First-principles predictions of bilayer graphene photoconductivity

Yijun Ge and Timothy S. Fisher

Mechanical and Aerospace Engineering Department,
University of California, Los Angeles, CA 90095
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We report calculations of electron-phonon coupling in bilayer graphene and its contribution to carrier scattering. In contrast to single-layer graphene, the Γ point low-energy LA′ and TA′ modes in bilayer graphene couple strongly with electrons with energies less than 200 meV, while optical modes dominate the high electron energy range. Based on a two-temperature model, heat transfer from electrons to the lattice is computed, and most of the energy couples into optical modes. A Drude model is used to calculate photoconductivity for bilayer graphene with different doping levels. Good agreement with prior experimental trends for both the real and imaginary components of photoconductivity confirms the model’s applicability. The effects of doping levels and electron-phonon scattering on photoconductivity are analyzed. We also extract acoustic and optical deformation potentials from average scattering rates and compare associated photoconductivity calculations with DFT results. The comparison indicates that momentum-dependent electron-phonon scattering potentials are required to provide accurate predictions.

I. INTRODUCTION

Bernal stacked bilayer graphene exhibits a significantly different band structure compared to single-layer graphene. The conduction and valence bands split into two subbands with a separation of 0.4 eV, and the linearity near the Dirac point is broken, accompanied by a reduction in the Fermi velocity. By breaking the inversion symmetry of the two layers, a band gap is induced and can be tuned through chemical doping [1] or gating [2], suggesting potential applications in transistors, optoelectronics and photonics [3, 4]. The performance of some of these devices depends strongly on the efficiency of carrier photoexcitation and subsequent hot carrier relaxation processes [5]. The purpose of this work is to develop a model for the coupling of electrons and phonons that can predict this decay process from first principles. A secondary objective is to compare these predictions to the commonly used deformation potential scattering approach.

Photoexcited carriers thermalize rapidly over a timescale of 100 to 200 fs and thus can be described by an effective electron temperature $T_e$. The hot carriers thereafter then scatter with phonons and transfer energy to the lattice. This process lasts for tens of picoseconds until the system returns to thermal equilibrium. Optical pump terahertz probe spectroscopy [6, 7] and angle-resolved photoelectron spectroscopy [8, 9] are the most often used methods for measuring electron-phonon coupling and carrier transport properties. The pump-probe method directly relates the measured optical transmission with and without photoexcitation to the photo-induced conductivity change in the material under study. The transition from negative to positive differential transmission has been observed in graphene sheets by changing electrostatic gating and the Fermi level [10][11]. The transition is explained as an interplay between Drude weight and scattering rates. Photoexcitation generates more electron-hole pairs in intrinsic graphene but only modifies the Fermi distribution in doped graphene and therefore increases absorption in the former case while inducing more scattering in the latter case. However, only phenomenological scattering rates have been used in prior studies, leaving details of the scattering processes unresolved [10–12].

Prior theoretical work on bilayer graphene’s electrical conductivity has focused on short-range scattering from impurities using tight-binding Hamiltonians [13, 14]. Viljas et al. [15] calculated electron-phonon heat transport based on a two-temperature model, with scattering rates obtained from an empirical deformation potential approach. Park et al. [16] calculated electron-phonon coupling strengths from first principles; however, they focused on phonon lifetimes. Details of electron-phonon scattering mechanisms and their contributions to the electro-thermal transport properties of bilayer graphene are still not well understood.

