

Generalized deformation potential and machine-learning approaches for electron-phonon coupling and thermoelectric transport in semiconductors

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The ability to compute electron-phonon coupling from first principles, using density functional perturbation theory and interpolation techniques, has enabled predictive calculations of electronic transport coefficients in crystalline materials. However, these methods are still computationally expensive. Here we present two inexpensive methods to obtain thermoelectric transport properties of semiconductors using a small number of electron-phonon matrix elements calculated from first principles. The first method combines models for coupling of electrons with different phonon modes whose parameters are obtained from ~ 10 matrix elements per electronic band and phonon mode calculated from first principles. Within this method, we formulate the acoustic deformation potential model for arbitrary crystal symmetries and band extrema locations. The second method uses machine learning to interpolate ~ 100 electron-phonon matrix elements per electronic band and phonon mode on dense reciprocal-space grids in the parts of the Brillouin zone relevant for transport. We apply both methods to two-dimensional MoS_2 and show very good agreement with the state-of-the-art method. The calculated thermoelectric properties also agree well with experiments. We find that the machine-learning method is more accurate and straightforward to implement compared to the model approach.

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I. INTRODUCTION

There has been significant recent progress in the development of methods and codes to calculate electron-phonon interactions and intrinsic electronic transport properties of bulk and two-dimensional (2D) materials from first principles [1–9]. These methods combine the Boltzmann transport equation (BTE) with approaches based on density functional theory (DFT) to compute the electronic and phonon band structure and the electron-phonon (el-ph) matrix elements on a reciprocal-space grid. In the case of semiconductors, these grids need to be very dense as the charge carriers contributing to transport occupy a narrow energy range near the Fermi level and, consequently, a small portion of the first Brillouin zone. Calculations on dense grids (of the order of 100 points per direction in reciprocal space, both for electrons and phonons) are particularly costly for el-ph matrix elements. To overcome this problem, they are usually computed on a small grid using density functional perturbation theory (DFPT) [10,11] (of the order of 10 points per direction in reciprocal space, both for electrons and phonons) and then interpolated to a much denser grid using the Wannier [12] or Fourier [13] interpolation.

Nevertheless, this approach is still computationally intensive, particularly when used for screening of materials with desired transport properties or predicting transport properties of materials with large unit cells (e.g., heterostructures).

One approach to reduce the cost of *ab initio* el-ph calculations in semiconductors is to use models for el-ph coupling based on the type of phonons participating in the interaction (e.g., the deformation potential models for acoustic, nonpolar optical and zone-edge phonons or the Fröhlich model for polar optical phonons) [14]. The parameters of those models can be calculated using a small set of el-ph matrix elements (of the order of 10 matrix elements per electronic band and phonon mode) obtained from the DFPT approach or its alternatives (e.g., the DFT-based frozen phonon approach) [15–20]. However, an accurate formulation of such models can be challenging, which is why they are often oversimplified. For example, the acoustic deformation model is frequently used by accounting for only one deformation potential parameter [21–23], although there can be up to six independent parameters describing the deformation potential tensor depending on crystal symmetry and band extrema location. Herring and Vogt [24] formulated a more general acoustic deformation potential approach for cubic semiconductors with band extrema along several high-symmetry lines, which uses two or three independent deformation potential parameters. In spite of the successful applications of the Herring and Vogt model to cubic semiconductors [15,17,18,25–27], the acoustic deformation potential model has not been laid out in sufficient detail for arbitrary crystal symmetries and band extrema locations.

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Machine-learning techniques could provide another route to faster simulations of el-ph coupling and electronic transport in bulk and 2D semiconductors. There have been several reports of using machine learning (ML) to predict physical properties determined by el-ph coupling, such as zero-point renormalization [28], thermoelectric figure of merit [29–34], and superconducting transition temperature [35–38], but without predicting el-ph matrix elements. One of the approaches to obtain el-ph matrix elements using machine learning uses deep neural networks to learn the key quantity of DFPT, i.e., the change of the Kohn-Sham potential due to atomic and other perturbations [39]. Another approach uses deep neural networks to construct atomic-orbital-based Hamiltonian matrices and gradients due to atomic displacements trained on first-principles calculations, from which el-ph matrix elements are obtained [40]. A recent work proposed a method to learn el-ph matrix elements from finite-difference first-principles calculations using neural networks [41]. Another relevant work used the Gaussian process regression to average over different momentum directions and obtain average el-ph matrix elements to speed up the calculations of thermoelectric transport properties [42]. However, other ML approaches to calculate el-ph matrix elements may be possible. For example, relatively small sets of calculated el-ph matrix elements for each phonon mode could be used as the training dataset to predict the el-ph matrix elements on very dense grids in relevant parts of the Brillouin zone, but this has not been attempted in the literature so far.

In this paper, we present computationally efficient first-principles based model and machine-learning approaches to electron-phonon scattering in semiconductors, which rely on explicit calculations of much smaller sets of electron-phonon matrix elements compared to the DFPT + Wannier approach. We use these methods to compute electronic thermoelectric transport properties of single-layer MoS₂, which exhibits large thermoelectric power factors near 300 K. Within the model approach, we generalize the Herring and Vogt acoustic deformation potential approach [24] for any crystal symmetry and band extrema location. We derive explicit formulas for hexagonal symmetry with conduction band valleys located along the Γ - K line in the Brillouin zone. We combine this model with the model of the Fröhlich interaction for polar optical phonons in 2D semiconductors [43,44] and the deformation potential models for other relevant phonons [14] to obtain el-ph scattering rates and thermoelectric transport properties of 2D MoS₂. Within this framework, the electron-phonon interaction is described by a compact set of physically transparent parameters that can be reused in subsequent studies without repeating the full first-principles workflow, e.g., for device modeling. We also develop a machine-learning approach that uses regression methods to predict el-ph matrix elements on very dense grids in regions of the Brillouin zone that contribute to electronic transport using a small training set of el-ph matrix elements calculated *ab initio* (of the order of 100 matrix elements per electronic band and phonon mode). The formulation of the machine-learning method is very general and can be straightforwardly applied to materials of any symmetry. Both approaches are in good agreement with the full first-principles (DFPT + Wannier) approach and experimental data for 2D MoS₂.

II. METHODOLOGY

A. Thermoelectric transport properties and electron-phonon coupling

The thermoelectric transport coefficients are calculated using the Boltzmann transport theory within the momentum relaxation-time approximation. The thermoelectric transport kernel function (L_β), with β denoting the order of the transport moment, can be expressed as [45]

$$L_\beta = \frac{2e^{2-\beta}}{V} \sum_{n,k} \left(-\frac{\partial f_{nk}^0}{\partial E_{nk}} \right) \tau_{nk} \bar{v}_{nk}^2 (E_{nk} - E_F)^\beta, \quad (1)$$

where e is the electronic charge, V is the crystal volume, E_{nk} is the energy of an electronic state with band index n and crystal momentum $\mathbf{k}$, $\bar{v}_{nk}$ is its average group velocity, τ_{nk} is the momentum relaxation time, and E_F is the Fermi energy. The electrical conductivity σ , the Seebeck coefficient S , and the power factor (PF) can then be written as

$$\sigma = L_0, \quad (2)$$

$$S = \frac{L_1}{TL_0}, \quad (3)$$

$$\text{PF} = S^2 \sigma. \quad (4)$$

The electron drift mobility μ (also referred to as the electron mobility from here on) is obtained from $\mu = \sigma/(en_c)$, where n_c is the carrier concentration.

