. Schlipf, and F. Giustino, Origin of low carrier mobilities in halide perovskites, *ACS Energy Lett.* **4**, 456 (2019).
- [61] H. W. Liu, P. Richard, Z. D. Song, L. X. Zhao, Z. Fang, G.-F. Chen, and H. Ding, Raman study of lattice dynamics in the Weyl semimetal TaAs, *Phys. Rev. B* **92**, 064302 (2015).
- [62] A. Kokalj, XCrySDen—a new program for displaying crystalline structures and electron densities, *J. Mol. Graph.* **17**, 176 (1999).
- [63] C.-C. Lee, S.-Y. Xu, S.-M. Huang, D. S. Sanchez, I. Belopolski, G. Chang, G. Bian, N. Alidoust, H. Zheng, M. Neupane, B. Wang, A. Bansil, M. Z. Hasan, and H. Lin, Fermi surface interconnectivity and topology in Weyl fermion semimetals TaAs, TaP, NbAs, and NbP, *Phys. Rev. B* **92**, 235104 (2015).
- [64] J. Xiang, S. Hu, M. Lv, J. Zhang, H. Zhao, G. Chen, W. Li, Z. Chen, and P. Sun, Anisotropic thermal and electrical transport of Weyl semimetal TaAs, *J. Phys.: Condens. Matter* **29**, 485501 (2017).
- [65] T. Ouyang, H. Xiao, C. Tang, M. Hu, and J. Zhong, Anisotropic thermal transport in Weyl semimetal TaAs: a first principles calculation, *Phys. Chem. Chem. Phys.* **18**, 16709 (2016).
- [66] G. E. Allemand, M. Giantomassi, and M. J. Verstraete, companion paper, First-principles calculations of transport coefficients in the Weyl semimetal TaAs, *Phys. Rev. B* **112**, 125122 (2025).
- [67] Z. Liu, S. Mishra, J.-M. Lihm, S. Poncé, and E. R. Margine, Phonon-limited carrier transport in the Weyl semimetal TaAs, *Mater. Cloud Archive* **2025**, 69 (2025).