1. Introduction

The graphene synthesis revealed exceptional properties for this material such as, high ambient temperature mobility, ambipolar effect, Klein tunneling, anomalous quantum Hall effect, etc [1]. This Breakthrough suggested many opportunities for the creation of other two dimensional (2D) materials. Among them, stanene, germanene and silicene are of particular interest because of their compatibility with current silicon technology [2]. Similar to graphene, the electrons in these 2D materials behave as massless Dirac fermions and exhibit a linear dispersion-band near the Fermi level due to their sp² electronic configuration [3]. The successful growth of Si, Sn and Ge- 2D monolayers has led to extensive investigation into the search for new hexagonal materials, such as phosphorene, borophene, aluminene and ZnO, with great potential for applications.

The materials consisting of column IV-elements of the periodic table are gapless in the absence of spin orbit coupling. This fact makes them less interesting for optoelectronic applications such as photovoltaic cells and light emitting diodes, which require a material with a nonzero band gap [4]. To overcome this deficiency, columns IV–IV hybrid materials have...
been introduced [5, 6]. The combination of silicon and carbon atoms creates silicene/graphene monolayer (SiC). This hybrid has a 2D planar honeycomb structure rather than a buckled one due to the strong π-bond through its perpendicular p$_x$ orbitals [7–9]. On the other hand, germanene/graphene hybrid (GeC) films are another column IV binary compound which can be prepared using deposition techniques such as laser ablation [10] and radio frequency reactive sputtering in Ar/CH$_4$ [11]. This material possesses excellent electro-catalytic properties and is promising for fuel cell and lithium–oxygen battery applications [12]. Both GeC and SiC sheets are direct band gap semiconductors and show strong excitonic effects with high binding energy [13, 14]. Meanwhile, the SnC monolayer, resulting from the combination of graphene and stanene, exhibits an indirect band gap. All these 2D graphene-based materials are good candidates for optoelectronic applications and are very promising for nanotechnology applications requiring catalytic performance for reduction and oxidation.

In a large group of semiconductors, a monotonic decrease of the energy gap has been observed as the temperature increases [15, 16]. This well understood phenomenon does not occur in some exceptional materials where band gaps exhibit two kinds of anomalous temperature dependence. In the non-monotonic anomalous case, the gap first increases at low temperatures and then decreases at high temperature [17]. In the monotonic anomalous case, the gap increases continuously with temperature. This behavior is observed for some perovskites [18], copper halides [19] and lead chalcogenides [20, 21]. Despite the abundance of experimental evidence, the understanding of anomalous gap dependence is explained by different, and sometimes even contradictory arguments, such as the role played by harmonic and anharmonic contributions [21, 22].

The temperature dependence of the electronic energies originates partially from the volume expansion [23] and results mainly from the electron–phonon (e–ph) interactions at constant volume [24]. In the latter case, the major contribution of the effect of e–ph interaction proves to be the most difficult to compute from first principles due to the huge number of k-points in the Brillouin zone required for convergence [25]. This can be avoided by using schemes based on Wannier functions. The spatial localization of the electronic and lattice Wannier functions allows to compute only a limited set of electronic and vibrational states as well as the corresponding e–ph interaction matrix elements from first principles. This requires low costs of a standard phonon dispersion calculation for a large number of k-points in the Brillouin zone [26].

Attention to the study of properties related to electron–phonon couplings (EPC) using ab initio computation has become more and more common for 2D materials. The obtained results subsequently explain many phenomena observed in honeycomb materials. The presence of Kohn anomalies in graphene and in the low buckled silicene is associated with their highest-branched optical modes [27, 28]. However, a negligible EPC is observed in germanene which shows very small square of the EPC matrix-element [28]. In stanene, the electron–phonon process is mainly dominated by the out-of-plane optical mode (ZO) leading to a hot carrier thermalization occurring at 250 fs [29]. In silicene, the low energy of out-of-plane acoustic phonon mode (ZA), derived from the weak sp$^3$ bond between its Si atoms, contributes to the high scattering rate and significant degradation in electron transport [30]. With access to the first-principles EPC, the effect of the scattering rate on the performance of MoS$_2$ and WSe$_2$ FET for a channel length of 10 nm shows a ballistic of 83% and 75% for WSe$_2$ and MoS$_2$ devices respectively [31].