The momentum relaxation times caused by electron-phonon interaction are calculated using Fermi's golden rule [46,47],

$$\begin{aligned} \tau_{nk}^{-1} = & \frac{2\pi}{\hbar} \sum_{\pm} \sum_{k',n'} \sum_{\lambda,q} |g_{nk\lambda q}^{n'k'}|^2 (1 - \cos \theta_{kk'}) \\ & \times \left[n(\omega_{\lambda q}) + \frac{1}{2} \mp \frac{1}{2} \right] \frac{1 - f^0(E_{n'k'})}{1 - f^0(E_{nk})} \\ & \times \delta_{k',k \pm q} \delta(E_{n'k'} - E_{nk} \mp \hbar\omega_{\lambda q}), \end{aligned} \quad (5)$$

where $\hbar$ is the Planck constant and $g_{nk\lambda q}^{n'k'}$ is the el-ph matrix element between electronic states $n\mathbf{k}$ and $n'\mathbf{k}'$ for a phonon mode λ with the wave vector $\mathbf{q}$ and the phonon frequency $\omega_{\lambda q}$. The angle between the wave vectors $\mathbf{k}$ and $\mathbf{k}'$ is denoted by $\theta_{kk'}$, $f^0(E_{nk})$ is the Fermi-Dirac distribution, and $n(\omega_{\lambda q})$ is the Bose-Einstein distribution. The Kronecker symbol $\delta_{k',k \pm q}$ represents the crystal momentum conservation. The absorption (emission) of a phonon is represented by the upper (lower) sign. The scattering rate for the electronic state $n\mathbf{k}$ can be obtained by excluding the terms $1 - \cos \theta_{kk'}$ and $[1 - f^0(E_{n'k'})]/[1 - f^0(E_{nk})]$ in Eq. (5). Details of the computational implementation of this approach can be found in Ref. [18].

B. Model approach

To develop an accurate model of electronic and thermoelectric transport in a material of interest, we need to analyze its electronic and phonon band structure. Monolayer MoS₂ has a hexagonal symmetry and is a semiconductor with a direct band gap located at the K and K' points of the Brillouin

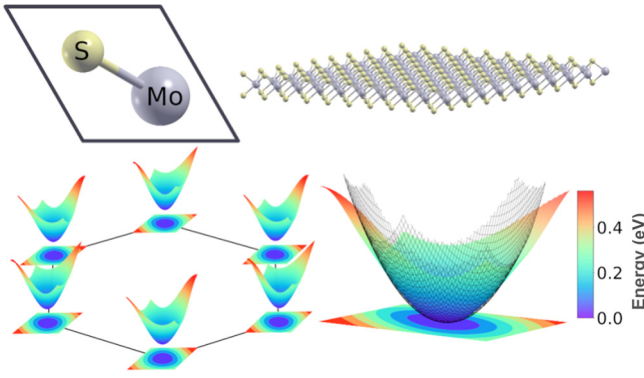


FIG. 1. Top left: Top view of the hexagonal unit cell of monolayer MoS₂. Top right: Atomic structure of a MoS₂ sheet. Lower left: The energy dispersion of the lowest conduction band of MoS₂, calculated using density functional theory (DFT) in the vicinity of the K and K' points in the hexagonal Brillouin zone. Lower right: The black curve is the dispersion of the conduction band obtained using the Kane model fitted to DFT results, shown in color.

zone (see Fig. 1). The electronic band structure of monolayer MoS₂ is shown in Supplemental Material [48]. The higher conduction band minima (CBM) are at least 300 meV above the lowest CBM at K and K' , so the transport properties of n -type MoS₂ are governed only by the lowest conduction band states near K and K' . The energy dispersion near the CBM at K and K' is nearly parabolic (Fig. 1) and can be described using the Kane model [50]. Since the lowest CBM are located at K and K' , we consider intravalley scattering mechanisms (within the K and K' valleys) originating from the phonon modes near Γ and intervalley scattering mechanisms (between the K and K' valleys) originating from the phonon modes near K .

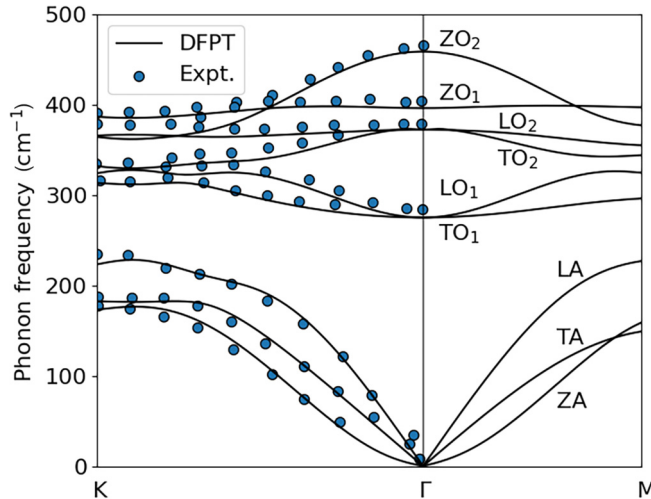


FIG. 2. The phonon dispersion of single-layer MoS₂ calculated using density functional perturbation theory, represented with solid lines. The experimental data taken from Ref. [52] are shown with circles [53]. The acoustic phonon branches are in-plane longitudinal (LA), in-plane transverse (TA), and out-of-plane (ZA). The optical modes are two in-plane longitudinal (LO) modes, two in-plane transverse (TO) modes, and two out-of-plane (ZO) modes.

The phonon band structure of 2D MoS₂ is shown in Fig. 2. The acoustic phonon branches are in-plane longitudinal (LA), in-plane transverse (TA), and out-of-plane (ZA). The optical modes are two in-plane longitudinal (LO) modes, two in-plane transverse (TO) modes, and two out-of-plane (ZO) modes. All the modes with the wave vectors corresponding to the Γ point are either odd or even with respect to the in-plane mirror plane containing Mo atoms. The el-ph matrix elements corresponding to the intravalley scattering of the electronic states at K and K' due to mirror-odd ZA, LO₁, TO₁, and ZO₂ modes at Γ are zero by symmetry. Odd-parity phonons can couple only electronic states of opposite parity since el-ph matrix elements are invariant under symmetry operations [51]. The el-ph matrix elements due to the mirror-odd phonons at Γ vanish exactly at the K and K' points since the initial and final electronic states are of the same parity. We therefore account for only mirror-even LA, TA, LO₂, TO₂, and ZO₁ modes in our treatment of intravalley scattering.

We describe the intravalley interaction of the electronic states near K and K' with LA and TA modes using the acoustic deformation potential approach [24], which we generalize to arbitrary crystal symmetries and band extrema locations. The intravalley scattering with the nonpolar optical mode (TO₂ near Γ) and the intervalley scattering with zone-edge phonons near K are described using the nonpolar optical/intervalley deformation potential approach [14]. The nonpolar optical deformation potential approach was modified to empirically include the effect of long-range interactions on the intravalley scattering with homopolar optical modes (ZO₁ near Γ). We use the Fröhlich-like model of the long-range dipole-dipole interaction to describe scattering due to the polar optical mode (LO₂ near Γ) [43,44]. We do not account for the long-range piezoelectric interaction associated with acoustic phonons, which is limited to low temperatures [54]. Charge screening effects on electron-phonon interaction are also not included in our analysis.

1. Intravalley acoustic scattering: Generalized deformation potential model

The interaction between electrons and acoustic phonons in the long-wavelength limit is characterized by a slowly varying potential, which can be expressed as [14,24,55]

$$H_{ep} = \sum_{\alpha\beta} \Xi_{\alpha\beta} \epsilon_{\alpha\beta}, \quad (6)$$

where Ξ is the deformation potential (DP) tensor, ϵ is the strain tensor, and α and β are the Cartesian coordinates. A second-rank symmetric tensor has a maximum of six independent components. However, depending on the material's symmetry and the position of the electronic band extrema in the Brillouin zone, symmetry constraints reduce the number of independent components in the DP tensor. In Supplemental Material [48], we outline a procedure to obtain the number of independent DP components for a crystal of any symmetry and any position of the electronic band extrema. Our method represents a generalization of the Herring and Vogt DP approach for cubic crystals whose band extrema lie along the Γ -L, Γ -X, and Γ -K directions [24].

TABLE I. Expressions for the six components of the deformation potential tensor for a bulk crystal with hexagonal symmetry and band extrema along the Γ - K direction.

Valley direction	Γ - K
$\Xi_1 = \Xi_{xx}$	$\Xi_d + \Xi_u$
$\Xi_2 = \Xi_{yy}$	$\Xi_d + \Xi_u - \Xi_p$
$\Xi_3 = \Xi_{zz}$	$\Xi_d - \Xi_u + \Xi_p$
$\Xi_4 = \Xi_{yz} = \Xi_{zy}$	0
$\Xi_5 = \Xi_{xz} = \Xi_{zx}$	0
$\Xi_6 = \Xi_{xy} = \Xi_{yx}$	0

For a three-dimensional (3D) unit cell with hexagonal symmetry, symmetry constraints dictate that the DP tensor elements can be characterized in terms of three independent components when the band extrema are along the Γ - K direction (see Supplemental Material [48]). These components have a direct physical interpretation. Using the Herring and Vogt definitions of volume dilation (Ξ_d), uniaxial stress (Ξ_u), and shear (Ξ_p) [48], we can express the DP tensor for a 3D material with hexagonal symmetry and band extrema along the Γ - K direction as shown in Table I. In the case of a 2D hexagonal crystal, the Ξ_3 component of the DP tensor is zero and the number of independent components reduces to two ($\Xi_d + \Xi_u$ and Ξ_p). The procedure to calculate these deformation potentials is outlined in Sec. III A and Appendix.