In this paper, we adopt a first-principles approach to obtain electron-phonon coupling constants and scattering rates from which effective acoustic and optical deformation potentials are extracted. A two-temperature heat transfer model is developed to predict the electron and lattice temperatures at different times, based on which we calculate photoconductivity using a Drude model. We explain the trends for real and imaginary parts of photoconductivity by analyzing the effects of doping levels and electron-phonon scattering, and further compare photoconductivity from DFT and the deformation-potential approach with previous experimental data.
II. ELECTRON PHONON INTERACTIONS, DEFORMATION- POTENTIAL AND HEAT TRANSFER

The development of density functional perturbation theory (DFPT) [17] has made first-principles calculations of electron-phonon coupling feasible in recent years. The temperature-independent electron-phonon coupling matrix $g$ describes the coupling strength of the transition from an initial electron state $|m,k\rangle$ to a final state $|n,k+q\rangle$, and is calculated as [18]:

$$g_{mn,v}(k,q) = \sqrt{\frac{\hbar}{2M\omega_{q,v}}} \langle n, k+q | V_{q,v} | m, k \rangle$$  \hspace{1cm} (1)

Here, $|m,k\rangle$ and $|n,k+q\rangle$ are wavefunctions for the initial and final Bloch states, $\Delta V_{q,v}$ is the self-consistent potential change experienced by electrons due to interaction with a phonon of wavevector $q$ in branch $v$, $M$ is the mass of carbon atoms, and $\omega_{q,v}$ is the phonon frequency.

After obtaining the electron-phonon coupling matrix, electron scattering rates are calculated based on Fermi’s golden rule and the relaxation time approximation:

$$\tau_{mk}^{-1}(T_e, T_{ph}) = \frac{2\pi}{\hbar} \sum_{n,q,v} |g_{mn,v}|^2$$  \hspace{1cm} (2)

$$\left\{ (f_{n,k+q} + n_{q,v})\delta(q_{m,k} + \hbar\omega_{q,v} - \epsilon_{m,k+q}) + (1 + n_{q,v} - f_{n,k+q})\delta(q_{m,k} - \hbar\omega_{q,v} - \epsilon_{m,k+q}) \right\}$$

In Eq. 2 the first and second terms on the right side denote phonon absorption and emission. $f$ is the Fermi-Dirac distribution at the electron temperature $T_e$, and $n$ is the Bose-Einstein distribution at the phonon temperature $T_{ph}$. The summation extends over all electronic bands with a final state momentum $k+q$, phonon wavevectors and phonon branches.

Similarly, the heat transfer rate per unit area from electrons to the lattice is computed as:

$$Q_{e-ph} = \frac{4\pi}{\hbar A} \sum_{k,q,m,n,v} \hbar\omega_{q,v}|g_{mn,v}(k,q)|^2$$

$$\left\{ f_{n,k+q} (1 - f_{m,k}) (n_{q,v} + 1) - (1 - f_{n,k+q}) f_{m,k} n_{q,v} \right\} \delta(q_{m,k} + \hbar\omega_{q,v} - \epsilon_{m,k+q})$$  \hspace{1cm} (3)

Here, $A$ is the unit cell surface area. The dynamic temperature evolution is governed by energy conservation as:

$$\begin{cases} C_e(T_e) \frac{dT_e}{dt} = -Q_{e-ph} \\ C_{ph}(T_{ph}) \frac{dT_{ph}}{dt} = Q_{e-ph} \end{cases}$$  \hspace{1cm} (4)

where $C_e$ and $C_{ph}$ are electron and phonon specific heats, respectively, and diffusive heat conduction has been neglected.

Even though first-principles calculations can be applied to any system in theory, the computations are extremely time-consuming. While Wannier function interpolation reduces computational cost greatly, the disentanglement procedure for complex material systems is quite involved, especially for interfaces consisting of dissimilar materials and having strong interactions.

For electron-phonon coupling calculations, the deformation-potential approach provides an alternative. Assuming that the perturbation of the potential felt by electrons is proportional to the change in unit cell volume, the deformation-potential approach is semiclassical and often obtained by fitting experimental mobility values. Here, we briefly discuss the derivation of the deformation potential for acoustic phonons.