Therefore, understanding the EPC from imaginary self energy, electron life time and carrier mobility in 2D hybrids is highly desirable and essential in order to facilitate their further applications. Considering the interest for graphene-based hybrids: GeC, SiC and SnC, this work studies the electron–phonon coupling involved in the temperature effect on the gap behavior. Using an ab initio approach based on the density functional theory (DFT), we investigate the behavior of the electronic hang gap thermal dependence in the three carbon based hybrids in the presence of electron–phonon interaction at constant volume. With the exception of SnC, which shows a non-monotonic anomaly, both GeC and SiC exhibit no anomalous behavior in their gap variation. To calculate the electron lifetime in these 2D materials, the imaginary part of electron’s self energy around the Fermi level and the corresponding scattering rate are determined in detail. The phonons contribution to the linewidth for an electron initially at the conduction band minimum (CBM) and the valence band maximum (VBM), as well as the variation of their corresponding lifetime with respect to the electron energy are discussed.

The present paper is organized as follows. In section 2, we present the computational method required for the calculation of the reported data. In section 3, we start by a comparative description of the temperature effect on the gap value. Then, we report a complete description of the behavior of SiC, GeC and SnC electron linewidth with respect to the electron energy and the temperature. From the plot of the scattering rate, we compute the electron lifetime and elucidate the role of phonon modes. Finally, in section 4, we end with a conclusion.

### 2. Computational method

In this work, three planar carbon-based hybrids are studied. The unit cell of each crystal contains two atoms: C and X (X = Si, Ge and Sn). As displayed in figure 1, each carbon atom is bonded to three X-atoms forming hexagonal structures.

Employing norm-conserving pseudo-potentials, the generalized gradient approximation of Perdew–Zunger exchange-correlation functional is used considering a plane-wave basis set with a kinetic-energy cutoff of 60 Ry [32]. The electronic states are computed using a k-sampling grid of $32 \times 32 \times 1$ in the Brillouin zone based on the Monkhorst–Pack scheme. The subsequent computational recipe is based on the scheme proposed in [24].

The vibrational frequencies, $\omega_{\alpha\beta}$, and the derivatives of the self-consistent Kohn–Sham potential with respect to the atomic displacements are calculated on $16 \times 16 \times 1 \, q$-point grids using density functional perturbation theory (DFPT) [26] as implemented in the Quantum-Espresso code [33].
These parameters are needed to evaluate the e–ph coupling matrix elements.

The many body perturbation theory (MBPT) is used to describe the behavior of electronic states as a function of temperature [34]. The electron–phonon coupling is perturbatively treated [35]. We consider the Fan and Debye–Waller self-energy terms corresponding respectively to the first and second order of the Taylor expansion in the displacement of the nuclei. The Green function is written as [24]:

$$G_{nk}(\omega, T) = \left[ \omega - \epsilon_{nk} - \Sigma_{\text{Fan}}^{\omega}(\omega, T) - \Sigma_{\text{DW}}^{\omega}(T) \right]^{-1}$$

where $\epsilon_{nk}$ is the Kohn–Sham ground-state eigenenergies of the frozen atoms, $\Sigma_{\text{Fan}}^{\omega}$ is the Fan contribution to the self energy given by:

$$\Sigma_{\text{Fan}}^{\omega} = \sum_{\omega'q\lambda} \frac{|q_{\omega'q\lambda}|^2}{N} \left[ N_{\omega\lambda}(T) + 1 - f_{\omega'q\lambda} - \omega_{\omega'q\lambda} - \omega_{\omegaq\lambda} \right]$$

and $\Sigma_{\text{DW}}^{\omega}$ is the Debye–Waller term expressed as follows [36]:

$$\Sigma_{\text{DW}}^{\omega} = -\frac{1}{2} \sum_{\omega'q\lambda} \Lambda_{\omega'q\lambda}^{\omega} \left[ N_{\omega\lambda}(T) + 1 \right] \left[ \epsilon_{nk} - \epsilon_{n'k} \right]$$

with $N_{\omega\lambda}$ and $f_{\omega'q\lambda}$ represent the distribution functions of Bose–Einstein and Fermi–Dirac, while $\omega_{\omega'q\lambda}$ and $N$ are the phonon frequencies and the number of points taken randomly to better map out the phonon transferred momentum [35]. $\Lambda_{\omega'q\lambda}^{\omega}$ is the second order electron–phonon matrix elements.

The first order electron–phonon matrix elements $g_{n'q'k'}$, which represent the probability amplitude for an electron to be scattered with emission or absorption of phonons are given by:

$$g_{n'q'k'} = \langle \psi_{n'k'} | \partial_{q'k'} | \psi_{nk} \rangle$$

where $n'$ and $n$ are initial and final electron band indices with wavevectors $k$ and $k' = q$, respectively, and $\partial_{q'k'}$ is the derivative of the self-consistent potential associated with a phonon of the wavevector $q$ in the branch $\lambda$. To calculate the imaginary part of the electron’s self-energy using the electron–phonon coupling using Wannier functions code (EPW) [37], the matrix elements were evaluated over a grid of $360 \times 360 \times 1$ q points.

Assuming the quasiparticle approximation (QPA), one can expand in first-order the self-energy frequency dependence around the bare energies. It follows that the temperature dependent quasi-particle energy is given by [24]:

$$E_{nk}(T) \approx \epsilon_{nk} + Z_{nk}(T) \left[ \Sigma_{\text{Fan}}^{\omega}(\epsilon_{nk}, T) + \Sigma_{\text{DW}}^{\omega}(T) \right]$$

where the renormalization factor is expressed as follows:

$$Z_{nk}(T) = \left[ -\frac{\partial R \sum_{\omega} \Sigma_{\text{Fan}}(\omega)}{\partial \omega} \right]^{-1}$$

We note that the imaginary part of the Fan’s self-energy ($\Sigma_{\text{Fan}}^{\omega}$) provides information on the rate of e–ph processes responsible for hot carrier thermalization, which is related to the intrinsic quasiparticle lifetime. The real part, however, informs us about the energy renormalization shift. Thus, in order to obtain the associated e–ph scattering rate, one should first compute the linewidth ($\Gamma_{nk}$) [37]:

$$\Gamma_{nk}^{\text{el–ph}} = \frac{2\Gamma_{nk}}{\hbar}$$

which just means that the quasiparticle lifetime corresponds to the inverse of the scattering rate $\tau^{-1}$.

Equation (4) states that the single particle energy $E_{nk}$ depends on temperature as follows [24]:

$$E_{nk}(T) = \epsilon_{nk} + \Delta E_{nk}(T).$$

The energy $\Delta E_{nk}(T)$ involves two contributions, namely:

$$\Delta E_{nk}(T) \approx \Delta E_{nk}(T)_{\text{har}} + \Delta E_{nk}(T)_{\text{anhar}}.$$  

The first term results from pure electron–phonon interactions and represents the harmonic contribution at constant volume. The second term corresponds to the effects flowing from the lattice expansion (variable volume). According to equation (8), it is obvious that the harmonic and anharmonic terms have some

![Figure 1](image-url)
En typically stands for a decreasing (decreasing) gap as function of temperature in contrast to a positive (negative) region of $E_g$.

### Results and discussion

#### 3.1. Temperature effect on the band gap

This part investigates the electron–phonon interaction in order to calculate and describe the temperature dependence of the electronic gap ($E_g$) for SiC, GeC and SnC hybrids. Figure 2 displays the variation of the band gap with respect to the temperature ($T$) for the three carbon-based hybrids.