We obtain electron-phonon matrix elements due to scattering with long-wavelength in-plane acoustic modes using the DP tensor described above. Since the acoustic phonon frequencies near the zone center are small, we use $n(\omega_{\lambda q}) \approx \frac{k_B T}{\hbar \omega_{\lambda q}}$

for both absorption and emission processes, where k_B is the Boltzmann constant, T is the temperature, and $|\mathbf{q}| \rightarrow 0$. At room temperature, the equipartition between absorption and emission processes holds, i.e., $n(\omega_{\lambda q}) \gg 1/2$. Therefore, if we neglect acoustic phonon energies when calculating the scattering rate given by Eq. (5), the scattering rates due to emission and absorption are approximately the same. If we assume that phonon frequencies change linearly with $\mathbf{q}$ in the long-wavelength limit, we obtain [18,24]

$$|M_{\lambda q}|^2 \equiv |g_{\lambda q}|^2 \times 2n(\omega_{\lambda q}) = \frac{k_B T I^2(\mathbf{k}, \mathbf{k}')}{A} \frac{\sum_{ij} \Xi_i \Xi_j f_i f_j}{\sum_{ij} c_{ij} f_i f_j}. \quad (7)$$

Here, $g_{\lambda q}$ is the el-ph matrix element between the lowest conduction band states with wave vectors $\mathbf{k}$ and $\mathbf{k}'$ and $I(\mathbf{k}, \mathbf{k}')$ is the overlap integral between the two Bloch states with the wave vectors $\mathbf{k}$ and $\mathbf{k}'$. A is the unit-cell area, c_{ij} are the components of the 6×6 elastic constant tensor, and f_i are the components of the 3×3 polarization tensor given as

$$\begin{aligned} f_i &= a_i q_i, \quad i = 1, 2, 3, \\ f_4 &= a_2 q_3 + a_3 q_2, \\ f_5 &= a_1 q_3 + a_3 q_1, \\ f_6 &= a_1 q_2 + a_2 q_1, \end{aligned} \quad (8)$$

where $\mathbf{a}$ is the atomic displacement for an acoustic phonon with wave vector $\mathbf{q}$. We calculate the polarization vectors by solving the generalized equation of motion for the atomic displacement in a hexagonal crystal [14],

$$\begin{pmatrix} c_{11}\alpha^2 + \frac{c_{11}-c_{12}}{2}\beta^2 + c_{44}\gamma^2 - \rho v_s^2 & \frac{c_{11}+c_{12}}{2}\alpha\beta & (c_{13}+c_{44})\alpha\gamma \\ \frac{c_{11}+c_{12}}{2}\alpha\beta & c_{11}\beta^2 + \frac{c_{11}-c_{12}}{2}\alpha^2 + c_{44}\gamma^2 - \rho v_s^2 & (c_{13}+c_{44})\beta\gamma \\ (c_{13}+c_{44})\alpha\gamma & (c_{13}+c_{44})\beta\gamma & c_{44}(\alpha^2 + \beta^2) + c_{33}\gamma^2 - \rho v_s^2 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = 0, \quad (9)$$

where ρ is the mass density and v_s is the speed of sound. The direction cosines of the wave vector $\mathbf{q}$ are denoted by α , β , and γ . In the case of a 2D hexagonal crystal, only c_{11} and c_{12} are not zero. We can obtain the matrix elements for the in-plane longitudinal and transverse acoustic branches along any $\mathbf{q}$ direction by substituting the polarization tensor components derived from Eq. (9) and the DP components from Table I in Eq. (7). The expressions for $\sum_{ij} \Xi_i \Xi_j f_i f_j / \sum_{ij} c_{ij} f_i f_j$ [see Eq. (7)] along the high-symmetry directions are listed in Table II.

2. Intravalley nonpolar optical phonon and intervalley scattering

Intervalley scattering between the K and K' valleys occurs via phonons near the K point. Scattering via phonons near the Brillouin zone edge typically has a weak wave-vector dependence [14]. The el-ph matrix element between the lowest conduction band states with wave vectors $\mathbf{k} \approx K$ and $\mathbf{k}' \approx K'$ can therefore be approximated as

$$g_{\lambda q} \approx g_{\lambda Q} = \sqrt{\frac{\hbar}{2m\omega_{\lambda Q}}} \Xi_{\lambda Q}, \quad (10)$$

where $\mathbf{Q}$ corresponds to the difference between the wave vectors of the K and K' points, m is the mass of the atoms in the unit cell, and $\Xi_{\lambda Q}$ is the deformation potential due to scattering between the valleys K and K' via the phonon mode λ . We also approximate the frequencies of zone-edge phonons to be equal to $\omega_{\lambda Q}$ when calculating the relaxation times using Eq. (5). These approximations are also valid for intravalley

TABLE II. Longitudinal acoustic (LA) and transverse acoustic (TA) mode contributions to the square of the electron-phonon matrix elements for the K valley [i.e., $\sum_{ij} \Xi_i \Xi_j f_i f_j / \sum_{ij} c_{ij} f_i f_j$ in Eq. (7)] along the high-symmetry directions. Ξ and c are the 6×6 deformation potential and elastic constant tensors, respectively. $\mathbf{q}$ is the phonon wave vector.

Valley	$\mathbf{q}$ direction	LA	TA
K	$\parallel$ to Γ - K	$\frac{(\Xi_d + \Xi_u)^2}{c_{11}}$	0
	$\parallel$ to Γ - M	$\frac{(\Xi_d + \Xi_u - \frac{1}{3}\Xi_p)^2}{c_{11}}$	$\frac{3\Xi_p^2}{8(c_{11} - c_{12})}$

scattering due to short wave-vector nonpolar optical phonons [14], i.e., we use Eq. (10) with $\mathbf{Q} = \mathbf{0}$ to approximate the el-ph matrix elements with $\mathbf{k} \approx K$ and $\mathbf{k}' \approx K$. The calculation of all these deformation potentials is given in Sec. III A.

3. Intravalley homopolar optical phonon scattering

It has been recently established that the el-ph matrix elements associated with the homopolar optical ZO_1 mode near Γ have a small long-range contribution [2,56,57]. Therefore, these el-ph matrix elements exhibit stronger wave-vector dependence compared to the zone-center nonpolar optical TO_2 mode. We parametrize the scattering due to the homopolar optical mode near Γ using the following form of the deformation potential:

$$\Xi^{\text{ZO}_1} = \sum_{i=0}^4 \Xi_i^{\text{ZO}_1} q^i. \quad (11)$$

The parameters $\Xi_i^{\text{ZO}_1}$ ($i = 0, 4$) are the Taylor series coefficients of the homopolar optical deformation potential expanded in powers of the phonon wave-vector magnitude q . Section III A describes the procedure to calculate these coefficients.

4. Intravalley polar optical phonon scattering

In addition to the deformation potential in the long-wavelength limit, the atomic displacements corresponding to the LO_2 mode of MoS_2 create long-range interactions between electrons and LO_2 modes. This long-range interaction can be described using the expression for the Fröhlich interaction in 2D crystals [43,44],

$$g_{\lambda q} = i \left[\frac{\pi}{2} \frac{e^2}{4\pi\epsilon_0 A} \frac{d}{A} \hbar\omega_{\text{LO}_2}(\epsilon_0 - \epsilon_\infty) \right]^{\frac{1}{2}} \times \frac{1}{\epsilon_\infty} \frac{2}{qd} \left[1 + (\epsilon_\infty qd)^{-1} \frac{e^{qd} - 1}{1 - (1 + \epsilon_\infty^{-1})(1 + e^{qd})/2} \right], \quad (12)$$

where ω_{LO_2} is the frequency of the LO_2 phonon at Γ , d is the effective dielectric thickness, ϵ_∞ is the high-frequency dielectric constant of the monolayer, and ϵ_0 is the dielectric constant of the vacuum. The procedure to calculate these parameters is outlined in Supplemental Material [48].