The potential perturbation $\Delta V(r)$ is related to the relative volume change $\Delta(r)$ by [19]:

$$\Delta V(r) = E_1 \Delta(r)$$  \hspace{1cm} (5)

where $E_1$ is the deformation potential, and $r$ denotes lattice sites. $\Delta(r)$ is calculated in the long wavelength limit as:

$$\Delta(r) = \frac{\partial u(r)}{\partial r}$$  \hspace{1cm} (6)

Here, $u(r)$ is the phonon displacement:

$$u(r) = \sum_{q} e_q (A_q e^{i\mathbf{q} \cdot \mathbf{r}} + A_q^* e^{-i\mathbf{q} \cdot \mathbf{r}})$$  \hspace{1cm} (7)

where $e_q$ is the normalized phonon eigenvector, and $2|A_q|$ is the oscillation amplitude. Considering equipartition in which all phonons are excited and $\hbar\omega_q \ll k_B T$, we can simplify the amplitude as $|A_q|^2 = \frac{k_B T}{2\rho A\omega_q^2} (\rho$ is the mass density) by connecting the classical wave energy to the quantum harmonic oscillators’ energy [20]. Combining Eqs. [5, 6] and [7] we find:

$$|\Delta V|^2 = \frac{E_1^2 k_B T L}{2\rho A v_q^2}$$  \hspace{1cm} (8)

where $v_q$ is the acoustic phonon group velocity. The transition probability $W_{kk'}$ from state $|k\rangle$ to state $|k'\rangle$ is calculated as:

$$W_{kk'} = \frac{2\pi}{\hbar} |\Delta V|^2 \delta(\epsilon_k + \hbar\omega_q - \epsilon_{k'}) \delta(|k + q - k'|)$$  \hspace{1cm} (9)

The scattering rate then becomes:

$$\tau^{-1}(\epsilon_k) = \sum_{k'} (1 - \cos \theta(k,k')) W_{kk'} \frac{1 - f(\epsilon_{k'})}{1 - f(\epsilon_k)}$$  \hspace{1cm} (10)
where \(\cos \theta\) is the angle between \(\mathbf{k}\) and \(\mathbf{k}'\).

Inserting Eq. 8 and 9 into Eq. 10 and considering valley and spin degeneracy, we obtain the scattering rate under the high-temperature and elastic-acoustic deformation approximations [21]:

\[
\tau^{-1}(\epsilon_k) = \frac{1}{4 \hbar^3 V_F^2} \frac{E_1^2}{\rho v_F^2} k_B T_L
\]

where \(V_F\) is the Fermi velocity. We assume an isotropic Fermi velocity \(V_F = 6 \times 10^5\) m/s in our calculations.

The average scattering rate is expressed as [21]:

\[
\langle \tau^{-1} \rangle = \frac{\int \mathrm{d} \epsilon D(\epsilon)\left(\frac{\partial f}{\partial \epsilon}\right)}{\int \mathrm{d} \epsilon D(\epsilon) \left(\frac{\partial f}{\partial \epsilon}\right)}
\]

(Eq. 12)

Inserting Eq. 12 into Eq. 10 gives:

\[
\sigma(\omega) = \frac{n e^2}{m^*} \frac{1}{\tau-1-i\omega} = n e \mu \frac{\tau^{-1}}{\tau-1-i\omega}
\]

(Eq. 15)

Here, \(n\) is the carrier density, \(e\) is the elementary charge, \(m^*\) is the effective mass, and \(\tau\) is the scattering rate. These terms are related to electron mobility via \(\mu = \frac{e \tau}{m^*}\), and \(\mu\) can be calculated from:

\[
\mu = \frac{e V_F^2}{2n} \int_0^\infty D(\epsilon)\left(\frac{\partial f}{\partial \epsilon}\right) \tau(\epsilon) d\epsilon
\]

(Eq. 16)

where \(D(\epsilon)\) is the density of states. Inserting Eq. 16 into Eq. 15 gives:

\[
\sigma(\omega) = \frac{e^2 V_F^2}{2} \int_0^\infty D(\epsilon)\left(\frac{\partial f}{\partial \epsilon}\right) \frac{1}{\tau-1-i\omega} d\epsilon
\]