The value of the bandgap of both SiC and GeC show a monotonic decrease as a function of temperature. It follows that these two materials are semiconductors with normal behavior. Meanwhile, SnC shows a different behavior. Indeed, by varying the temperature from 0 K to 100 K, the band gap of the SnC configuration also increases as plotted in figure 2. Thus, SnC has an anomalous trend in this temperature range. However, for a temperature above 100 K, the gap of SnC starts to decrease. This gap behaviour makes SnC hybrid a semiconductor of non-monotonic anomaly kind.

The projected phonon density of state in figure 3 reveals that the heavier is the atom the smaller is his contribution to the optical modes. In the three hybrids, all optical modes are mainly dominated by carbon atoms, while the acoustical modes are mostly dominated by the heaviest atoms, namely Si, Ge and Sn in SiC, GeC and SnC respectively.

To shed more light on the gap behavior for the three binary compounds, figure 4 plots the generalized Eliashberg spectral function for the CBM and VBM states to visualize the electronic gap ($E_g$) for SiC, GeC and SnC hybrids. Figure 2 displays the variation of the band gap with respect to the temperature ($T$) for the three carbon-based hybrids.

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Generally, the Eliashberg function, defined in equation (9) is positive for the valence band maximum and negative for conduction band minimum. This opposite trend leads to the reduction of the gap. Regarding equation (10), a positive region of $g^2 F_n k$ corresponds to a temperature increasing of the gap energy while its negative region stands for a decreasing of $E_g (T)$. For the carbon based hybrids, one deduces that in SiC, the VBM and CBM Eliashberg functions are all normal for all phonon modes leading to a gap decreasing. For GeC, the CBM contributions are negative for all phonons while for the VBM, the contribution for the Eliashberg function are positive except for phonon with frequency around $250 \text{ cm}^{-1}$. Therefore, the resulting Eliashberg function arising from VBM and CBM contribution show a gap decreasing. Finally, the curve associated to the SnC sheet shows a strong anomalous behavior for the VBM due to the contribution of the high optical phonon modes. This anomalous behavior leads to the non monotonic variation of the gap when increasing the temperature.

### 3.2. Electron linewidth versus temperature

The following part investigates the electron linewidth arising from the electron–phonon interaction and determines the electron lifetime for all structures. Figure 5 displays the pooling of the electronic band structure of stanene and the imaginary part of the self energy $\Gamma_{nk}$ on a fine electron wave-vector k-grid for two different temperatures namely, 0 K and 300 K. The temperature 300 K is chosen rather than other temperatures in order to investigate hot carrier behaviour at room temperature.

At 0 K, the variation of electron linewidth as a function of the electron energy is plotted in figure 5 along k-points on the high symmetry line for SiC, GeC and SnC respectively. The band structures of SiC, GeC and SnC show that the states in SnC are more closer from each other compare to SiC and GeC explaining the smaller linewidth for SnC with respect to SiC and GeC, which is more observable in the unoccupied states. Recall that the imaginary part $\Gamma_{nk}$ of the Fan’s self-energy provides information on the rate of e–ph processes responsible for hot carrier thermalization [39]. The following focus on the carriers thermalization and their lifetime around the Fermi level for the three monolayers.

At 300 K, figures 5(d)–(f) show that the imaginary part of the self energy is more sensitive to the temperature in the conduction bands compared to valence bands. This is due to the fact that, the carrier in the conduction band are
free to move which makes them very susceptible to any external perturbation such as temperature. This sensitivity also depends on the gap value as it gets increased when the gap value is decreasing. Indeed, when increasing the temperature, the electron linewidth in the SiC structure changes less significantly with respect to its two counterparts GeC and SnC having smaller gaps. Moreover, compared to GeC, the linewidth in SnC is more sensitive to temperature at the vicinity of the $M$-point. However, far from this symmetric point and around the Fermi level, the thermal sensitivity is quite similar in both GeC and SnC. The very small density of states makes the imaginary self energy very small and unchanged in term of temperature dependence compared to other energy levels. The obtained results are in good accordance with the high thermal sensitivity observed for bulk silicon and bulk germanium due to their small gap values of 1.17 eV and 0.74 eV respectively [46]. Finally, the used method gives accurate variation of the linewidth with respect to the electron energy for the three carbon based hybrids as this method allows to extract information about the linewidth for each energy level. This is promising for determining the exact relaxation time and engineering hot carriers cells [40].