C. Machine-learning approach

Our machine-learning method to compute el-ph matrix elements relevant for thermoelectric transport in semiconductors is based on regression approaches, which are used to predict el-ph matrix elements near band extrema on a very dense grid using a relatively small training dataset calculated using the DFPT+Wannier approach. Our method is straightforward because it is possible to fairly accurately describe those el-ph matrix elements using the analytical formulas of the model approach.

The ML approach to calculate el-ph matrix elements near band extrema from a training dataset is carried out using the SCIKIT LEARN package [58]. The training datasets can be chosen in different ways. We tested the training dataset consisting

of first-principles el-ph matrix elements where the initial electronic state $\mathbf{k}$ is located at the K point and the phonon wave vectors $\mathbf{q}$ are uniformly distributed along selected directions in the first Brillouin zone, which include high-symmetry directions [as sketched in the inset of Fig. 3(a)]. We will refer to this type of training dataset as “uniform”. We also used the training datasets consisting of $\mathbf{k} = K$ and randomly chosen $\mathbf{q}$ points in all directions of the first Brillouin zone. In both datasets, the Γ point is included in the $\mathbf{q}$ -point set and the magnitude of the phonon wave vectors varies between 0 and 35% of the distance between the Γ and K points. We sample only this small part of the Brillouin zone as only the phonon wave vectors near Γ contribute significantly to intravalley scattering. We do not use machine learning for intravalley nonpolar and intervalley scattering since they are well described by only one el-ph matrix element (as described in Sec. II B 2). In this case, we explicitly calculate that matrix element using DFPT and then use analytical formulas of Sec. II B 2 to compute the scattering.

For intravalley scattering due to acoustic modes (LA and TA), we use the *Polynomial Features* (PFR) algorithm to obtain el-ph matrix elements near band extrema since the acoustic deformation potential model gives the polynomial (linear) dependence on the phonon wave vector. The PFR approach generates a matrix consisting of all possible combinations of polynomials with degrees less than or equal to the user-stated input value. The specified degree for all acoustic modes were set at 5.

For intravalley scattering due to the polar and homopolar optical modes (LO_2 and ZO_1), the *Gaussian Process Regressor* (GPR) algorithm is used to compute el-ph matrix elements near band extrema. This is done because the dependence of these matrix elements on the phonon wave vector is more complicated than that for intravalley acoustic scattering, as can be seen from our model approach. GPR uses the Gaussian process for regression and hence a prior mean and covariance must be defined. We use the mean of the training set data as the prior mean. The prior’s covariance is obtained by implementing a kernel object. We implement the radial-basis function (RBF) kernel (or “squared-exponential kernel”). The RBF kernel defined on two feature vectors, labeled as x and x' , is expressed as

$$K(x, x') = \exp \left(\frac{-|d(x, x')|^2}{2l^2} \right), \quad (13)$$

where the hyperparameters $d(x, x')$ and l are the Euclidean distance and the length scale of the kernel, respectively. These hyperparameters are then obtained by maximizing the log-marginal likelihood.

The el-ph matrix elements obtained as described above are then used in Eq. (5) to compute el-ph relaxation times and scattering rates. At present, we approximate the electronic band structure with the nearly parabolic (Kane) model [50] and treat the frequencies of the phonon modes as in our model approach (acoustic phonon frequencies depend linearly on q , while all other phonon frequencies are independent of the phonon wave vector and their values are taken at Γ or K). The electronic and phonon band structures could also be

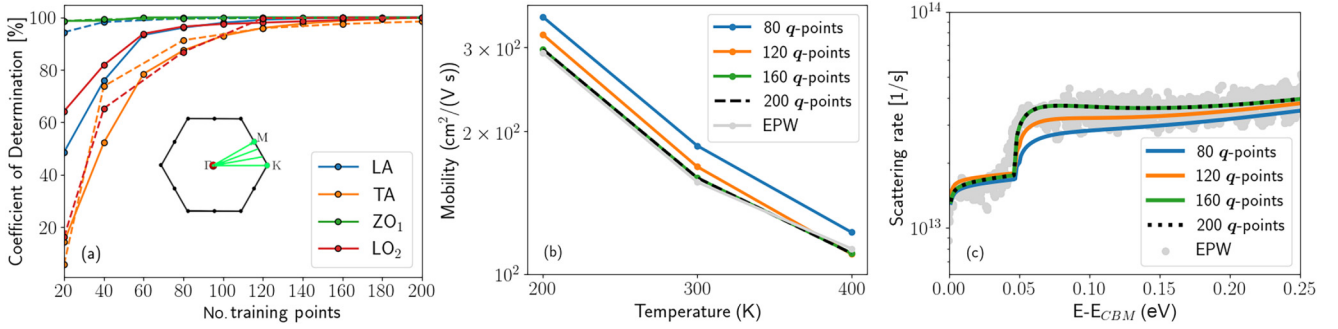


FIG. 3. (a) Coefficient of determination for phonon-mode resolved electron-phonon matrix elements as a function of the size of the training dataset. The results corresponding to the datasets consisting of one k point located at K and uniformly distributed q points along selected lines in the Brillouin zone (the “uniform” datasets) are shown by solid lines. The results obtained from the datasets with one k point located at K and randomly chosen q points are shown by dashed lines. LA and TA correspond to longitudinal and transverse acoustic phonons, respectively. ZO₁ and LO₂ stand for the homopolar and polar optical phonons, respectively. Inset: Selected directions in the first Brillouin zone along which the training dataset of first-principles electron-phonon matrix elements was uniformly distributed. (b) Electron drift mobility vs temperature and (c) scattering rate vs energy with respect to the conduction band minima at K and K' , obtained using the “uniform” training dataset for different dataset sizes, as well as the EPW code.

interpolated using a similar ML approach as described here, which may be addressed in future work.

D. First-principles calculations

The DFT calculations of the electronic band structure of single-layer MoS₂ are carried out using the QUANTUM ESPRESSO code [59,60]. We used a $24 \times 24 \times 1$ reciprocal-space k -point grid for plane waves and the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional with spin-orbit coupling (SOC) [61]. The kinetic and charge density energy cutoff used in our DFT calculations are 70 and 280 Ry, respectively. We utilize the 2D Coulomb cutoff approach to avoid interaction between MoS₂ layers [62]. The vacuum spacing is 22 Å along the direction perpendicular to the plane of the MoS₂ layer.

We compute the phonon dispersion of single-layer MoS₂ using density functional perturbation theory (DFPT) and the QUANTUM ESPRESSO code. A $12 \times 12 \times 1$ phonon wave-vector q -point grid is used in this calculation. The el-ph matrix elements are calculated on the coarse $24 \times 24 \times 1$ electron wave vector k -point and $12 \times 12 \times 1$ phonon wave-vector q -point grids. We then use the Wannier interpolation approach, as implemented in the EPW code [5,63], to interpolate these matrix elements onto dense $204 \times 204 \times 1$ k - and q -point grids by contriving 22 Wannier orbitals. The initial guesses are the d orbitals for the Mo atoms and the p orbitals for the S atoms which are inclusive of both spin-up and spin-down orbitals. The values of quadrupoles for the accurate treatment of long-range interactions are taken from Ref. [57].

III. RESULTS AND DISCUSSION

A. First-principles parameters for the model approach

The energy dispersion near the CBM at K and K' can be expressed with the Kane Hamiltonian [50],

$$\frac{\hbar^2 k^2}{2m^*} = E(1 + \alpha_p E), \quad (14)$$

where $\hbar$ is the Planck constant, m^* is the effective mass, k is the magnitude of the wave vector with respect to the CBM, E is the electronic energy with respect to the CBM, and α_p is the measure of the deviation from the parabolic dispersion relation. The effective mass and the nonparabolic factor are calculated by fitting Eq. (14) to the conduction band energy dispersion obtained from DFT, as shown in Fig. 1. Our calculated effective masses and the nonparabolic factor are shown in Table III, along with structural parameters. The calculated lattice constant, the monolayer thickness, and the band gap are nearly identical to those obtained in a recent study at the PBE level of theory (less than 0.1% difference) [2], while there is a 3.7% difference for the effective mass. To the best of our knowledge, no literature values are available for the nonparabolicity parameter α_p .