(Eq. 17)
temperature $T_e$ higher than the lattice temperature $T_{ph}$ for the pump-off case. Photoconductivity is therefore the difference between the pump-on and pump-off conductivities $\Delta \sigma(\omega) = \sigma(T_e = T_{ph}, \omega) - \sigma(T_e = T_{ph}, \omega)$. By converting the integral over energy space to a summation over the $k$ space, we find:

$$
\frac{\Delta \sigma(\omega)}{G_0} = \frac{\hbar v_F^2}{4NkA} \left\{ \sum_k -\frac{\partial f(k, T_e \neq T_{ph})}{\partial \epsilon(k)} \int \frac{d\omega}{2\pi} \left[ \tau^{-1}(k, T_e \neq T_{ph}, T_{ph}) - i\omega \right] + \sum_k -\frac{\partial f(k, T_e = T_{ph})}{\partial \epsilon(k)} \int \frac{d\omega}{2\pi} \left[ \tau^{-1}(k, T_e = T_{ph}, T_{ph}) - i\omega \right] \right\} \tag{18}
$$

where $G_0 = \frac{2e^2}{h}$ is the conductance quantum.

**IV. RESULTS AND DISCUSSION**

Electronic structure was computed with the Quantum-Espresso package [22] using a norm-conserving pseudopotential in the local density approximation. A cutoff energy of 140 Ry and a Monkhorst-Pack $24 \times 24 \times 1$ k-space grid are chosen in the self-consistent calculations. Phonon dispersion calculations were performed with DFPT and a $12 \times 12 \times 1$ q-space grid. Due to the high computational cost of calculating energies and coupling matrix elements, we use an interpolation scheme based on maximally localized Wannier functions on a dense $1000 \times 1000 \times 1$ k-mesh and q-mesh with the EPW package [23].

In single-layer graphene, the electron-phonon coupling matrix elements for TO and LO modes are significantly greater than those of acoustic modes in the low electron energy range, causing an order of magnitude larger scattering rates [24]. However, there are two major differences in the case of bilayer graphene. The first is that the magnitudes of the electron-phonon coupling matrix elements are roughly half those of single layer graphene, possibly due to the splitting of the two conduction bands and valence bands (see Fig. 1 (a)). The second is the emergence of LA’ and TA’ modes, as indicated by the inset of Fig. 1 (b).

To differentiate between different phonon branches and to understand how phonons of different wavevectors couple with electrons, we chose a small region of the radius $0.06 \times 2\pi/a$ ($a$ is the lattice constant) near the phonon $\Gamma$ and K points in reciprocal space and split it into four rings. The shaded blue regions in the insets of Fig. 3 (a) and 4 indicate the corresponding range of wavevectors in intrinsic bilayer graphene. Fig. 2 shows that in the high electron energy range ($>200$ meV) near the phonon $\Gamma$ point, LA’ and TA’ modes are dominant and confined to small phonon wavevectors ($<0.026 \times 2\pi/a$). Unlike single-layer graphene, bilayer graphene scattering rates are not linearly proportional to the energies from the Dirac $K$ point because LA’ and TA’ modes do not ex-

**FIG. 2**: Intrinsic bilayer graphene electron scattering rates near the phonon $\Gamma$ point at $T_e = 300$ K. (a) Phonon wavevectors $0 - 0.013 2\pi/a$. LA’ and TA’ modes dominate for electron energies less than 200 meV. (b) Phonon wavevectors $0.013 - 0.026 2\pi/a$. (c) Phonon wavevectors $0.026 - 0.04 2\pi/a$. (d) Phonon wavevectors $0.04 - 0.06 2\pi/a$. Optical modes only participate in phonon emission processes.

**FIG. 3**: Intrinsic bilayer graphene electron scattering rates at the phonon K point at $T_e = 300$ K. (a) Phonon wavevectors $0 - 0.013 2\pi/a$ from the phonon K point. (b) Phonon wavevectors $0.013 - 0.026 2\pi/a$ from the phonon K point. (c) Phonon wavevectors $0.026 - 0.04 2\pi/a$ from the phonon K point. (d) Phonon wavevectors $0.04 - 0.06 2\pi/a$ from the phonon K point. Acoustic phonons rarely participate in scattering events at the phonon K point. Optical modes, especially the TO mode, dominate over all energy ranges.
hibit a linear dispersion near the phonon Γ point (see Fig. 1 (b)).