### 3.3. Scattering rate and lifetime

Based on equation (6), the electron–phonon scattering rate is plotted with respect to the electron energy in figure 6 for the three hybrids SiC, GeC and SnC. Only the electron–phonon contribution is considered as it is the most dominant near the Fermi level compared to the electron-electron interaction. Indeed, as reported in [41, 42], hot electrons essentially interact with phonon because of the small density of state and the low energy range around the Fermi level.

Figure 6 shows a very small change of the scattering rate in term of temperature for the SiC hybrid. The shifting is more observable in GeC compared to SiC, and the displacement of the scattering rate is much more visible for SnC. All these observations are in good agreement with the results obtained for bulk germanium, bulk silicon [46] and diamond [43].

Hot carrier relaxation time, that is inversely proportional to the imaginary part of the self energy, shows in figure 7 a high value near the band edges. Moreover, electronic energy regions with many bands results in a faster electron–phonon relaxation time of hot electrons by phonon emission. This behaviour is due to the large number of possible transitions. The hot electron lifetime plot corresponding to the SiC structure indicates that hot carrier relaxation near the band edge is characterized by relaxation time around 90 fs while faster relaxation time of 10–20 fs are found at energy more than 75 meV away from the band edge. For GeC, the analysis of figure 6(d) reveals hot electron lifetime around 100 fs near the Fermi level at room temperature. For an energy ranging from 200 meV up to the Fermi level, the relaxation time is much shorter at less than 50 fs. Finally around the edge of the band of SnC, the gap is characterized by a relaxation time limiting the thermalization of the rate of hot electrons in the interval ranging from 100 fs to 120 fs. At 100 meV away, the hot electron relaxation time ranges in the interval [10,90] fs. In the three carbon-based hybrids, the relaxation time observed near the band edges are slower than the 400 fs found for graphene [44].
3.4. Linewidth and scattering rate phonon dependency

In general, the electron scattering rate arises from the contribution of acoustic and optical phonons together. Figure 8 provides a quantitative analysis of the contributions from the individual phonon modes. In SiC hybrid, the scattering rate is mainly dominated by the out of plane acoustic mode (ZA) over all energy levels. More precisely, ZA mode is followed by the transversal acoustic mode (TA) mode at VBM, while ZA is followed by the longitudinal acoustic mode (LA) mode at CBM. For higher energy levels, ZA is followed by the optical transversal mode (TO). When the Si atom is replaced by the much heavier Ge atom, the optical modes contribution is getting much important. As shown in figures 8(c) and (d),

![Graphs showing electron scattering rate and linewidth](image)

**Figure 8.** Electron scattering rate associated with acoustic (in the first line) and optical (in the second line) modes, respectively for SiC, GeC and SnC monolayers.

![Graphs showing electron linewidth variation](image)

**Figure 9.** Electron linewidth variation in terms of electron wavevector $k$ projected on the six phonon modes for SiC, GeC and SnC, where the initial electron state is at the VBM. The contribution for each phonon mode is displayed for the same electron energy for (a), (c) and (e) acoustic phonon branches LA (red continuous), TA (green dashed) and ZA (blue dashed–dotted); and (b), (d) and (f) the optical phonon branches LO (red continuous), TO (green dashed) and ZO (blue dashed–dotted). On the top figures correspond to the acoustic contribution and the bottom are the optical contribution. $\Gamma$, $K$ and $M$ describe the high symmetry point of electron wavevector.
the electron scattering is mostly due to the presence of TO followed by ZA modes for higher electron energy ranges in GeC. At the band edges of GeC, the CBM arise essentially from both ZA and ZO mode while the VBM is dominated by ZA and TA. Unlike SiC, the major contribution arises from the optical modes in SnC. Indeed, both the VBM and the CBM are mainly dominated by ZO mode followed by TA mode. For higher energy in the conduction band, ZO is followed by ZA.