The parameters describing el-ph coupling were obtained as follows. The independent components of the DP tensor for LA and TA modes were computed from the calculations of ≈ 10 el-ph matrix elements in the limit of small phonon wave vectors along selected high-symmetry lines using DFPT calculations and the Wannier interpolation, as described in Appendix. Our computed values of $\Xi_d + \Xi_u$ and Ξ_p are given in Table IV, together with the values of elastic constants computed using DFPT and a finite-difference method. Our elastic constant values are in excellent agreement with pre-

TABLE III. Calculated lattice constant a_0 , monolayer thickness h_z , band gap E_g , effective mass m^* , and nonparabolic factor α_p of monolayer MoS₂.

Parameters	Calculation	Experiment
a_0 (Å)	3.188	3.16 ^a
h_z (Å)	3.133	
E_g (eV)	1.6	1.88 ^b
m^* (m_e)	0.405	
α_p	0.7	

^aReference [64].

^bReference [65].

TABLE IV. Parameters related to electron-phonon interaction used in our model approach (see the text for definitions), calculated from first principles.

Intravalley	Parameters
In-plane acoustic modes	
$\Xi_d + \Xi_u$ (eV)	7.20
Ξ_p (eV)	2.63
c_{11} (N/m)	132.7
c_{12} (N/m)	33
Homopolar mode	
ω_{ZO_1} (meV)	49.17
$\Xi_0^{ZO_1}$ ($\frac{eV}{\text{\AA}}$)	2.89
$\Xi_1^{ZO_1}$ (eV)	-12.58
$\Xi_2^{ZO_1}$ (eV $\text{\AA}$)	28.65
$\Xi_3^{ZO_1}$ (eV $\text{\AA}^2$)	-107.61
$\Xi_4^{ZO_1}$ (eV $\text{\AA}^3$)	184.96
Polar mode	
ω_{LO_2} (meV)	46.2
d ($\text{\AA}$)	5.48
ϵ_∞	16.76

viously reported PBE values [66]. The deformation potentials for the homopolar optical mode were obtained in a similar manner as acoustic deformation potentials. They were fitted along the Γ - K direction and it was checked that the same fits were obtained along the Γ - M direction. The deformation potentials for intervalley and intravalley nonpolar optical phonon scattering were calculated using Eq. (10), where the el-ph matrix elements $g_{\lambda Q}$ were obtained using DFPT for all relevant phonons, with the wave vectors corresponding to the Γ and K points. Their values and the corresponding phonon frequencies are listed in Supplemental Material [48]. Our deformation potential values are of the same order of magnitude as reported in Refs. [67,68], which used the local density approximation and supercell/DFPT methods to calculate el-ph matrix elements without an accurate treatment of long-range interactions. Our el-ph matrix elements agree well with the state-of-the-art DFPT + Wannier results obtained using PBE and accurately treating long-range interactions [2,57]. The computational cost of extracting deformation potential parameters is discussed in Supplemental Material [48]. Finally, we computed the values of the effective dielectric thickness d and the high-frequency dielectric constant ϵ_∞ that quantify the 2D Fröhlich interaction using the capacitor stack model (see Supplemental Material [48]). These values are given in Table IV and are in excellent agreement with those reported in Ref. [44], with deviations of approximately 0.2% for d and 2% for ϵ_∞ .

B. Training datasets for the machine-learning approach

We verify the accuracy of the ML approach using the “uniform” and random training datasets explained in Sec. IIC. For this, we compute the coefficient of determination for the el-ph matrix elements obtained from regression compared to those obtained using the DFPT + Wannier approach and the EPW code. These matrix elements were calculated for the initial

electronic state $\mathbf{k}$ located at K and the phonon wave vectors $\mathbf{q}$ located in the circle centered at the Γ point with the radius of 35% of the distance between the Γ and K points. Figure 3(a) shows those coefficients of determination for the “uniform” and random datasets as a function of the size of the training set. We can see that the results obtained using the random datasets have a higher accuracy for somewhat smaller datasets compared to those obtained from the “uniform” datasets, except in the case of the polar optical phonon. Both types of training datasets yield all the coefficients of determination above 90% for the dataset sizes of ~ 100 .

Figure 3(b) shows the electron drift mobility as a function of temperature for the “uniform” datasets with different sizes, as well as that calculated using the EPW code, which computes the mobility using a linearized Boltzmann transport equation. This figure shows that the very accurate results for the mobility, compared to the state-of-the-art DFPT + Wannier approach, can be obtained with the “uniform” training datasets containing more than 100 $\mathbf{q}$ points and converging for the datasets containing 160 $\mathbf{q}$ points. Figure 3(c) illustrates the same point by showing the total scattering rate as a function of the energy with respect to the CBM, obtained using our ML approach and the DFPT + Wannier approach. For the results obtained using the ML approach from now on, we use the “uniform” training dataset with 160 $\mathbf{q}$ points. The computational cost of the ML approach is discussed in Supplemental Material [48].

C. Accuracy of the model and machine-learning approaches

We first compare the el-ph matrix elements obtained using our model and ML approaches with those obtained from DFPT and the Wannier interpolation computed with the EPW code. In Figs. 4(a)–4(d) and 5(a)–5(d), we plot the scaled el-ph matrix elements $\bar{g}_{\lambda q} = g_{\lambda q} / \sqrt{\hbar/2m\omega_{\lambda q}}$ (for an easy extraction of deformation potentials, see Eq. (10) and Ref. [16]) arising from the interaction with LA, TA, polar optical, and homopolar optical phonons, respectively, where the K point is the initial electronic state. The EPW results are shown in black in both figures, while the results from the model and ML approach are shown in color. It is evident that both the model and ML el-ph matrix elements match those of the DFPT + Wannier approach well for all phonon modes.

The model and ML el-ph matrix elements also accurately capture the phonon wave-vector dependence of the el-ph matrix elements obtained using the EPW code; see Figs. 4 and 5. In all these approaches, the el-ph matrix elements corresponding to LA, LO₂, and ZO₁ phonons are isotropic, while those related to TA phonons are highly anisotropic [67]. The el-ph matrix elements due to the polar optical (LO₂) phonon mode steeply increase towards the Γ point, but do not diverge [43,44]. The el-ph matrix elements due to the homopolar (ZO₁) mode exhibit a cusp near the Γ point due to the long-range interaction [56,57]. Both the model and ML approaches correctly describe the different behavior of el-ph matrix elements with respect to the phonon wave vector for all phonon modes.

Next we analyze the phonon-resolved scattering rates of single-layer MoS₂ obtained from our approaches and the EPW code. In Figs. 4(e) and 5(e), we plot the scattering rates as a

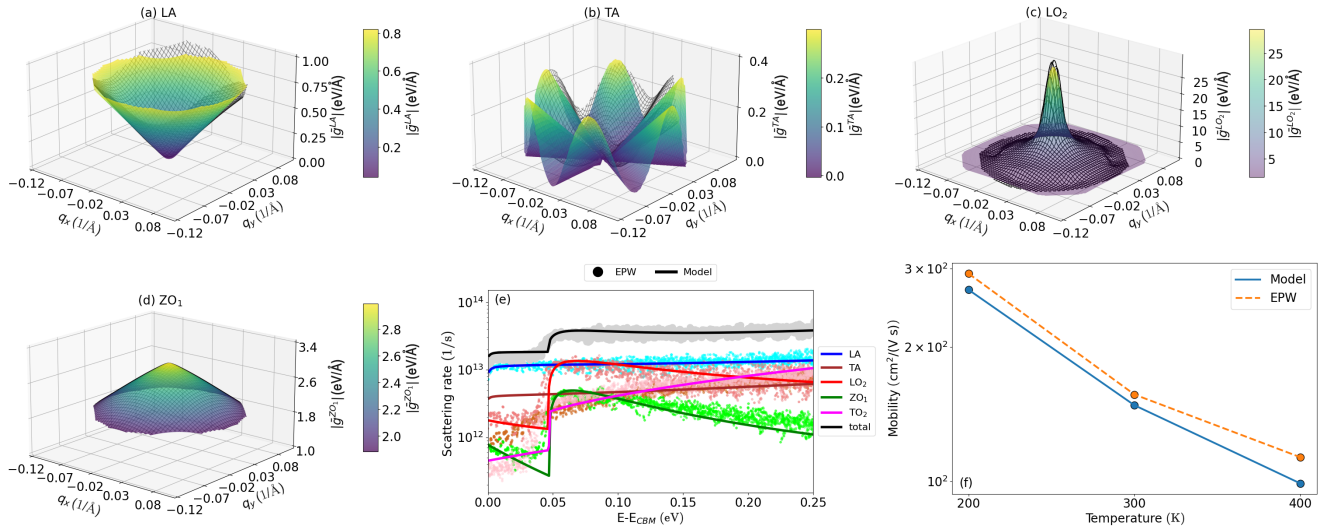


FIG. 4. Phonon-mode resolved scaled electron-phonon matrix elements with the initial electronic state at the K point as a function of the phonon wave vector. The results shown in color are obtained using the model approach. The black curves are the results obtained using the EPW code. (a)–(d) Longitudinal acoustic (LA), transverse acoustic (TA), polar optical (LO_2), and homopolar optical (ZO_1) phonons, respectively. (e) Scattering rates vs energy with respect to the conduction band minima at K and K' . Solid lines represent the model results, while the dots correspond to the EPW results. (f) Electron mobility vs temperature. Solid lines represent the model results, while dashed lines correspond to the EPW results.