**FIG. 4:** Intrinsic bilayer graphene electron scattering rates near the phonon Γ point at $T_e = 700$ K. (a) Phonon wavevectors $0 - 0.013 \ 2\pi/a$. (b) Phonon wavevectors $0.013 - 0.026 \ 2\pi/a$. (c) Phonon wavevectors $0.026 - 0.04 \ 2\pi/a$. (d) Phonon wavevectors $0.04 - 0.06 \ 2\pi/a$. The increase of electron temperature does not change acoustic mode scattering rates, but does cause more optical mode scattering in the low energy range.

In Fig. 2 (a), the absorption process is slightly stronger than the emission process at $E - E_f < 100$ meV for the LA' mode because final states have higher densities of states. However, for high energy electrons the emission process is more active because the final states have higher occupations. This phenomenon is also observed in Fig. 4 where the transition happens at higher electron energy as the increase of temperature also increases the final state occupations.

As shown in Fig. 2 (b), (c) and (d), optical modes only participate in the emission process, because almost no phonons with energies higher than 200 meV are excited at 300 K. This is also true for K-point phonons in Fig. 3. Optical modes, especially the TO mode, dominate over acoustic modes in all energy ranges at the phonon K point.

We also investigate temperature effects on scattering rates by increasing the electron temperature $T_e$ from 300 K to 700 K with the phonon temperature $T_{ph}$ fixed at 300 K in Figs. 4 and 5. Fig. 4 demonstrates that increasing the electron temperature does not influence the acoustic modes while causing more optical phonon emission at the phonon Γ point in the low energy range as a consequence of more available final states, but the increase compared with Fig. 2 is not very significant. The effects on K-point phonons are similar, as shown in Fig. 5. The scattering starts to involve the TO absorption process due to the expansion of the Fermi window.

In order to explore the effects of doping levels on photoconductivity, we first calculate the temperature change with time and the corresponding heat flow into Γ-point and K-point acoustic and optical phonons based on the two-temperature model. We choose a starting electron temperature $T_e = 2000$ K and lattice temperature $T_{ph} = 300$ K, and allow the system to decay for bilayer graphene with Fermi levels 10 meV, 20 meV, 40 meV, and 60 meV respectively. Fig. 6 (a) shows that the thermalization process for bilayer graphene with $E_{fermi} = 10$ meV requires 60 ps to reach equilibrium, and the phonon temperature remains almost constant around 303 K because of the large phonon heat capacity. The electron temperature drops rapidly to 1200 K during the first 0.4 ps. Therefore even if the initial electron temperature may not be a precise estimate, further calculations are not severely affected. From Fig. 6 (b), at temperatures above room temperature, most of the heat loss by electrons flows to the optical phonons near the phonon K point. This result is not surprising because optical phonons have higher energies than acoustic phonons. As the electron temperature approaches 303 K after around 40 ps, the energy diverted to Γ point optical modes is lower than acoustic modes because optical modes rarely interact with low energy electrons near the Γ point.

Using the electron and phonon temperatures obtained...
FIG. 6: Two-temperature model. (a) Electron and lattice temperature changes vs time. The thermalization process takes 60 ps to reach equilibrium. The electron temperature drops drastically by 800 K in the first 0.4 ps. The lattice temperature remains almost constant around 303 K. (b) Heat flux to the phonon Γ point and K point acoustic and optical modes. Most of the heat is diverted to K-point phonon optical modes. After 40 ps, Γ point acoustic modes heat transfer exceeds Γ point optical modes.