To shed more light on the $k$-dependence of the imaginary part of the self energy in the three binary compounds, figures 9 and 10 display the linewidth variation over the high symmetry line of BZ and electron state being at the CBM and VBM. In these figures, the linewidth is projected over acoustic and optical phonon modes to (i) show their different contribution depending on the high symmetry directions related to real space and to (ii) deduce information regarding the linewidth and which phonon plays crucial role in this direction.

3.4.1. VBM. For electron state at the VBM, the examination of acoustic modes contributions plotted in figure 9 shows that the LA mode is lower compared to TA and ZA in all configurations. Over the $\Gamma - K$ and $M - \Gamma$ directions, the highest contribution in the linewidth is attributed to the ZA mode for SiC and also for GeC but with smaller amplitude. This result matches very well with their counterparts silicene and germanene [45]. In SnC, figure 9(c) reveals that the linewidth arise mainly from both ZA and TA modes with a ZA magnitude very small compared to GeC and SiC. At $K$-point, all acoustic modes have no contribution in the electron linewidth due to the weak interaction occurring because of the lack of states at the band edges as shown in figure 9.

For optical phonon, the curves plotted in figures 9(b)–(f) show that in SiC, the linewidth is dominated by ZO mode all over the high symmetry line, followed by LO and TO. In both GeC and SnC, the main contribution arises also from the out of plane mode ZO.

3.4.2. CBM. For electron state at the CBM, figure 10 plots the electron linewidth projected over phonon modes. In SiC, the largest contribution comes from ZA mode over the high symmetry line, however the linewidth is shared into three parts over the high symmetry line as displayed for GeC. Indeed, the linewidth is dominated by the TO and ZA in the $\Gamma - K$ region and only by ZA in the interval $M - \Gamma$. While, the major contribution is attributed to the LO mode along $K - M$. In SnC, the electron linewidth is dominated by ZO mode for all the BZ high symmetry line. It is worth noting that in SiC and GeC, the linewidth is zero for all phonon modes at $K$-point. However, for both TO and ZO mode, the linewidth is not zero in SnC. This difference is due to the indirect gap of SnC as the band edge is located at $K$-point for VBM and at $\Gamma$-point for CBM.

Finally, by evaluating the linewidth over the typical edge of the Brillouin zone in SiC, GeC and SnC, one can deduce that there exists a large variation in the magnitude of the electron–phonon coupling along the different crystallographic directions.

4. Conclusion

Using ab initio calculations, we reported a theoretical description of the electron–phonon coupling effects on the gap,
 linewidth and scattering rate in two-dimensional SiC, GeC and SnC materials. In addition to the study of the thermal sensitivity of the linewidth, we investigated its k-resolved behavior. This type of study is important for transport phenomena where phonons play a crucial role and therefore has an impact on the engineering concepts of devices based on nanostructures. While the band gap in SiC and GeC showed a normal monotonic dependence to temperature, its behavior was rather anomalous in the SnC semiconductor. It has been found that the out-of-plane acoustic transverse mode ZA efficiently couples to the electronic states at the SiC band edge, while the linewidth mainly arises from the ZA and ZO modes in GeC. In SnC, the optical mode, namely ZO, was predominant. The hot carrier thermalization losses in SiC, GeC and SnC under solar lighting were also calculated. It was found that, under sunlight illumination, the hot carriers thermalize within 90 fs, 100 fs and 120 fs for SiC, GeC and SnC respectively. This work highlights the microscopic origin of the thermalization of hot electrons, which is difficult to deduce from experiments and opens the way toward the study of materials for renewable energies by means of ab initio calculations of hot electrons.

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