function of the electronic energy with respect to the CBM for the phonon modes that are mirror-even at Γ (the scattering due to the phonon modes that are mirror-odd at Γ is much weaker). The circular points correspond to the EPW calculations, while the solid lines correspond to our model approach [Fig. 4(e)] and our ML approach [Fig. 5(e)]. We can see that the ML approach is almost as accurate as the DFPT + Wannier approach, while the model becomes somewhat less accurate for the TA modes, likely due to the neglect of the piezoelectric

long-range interaction, which is included in the EPW and ML calculations.

All three methods used show that the largest scattering rate is due to LA phonons [Figs. 4(e) and 5(e)], exhibiting a weak energy dependence in the energy interval considered because it is proportional to the density of states. The scattering due to the polar optical (LO_2) mode is the second strongest scattering mechanism in the middle of the energy interval considered, with the characteristic energy dependence indicating the

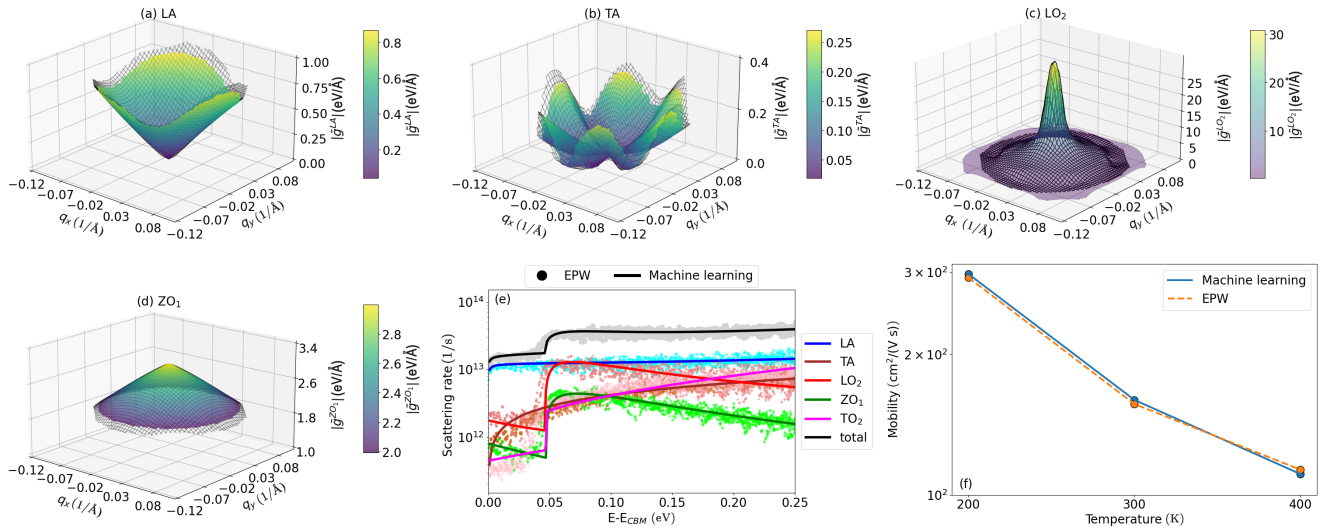


FIG. 5. Phonon-mode resolved scaled electron-phonon matrix elements with the initial electronic state at the K point as a function of the phonon wave vector. The results shown in color are obtained using the machine-learning approach. The black curves are the results obtained using the EPW code. (a)–(d) Longitudinal acoustic (LA), transverse acoustic (TA), polar optical (LO_2), and homopolar optical (ZO_1) phonons, respectively. (e) Scattering rates vs energy with respect to the conduction band minima at K and K' . Solid lines represent the machine-learning results, while the dots correspond to the EPW results. (f) Electron mobility vs temperature. Solid lines represent the machine-learning results, while dashed lines correspond to the EPW results.

onset of phonon emission near 50 meV. The homopolar (ZO_1) phonon has a similar energy dependence compared to the polar optical phonon, but it is the weakest scattering mechanism overall. The scattering rates due to the TA and TO_2 modes increase with energy, with the scattering rate due to the TO_2 mode becoming the second strongest scattering mechanism at higher energies.

Finally, we compare the mobility calculated using the model and ML approaches with that obtained using the DFPT + Wannier approach; see Figs. 4(f) and 5(f). It is clear that the ML approach is almost as accurate as the more rigorous DFPT + Wannier approach, while the model approach is somewhat less accurate. Furthermore, the ML approach is very easy to implement, unlike the model approach, which needs to be carefully formulated and parameters calculated.

The experimentally reported room-temperature mobilities for monolayer MoS_2 vary by an order of magnitude [between ~ 15 and $\sim 150 \text{ cm}^2/(\text{Vs})$] [69–72]. These discrepancies are commonly attributed to differences in the quality of samples, substrates, and contacts. The room-temperature mobility obtained with our ML model and the EPW framework are 159 and $156 \text{ cm}^2/(\text{Vs})$, respectively, and are close to the maximal mobility value of $148 \text{ cm}^2/(\text{Vs})$ reported by Yu *et al.* [70].

There have been several first-principles studies of the electron mobility of 2D MoS_2 in recent years [2,47,54,57,67,68,73–78]. The reported first-principles values of mobility vary between ~ 110 and $\sim 410 \text{ cm}^2/(\text{Vs})$. This may stem from different exchange-correlation functionals leading to different energy differences between the K/K' and Q valleys (the Q valleys are closest in energy to the K/K' valleys), but also from different methods to calculate electron-phonon matrix elements (using supercells, linearly or Wannier interpolated DFPT). The conceptual framework to accurately include the effect of long-range interactions in 2D materials was developed and applied to MoS_2 only in Refs. [2,57]. Reference [2] reported a room-temperature electron drift mobility of $132 \text{ cm}^2/(\text{Vs})$, in good agreement with our results.

D. Thermoelectric transport properties of 2D MoS_2 at 300 K

In this section, we obtain the thermoelectric transport coefficients of 2D MoS_2 at room temperature and compare them with the available experimental data [70–72,79,80]. Previous studies of thermoelectric transport in 2D MoS_2 either did not properly account for the effect of long-range interactions on el-ph scattering or employed simpler scattering models than those developed in this work [81–86]. Furthermore, no comparisons were made with experimental data on thermoelectric transport coefficients [79,80].

Here we will present only the ML results, as the results of the model approach are very similar. Figure 6(a) illustrates our calculated chemical potential as a function of electron concentration and shows excellent agreement with the experimental data [79,80]. In Fig. 6(b), we compare the conductivity obtained using our ML approach and measured or estimated experimentally [70–72,79,80]. We find the standard behavior seen in semiconductors, i.e., there is an increase in conductivity due to the increase in carrier concentration.

References [79,80] reported the conductivity values in the units of S/m , obtained by taking the effective monolayer thickness $h_z^{\text{eff}} = 6.6 \text{ \AA}$, which includes the bare S-S nuclear separation ($h_z = 3.13 \text{ \AA}$) together with the finite spatial extent of the sulfur electron clouds on outer surfaces of the S-Mo-S monolayer. Therefore, we use the same value of the effective monolayer thickness as Refs. [79,80] in our conductivity calculations. Moreover, we estimated the conductivity values from Refs. [70–72] using the measured mobility values, the quoted carrier concentration values, and $h_z^{\text{eff}} = 6.6 \text{ \AA}$. Similarly to the mobility values, there is almost an order of magnitude difference between the conductivity values obtained from experiments, reflecting the sample, substrate, and contact quality. Our conductivity values are in very good agreement with experiments for the sample with the highest mobility [70].