from the two-temperature model, we calculate photoconductivities at four specific times, \( t = 2.8 \) ps, \( t = 4.8 \) ps, \( t = 5.8 \) ps and \( t = 6.8 \) ps, and compare with prior experimental results. We show only \( t = 2.8 \) ps and \( t = 5.8 \) ps in this paper. The case \( E_{\text{fermi}} = 10 \) meV matches with experimental values best in terms of both trend and intersection of the real and imaginary parts at all four times. The negative imaginary part can be qualitatively explained by an increase of temperature that amplifies overall scattering rates. The imaginary part goes to 0 as the probe frequency increases to values considerably larger than the overall scattering rates, because the effect of increased scattering become insubstantial and eventually diminishes. At \( t = 2.8 \) ps, the real part of photoconductivity decreases significantly with doping level at low probe frequencies due to enhanced electron-phonon scattering. Note that at \( t = 5.8 \) ps, the conductivity for \( E_{\text{fermi}} = 40 \) meV is higher than that for \( E_{\text{fermi}} = 60 \) meV because the heat loss to phonons is more severe for \( E_{\text{fermi}} = 60 \) meV. Thus the electron temperature is lower than that for \( E_{\text{fermi}} = 40 \) meV at the same time even though the former has higher density of states. As the decay proceeds, the real part of photoconductivity increases because the electron temperature decreases and weakens electron-phonon scattering. The real part also increases with probe frequency because the scattering time is comparably longer for carriers to react to electric field oscillations. Similarly, differences in conductivity between different doping levels are smaller at high frequencies where the scattering effects are less prominent.

Assuming \( T_e = T_L = 300 \) K and following the approach in [25], we combine contributions from the deformation potential and gauge field, and then extract an effective deformation potential coupled to a single phonon mode. The calculated \( E_{1,\text{eff}} \) is 22 eV with Eq. 13 for an effective phonon group velocity of \( v_{\text{ph}} = 2 \times 10^4 \) m/s. Fig. 2 indicates that both LO and TO modes contribute to scattering, and we use a single phonon optical deformation potential to represent LO and TO modes at the phonon Γ point. The corresponding phonon frequency \( \omega_{\text{LO/TO,Γ}} \) is 200 meV. At the phonon K point, electrons mainly interact with the TO mode; therefore we use the K-point TO phonon frequency \( \omega_{\text{TO,K}} \) in Eq. 14. The calculated \( D_{\text{LO/TO,Γ}} \) is 1.8 eV/˚A, and \( D_{\text{TO,K}} \) is 2.5 eV/˚A.

We further use the derived deformation potentials to calculate photoconductivity for \( E_{\text{fermi}} = 10 \) meV at four times. As shown in Fig. 8, the real part of photoconductivity calculated using the acoustic-deformation potential deviates significantly from the experimental data, as opposed to DFT predictions. The inclusion of an optical-deformation potential slightly improves the predictions for both real and imaginary parts; however the deviation from experiments and DFT results is still large. This indicates that momentum-dependent electron-phonon scattering potential and scattering rates are likely required to achieve accuracy in photoconductivity calculations.

Because defects indeed exist in the experimental bilayer graphene samples even though the concentration may be low, we expect a discrepancy between our calculations and measurements. Apart from electron-phonon scattering, short-range scattering also occurs in reality. Another factor is the indeterminism of the electron temperature, without which the calculated photoconductivity is not accurate. The two-temperature model could also be a source of discrepancy, but its effects are likely not significant. Phonon temperatures could depend on branches and their positions in reciprocal space; however they should always be around 300 K because of their large heat capacities.
FIG. 7: Photoconductivity evolution. Squares and circles are experimental data [7] for real and imaginary parts of photoconductivity, solid lines denote calculated real parts, and dashed lines denote calculated imaginary parts. The electron and lattice temperatures at each time step are obtained from our previous two-temperature calculations.