The discrepancy between our calculations with other experimental data can be attributed to extrinsic disorder effects,¹ such as charged impurities and substrate-induced scattering. To assess this effect quantitatively, we model ionized impurity scattering using a screened Coulomb potential of an impurity as a perturbation (see Supplemental Material [48]) and add it to phonon scattering via Matthiessen's rule. We consider impurity densities up to $2 \times 10^{12} \text{ cm}^{-2}$, which is consistent with experimentally inferred values for monolayer MoS_2 [70,87]. For impurity concentrations in this range, the calculated conductivities fall within the range of experimentally reported values (see Supplemental Material [48]).

In Fig. 6(c), we plot the conductivity resolved by each mirror-even phonon mode to determine the dominant contributions to the thermoelectric transport coefficients. We find that the LA phonon mode has the largest contribution throughout the whole range of carrier concentrations. At very high electron concentrations ($\sim 5 \times 10^{13} \text{ cm}^{-2}$), we find that the polar optical (LO_2) phonon has a comparable contribution to conductivity to that of LA phonon mode, while other modes contribute much less. These conclusions are in accordance with the plots of scattering rates shown in Figs. 4(e) and 5(e), which also show that LA and, to a much lesser extent, LO_2 modes are the largest contributors to transport in the range of Fermi energies corresponding to realistic carrier concentrations; see Fig. 6(a).

The absolute value of the Seebeck coefficient versus carrier concentration is illustrated in Fig. 6(d). We find the standard semiconductor behavior of the Seebeck coefficient, i.e., the absolute value of S decreases with increasing carrier concentration. For different experimental samples, we find different values of the Seebeck coefficient. For example, the highest measured Seebeck coefficient varies from $\sim 280 \text{ } \mu\text{V/K}$ to $\sim 380 \text{ } \mu\text{V/K}$ for the carrier concentrations of $\sim 10^{12} \text{ cm}^{-2}$

¹In principle, another potential source of discrepancy could be the use of the momentum relaxation-time approximation instead of the numerical solution of the linearized BTE. The momentum relaxation-time approximation is accurate when transport is dominated by quasi-elastic intravalley acoustic phonon scattering, as is the case here. Indeed, the momentum relaxation-time approximation was shown to yield mobility values nearly identical to those obtained from the linearized BTE for phonon-limited transport in MoS_2 [74].

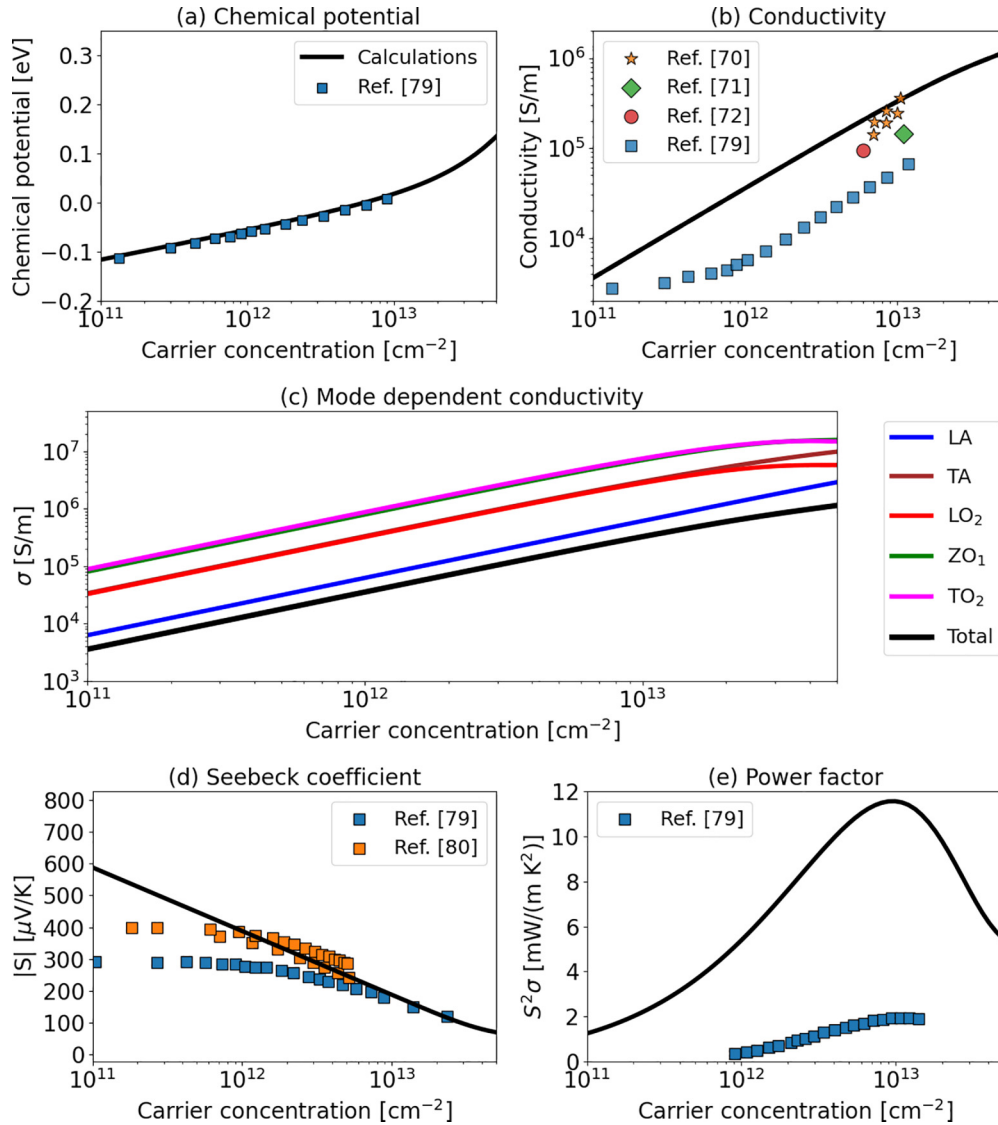


FIG. 6. Thermoelectric transport properties of monolayer MoS₂ at 300 K as a function of carrier concentration: (a) chemical potential, (b) electrical conductivity, (c) phonon-mode resolved conductivity, (d) Seebeck coefficient, and (e) power factor. The solid lines correspond to our results using the machine-learning approach. The squares represent the experimental data taken from Refs. [79,80]. The other symbols represent estimates of conductivity taken from Refs. [70–72].

[79,80]. Our predicted values of the Seebeck coefficient are within the experimental data for higher carrier concentrations ($\sim 10^{12}$ – 10^{13} cm⁻²), as seen in Fig. 6(d). However, at lower carrier concentrations ($< 10^{12}$ cm⁻²), our results overestimate the measured Seebeck coefficient. A likely reason for this is that our calculations consider only the lowest conduction band contribution to transport, whereas at such low carrier concentrations, thermally activated holes from the highest valence band may also contribute to transport, effectively reducing the total Seebeck coefficient. Ionized impurity scattering has an almost negligible effect on the calculated Seebeck coefficient values.

The power factor as a function of the carrier concentration is shown in Fig. 6(e). Ng *et al.* [79] measured the highest power factor of $S^2\sigma|_{\text{exp}} = 2.0 \times 10^{-3}$ W/(m K²) with the optimal carrier concentration of $n \sim 1.3 \times 10^{13}$ cm⁻², while

Hippalgaonkar *et al.* [80] measured the highest power factor to be $S^2\sigma|_{\text{exp}} = 3.3 \times 10^{-3}$ W/(m K²). Our calculations predict the maximal power factor of 11.6 mW K⁻² m⁻¹ (for the effective thickness of $h_z^{\text{eff}} = 6.6$ Å) with the optimal carrier concentration of $n = 10^{13}$ cm⁻². When ionized impurity scattering is included (see Supplemental Material [48]), with impurity densities up to 2×10^{12} cm⁻², the maximal power factor is achieved for carrier concentrations in the range $(1\text{--}2) \times 10^{13}$ cm⁻², with peak values ranging from 2 to 11.6 mW K⁻² m⁻¹. At high impurity concentrations, the calculated power factor shows good agreement with experimentally measured values, confirming that impurity scattering is likely the dominant mechanism limiting thermoelectric performance in these samples (see Supplemental Material [48]).

Importantly, the predicted phonon-limited room-temperature power factor of single-layer MoS₂ is larger

than those of the commercial thermoelectric materials bismuth telluride [23,88] and lead telluride [21,89,90] by a factor of ~ 2 –4. The large power factor can be attributed to the large effective mass of monolayer MoS₂ and its 2D density of states. Heterostructures of MoS₂ have been shown to enhance the power factor [79,80] and reduce the lattice thermal conductivity [91], so they are promising candidates for next-generation thermoelectric generators.

IV. SUMMARY AND CONCLUSIONS

We have developed computationally inexpensive model and machine-learning approaches combined with first-principles calculations that provide an accurate description of electron-phonon interaction in semiconductors. We have applied these methods to calculate thermoelectric transport properties of two-dimensional MoS₂. The model approach includes the Fröhlich model to describe polar optical modes, while the deformation potential models describe electron-phonon scattering processes due to other modes. The different aspect of our model approach is the generalization of the acoustic deformation potential approach for arbitrary crystal symmetries and arbitrary locations of band extrema. All the parameters for the model approach can be computed using state-of-the-art density functional perturbation theory (DFPT). In the machine-learning approach, we use regression to obtain electron-phonon matrix elements on dense wave-vector grids in the regions of the Brillouin zone relevant for transport, starting from relatively small wave-vector grids obtained using DFPT.

We have shown that both the model and machine-learning approaches show very good agreement with the DFPT + Wannier approach for dense wave-vector grids. The thermoelectric transport coefficients derived from both models are also in good agreement with the available experimental data and accurately capture the high thermoelectric power factor of 2D MoS₂. We find that the dominant scattering mechanism is due to longitudinal acoustic phonon modes.

We highlight that both the model and machine-learning approaches can predict accurate thermoelectric transport coefficients for a variety of materials at a much reduced computational time compared to the standard DFPT + Wannier approach. In this work, the electron-phonon matrix elements in both the model and machine-learning approaches were obtained from the DFPT + Wannier calculations primarily because such a benchmark was needed for the validation of both approaches. However, neither method intrinsically requires the Wannier interpolation: the relevant parameters can be extracted directly from DFPT calculations using a small number of phonon wave vectors, which can drastically reduce the computational cost. The ML approach can be two orders of magnitude faster than the DFPT + Wannier approach and has comparable accuracy. The ML approach is also straightforward to implement. The model approach is less accurate than the DFPT + Wannier and ML approaches (but still fairly accurate) and can be three-orders-of-magnitude faster than the DFPT + Wannier approach. However, the model approach may require considerable effort to be formulated for each material of interest. Therefore, the ML approach may be the most

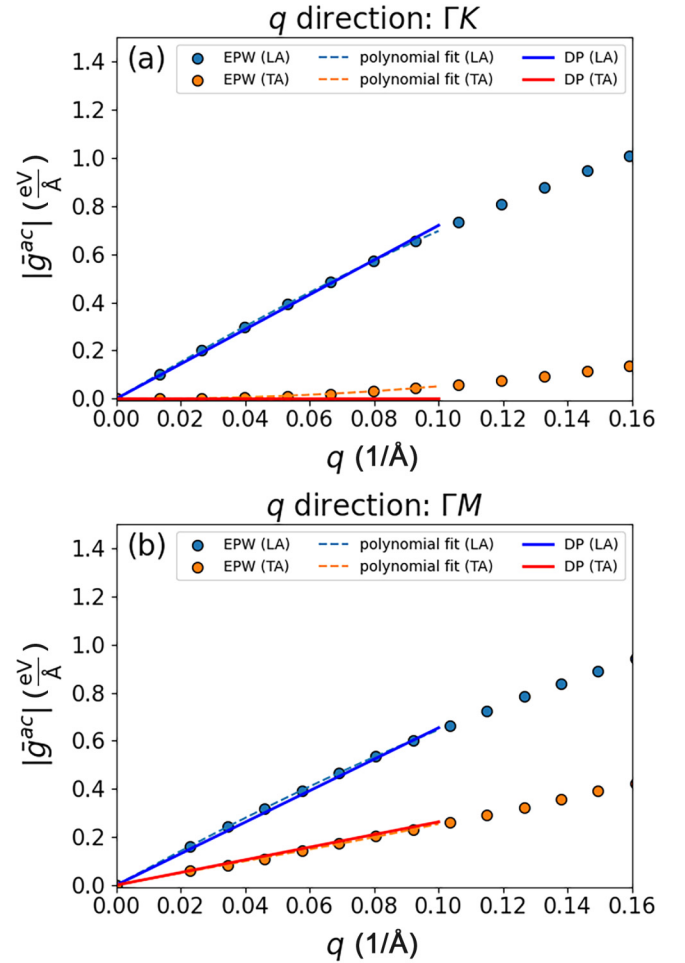


FIG. 7. Scaled electron-phonon matrix elements due to acoustic modes between the electronic states at K and $K + \mathbf{q}$ as a function of the phonon wave vector $\mathbf{q}$, whose directions are indicated at the top of each panel. Orange and blue dots represent the matrix elements calculated using density functional perturbation theory and the Wannier interpolation for transverse and longitudinal acoustic modes, respectively. Dashed lines are the third-order polynomial fits to those matrix elements. Solid lines are obtained using the computed values of deformation potentials (DPs) given in Table II for transverse and longitudinal acoustic modes in the long-wavelength limit.

advantageous method among the three for screening different material systems.

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

APPENDIX: INTRAVALLEY NONPOLAR OPTICAL AND INTERVALLEY DEFORMATION POTENTIALS

To obtain the independent DP components, we adopt the method described by Murphy *et al.* [16] and D'Souza *et al.* [18]. In this method, we relate the el-ph matrix elements obtained from DFPT and the Wannier interpolation with deformation potentials along high-symmetry lines using Eq. (7) and Table II.

In DFPT, the el-ph matrix element from a state $\mathbf{k}$ and band index n to a state $\mathbf{k} + \mathbf{q}$ and band index n' is given as [92]

$$g_{nk,\lambda\mathbf{q}}^{n'\mathbf{k}+\mathbf{q}} = \sqrt{\frac{\hbar}{2\omega_{\lambda\mathbf{q}}}} \sum_{b,i} \sqrt{\frac{1}{m_b}} e_{b,i}^{q\lambda} \times \langle u_{n'\mathbf{k}+\mathbf{q}} | \partial_{b,i,\mathbf{q}} v^{\text{KS}} | u_{n\mathbf{k}} \rangle, \quad (\text{A1})$$

where $u_{n\mathbf{k}}$ is the lattice periodic part of the wave function given as $\frac{1}{\sqrt{N_l}} u_{n\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}$, where N_l is the number of primitive cells.

$e_{b,i}^{q\lambda}$ is the i th Cartesian component of the phonon eigenvector associated with atom b of mass m_b . $\mathbf{q}$ and λ are the wave vector and branch of the phonon with frequency $\omega_{\lambda\mathbf{q}}$ that is involved in the scattering event. $\partial_{b,i,\mathbf{q}} v^{\text{KS}}$ is the lattice periodic part of the first-order expansion of the perturbed Kohn-Sham potential [92].

The el-ph matrix elements are calculated using DFPT and the Wannier interpolation between the electronic states at K and $K + \mathbf{q}$ using Eq. (A1) as $|\mathbf{q}| \rightarrow 0$ along two directions, $\mathbf{q} \parallel$ to $\Gamma-K$ and $\mathbf{q} \parallel$ to $\Gamma-M$. The DFPT electron-phonon matrix elements divided by the phonon amplitude $\sqrt{\hbar/2m\omega_{\lambda\mathbf{q}}}$ are then plotted and fitted to a third-order polynomial; see Fig. 7. We fit the linear coefficient terms to the expressions given by Eq. (7) and Table II using a linear regression technique and obtain the linearly independent deformation potentials for the K valley. The calculated independent components are shown in Table IV. It is clear from Fig. 7 that in the long-wavelength limit ($\mathbf{q} \rightarrow 0$), analytical expressions accurately describe the first-principles matrix elements. We note that when $\mathbf{q}$ is parallel to $\Gamma-K$, the deformation potential due to the TA phonon mode vanishes. However, the nonlinear coefficients of the DFPT + Wannier matrix elements do not vanish and they are the consequence of long-range piezoelectric interaction.

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