V. CONCLUSIONS

This paper demonstrates first-principles methods for the calculation of electron-phonon coupling, based on which an effective acoustic deformation potential $E_1 \text{ eff} = 22$ eV is estimated for bilayer graphene. The Drude model with DFT-calculated scattering rates predicts the correct trend for real and imaginary parts of photoconductivity. By increasing the doping level, the electron-phonon scattering is enhanced especially for low probe frequencies. The comparison between our DFT and deformation-potential approach calculations indicates that first-principles methods result in less deviations from experiments. The small deviations from experimental values could derive from several causes such as defects in the sample, short-range scattering, and electron temperature inaccuracies. The initial electron temperature is related to the incident light frequencies, intensities and the sample area illuminated. A possible direction of the future work could be determining the initial electron temperature accounting for fast electron-electron scattering that involves many-body effects.

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[1] W. J. Yu, L. Liao, S. H. Chae, Y. H. Lee, and X. Duan, Nano letters 11, 4759 (2011).
[2] Y. Zhang, T.-T. Tang, C. Girit, Z. Hao, M. C. Martin, A. Zettl, M. F. Crommie, Y. R. Shen, and F. Wang, Nature 459, 820 (2009).
[3] F. Bonaccorso, Z. Sun, T. Hasan, and A. Ferrari, Nature photonics 4, 611 (2010).
[4] Q. Bao and K. P. Loh, ACS nano 6, 3677 (2012).
[5] K.-J. Tielrooij, J. Song, S. A. Jensen, A. Centeno, A. Pesquera, A. Z. Elorza, M. Bonn, L. Levitov, and F. Koppen, Nature Physics 9, 248 (2013).
[6] P. A. George, J. Strait, J. Dawlaty, S. Shivaraman, M. Chandrashekh, F. Rana, and M. G. Spencer, Nano letters 8, 4248 (2008).
[7] S. Kar, V. L. Nguyen, D. R. Mohapatra, Y. H. Lee, and A. Sood, ACS nano 12, 1785 (2018).
[8] T. Ohta, A. Bostwick, J. L. McChesney, T. Seyller, K. Horn, and E. Rotenberg, Physical Review Letters 98, 206802 (2007).
[9] S.-i. Tanaka, M. Matsunami, and S.-i. Kimura, Scientific reports 3, 3031 (2013).
[10] S.-F. Shi, T.-T. Tang, B. Zeng, L. Ju, Q. Zhou, A. Zettl, and F. Wang, Nano letters 14, 1578 (2014).
[11] A. Frenzel, C. Lui, Y. Shin, J. Kong, and N. Gedik, Physical review letters 113, 056602 (2014).
[12] J. Heyman, J. Stein, Z. Kaminski, A. Banman, A. Massari, and J. Robinson, Journal of Applied Physics 117, 015101 (2015).
[13] S. Adam and S. D. Sarma, Physical Review B 77, 115436 (2008).
[14] A. Ferreira, J. Viana-Gomes, J. Nilsson, E. R. Mucciolo, N. M. Peres, and A. C. Neto, Physical Review B 83, 165402 (2011).
[15] J. Viljas and T. Heikkilä, Physical Review B 81, 245404 (2010).
[16] C.-H. Park, F. Giustino, M. L. Cohen, and S. G. Louie, Nano letters 8, 4229 (2008).
[17] S. Baroni, S. De Gironcoli, A. Dal Corso, and P. Giannozzi, Reviews of Modern Physics 73, 515 (2001).
[18] P. K. Lam, M. M. Dacorogna, and M. L. Cohen, Physical Review B 34, 5065 (1986).
[19] J. Bardeen and W. Shockley, Physical Review 80, 72 (1950).
[20] M. Lundstrom, Fundamentals of carrier transport (Cambridge university press, 2009).
[21] E. Hwang and S. D. Sarma, Physical Review B 77, 115449 (2008).
[22] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, et al., Journal of physics: Condensed matter 21, 395502 (2009).
[23] S. Poncè, E. R. Margine, C. Verdi, and F. Giustino, Computer Physics Communications 209, 116 (2016).
[24] A. K. Vallabhaneni, D. Singh, H. Bao, J. Murthy, and X. Ruan, Physical Review B 93, 125432 (2016).
[25] K. Kaasbjerg, K. S. Thygesen, and K. W. Jacobsen, Physical Review B 85, 165440 (2012).