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Theoretical Study of Electronic and Thermoelectric Properties of Ultra-Thin Silicene and Germanene

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ABSTRACT

In this study, we used the Non-Equilibrium Green Function (NEGF) and Density Functional Theory (DFT) to analyze the nanoscale electronic properties of silicene and germanene structures, the band structure and Density of State (DOS) for the unit cell of silicene and germanene are found that the energy gap is (0 eV) in both. A comparison was made between silicene and germanene in terms of electrical and thermal properties, by calculating the transmission coefficient T(E) for silicene patterns (Si1, Si2, Si3, and Si4) and germanene patterns (Ge1, Ge2, Ge3, and Ge4). The results show that T(E) decreases with increasing etching depth, which also leads to a decrease in electronic conductivity. Moreover, the value of the Seebeck coefficient (S) increases with increasing drilling depth, and also the sign of S varies from a positive value for (Si1, Si4, Ge1, Ge2, Ge4) to a negative value for (Si2, Si3, Ge3) at Fermi level (E_f) equal to (0 eV). The highest value of the figure of merit is about (1.8) for the Ge4 structure.

دراسة نظرية للخواص الكهربائية والكهروحرارية للسيليسين والجرمانيين الرقيق للغاية

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الملخص

في هذه الدراسة، استخدمنا دالة كرين غير المتوازنة (NEGF) ونظرية الكثافة الوظيفية (DFT) لتحليل الخصائص الإلكترونية ذات المقياس النانوي لهياكل السيليسين والجيرمانين، وهيكل النطاق وكثافة الحالة DOS لوحدة الخلية من السيليسين والجيرمانيين. وجد أن فجوة الطاقة هي (0 eV) في كليهما. تم إجراء مقارنة بين السيليسين والجيرمانين من حيث الخواص الكهربية والحرارية، وذلك بحساب معامل النقل T(E) لأنماط السيليسين (Si1 و Si2 و Si3 و Si4) وأنماط الجرمانين (Ge1 و Ge2 و Ge3 و Ge4). أظهرت النتائج أن T(E) يتناقص مع زيادة عمق التنميش، مما يؤدي إلى انخفاض في التوصيل الإلكتروني أيضًا. علاوة على ذلك، تزداد قيمة معامل سيبيك (S) مع زيادة عمق الحفر، كما تختلف علامة S من قيمة موجبة لـ (Si1، Si4، Ge1، Ge2، Ge4) إلى قيمة سالبة لـ (Si2، Si3، Ge3) عندما تكون طاقة مستوى فيرمي (E_f) مساوية لـ (0 eV). أعلى قيمة للكفاءة (ZT) هي حوالي (1.8) لهيكل Ge4.

الكلمات المفتاحية : سيليسين، جرمانيين، نظرية الكثافة الوظيفية (DFT)، هيكل النطاق.

Introduction

Graphene is the first two-dimensional atomic crystal available to us, and it has extreme mechanical strength, exceptionally high thermal and electrical conductivity, and many other properties, all of which make it very special for many applications [1]. Inspired by the future properties of graphene, there is growing interest, as other 2D lattices such as silicene and germanene are being studied. In fact, silicene - the silicon analogue of graphene - too. Its two-dimensional structure leads to many interesting physical and chemical properties, which attract great interest [2–5]. Even more interesting than graphene is silicene, especially for thermoelectric applications [6]. It has been reported that graphene has the highest intrinsic limit for electrical mobility at room temperature [7], which is a good reason for thermoelectric uses. However, experiments have shown that the heat conductivity of a single layer of suspended graphene is between ((4.84 ± 0.44) × 10^3 to (5.30 ± 0.48) × 10^3 W/m k) at room temperature [8], and this is approximately the highest found thermal conductivity of any material while extremely high thermal conductivity helps electronics get rid of heat, but it makes graphene less useful as a thermoelectric material because the efficiency of energy transfer is inversely proportional to thermal conductivity [9]. Graphene doesn't have an energy gap, so its Seebeck value is very small [10]. But silicene could be a great way to turn heat energy into something useful. First, from the electronic structure perspective, many studies show that silicene is the same as graphene [11], which means that it conducts electricity just as well as graphene. Second, unlike graphene, The atoms in silicene are bent, which causes an energy gap that isn't zero and makes the Seebeck coefficient bigger [12]. Therefore, there is a very important need to determine the thermal transfer properties of silicene. It has some of the same electronic properties as graphene and has shown great promise in other fields, such as nanoelectronics [13–15]. In addition, silicene is more readily integrated into devices than graphene. Several crucial mechanisms have not been investigated with electronic devices based on silicon. In theoretical research, silicene and other nanostructures can be studied by employing the popular classical molecular dynamics simulation [16]. Unfortunately, we did not find interatomic potential to accurately characterize the unique properties of silicene, for example, the low-bending structure and corresponding torsional distance that emerge through reproducing experiments [17] and preliminary calculations [18]. From early studies, Ge was thought to form a single-layer hexagonal lattice called germanene [19]. In theory, germanene has a Dirac point, and its structural and electronic properties are very close to those of silicene. This is because the bulk Si and Ge have a small electronic gap, which makes the Seebeck value much higher [20]. In this study, we are going to investigate more details about fully crystalline and deformation of two dimensions Si and Ge, such as thermal conductance and electrical features using density functional theory combined with nonequivalent green theory.

Theoretical methods

The purpose of this research was to make a comparison between the characteristics of germanene and silicene by examining the properties of each of them and optimizing the structure of both of them using the density functional theory applied in the SIESTA code [21], Density Functional Theory (DFT) In comparison to the electronic form of structure based on the wave function, it is understood that the DFT approach is based on the density principle. Owing to its imperfect existence, several improvements were made to this hypothesis. Centered on the approximation of born-oppenheimer and of Hartree-Fock theories (HF) and variational theorems, the DFT was introduced. The Hohenberg-Kuhn scientist theory (HK) using the Generalized Gradient Approximation (GGA), and transforming the Perdew-Burke-Ernzerhof interaction [22,23] and correlation parameters. Dual polarization basis sets are applied with a (51 × 51 × 1) Monkhorst-Pack lattice starting from point k in the Brillouin zone integration when all forces on each atom are below the (40 eV A^{-1}) tolerance limit. The band structure and density of state are calculated, we first use the SIESTA [24], software of density functional theory to obtain the average material-specific Hamiltonian field for each structure. This is done by looking at the geometry optimized for each intersection. Then, using the Landauer formula, we combine the DFT method with the Gollum quantum transport code [25–27] to obtain the Transport coefficient T(E) and the thermoelectric properties.

Results and discussion

Figure 1(a,b) shows the density of state and band structure of the unit cell of silicene and germanene under this study, as we can see from this figure that the unit cell consists of two atoms with a bond length of (2.36 Å for silicene and 2.49 Å) for germanene. As we can see, the difference between silicene and germanene's band gap is closed at (Ef = 0 eV), this means that the structure of silicene and germanene is a semi-metal, and this result agrees with many studies [28,29]. The structure of germanene is more twisted than that of silicene. This was found after calculating the torsional modulus for both germanene and silicene, where the torsion modulus value for germanene was (0.841 Å) and for silicene (0.802 Å), it is slightly higher than the values reported in [30–32]. This could be because the way the tools work is different. To study the energy gap of both silicene and germanene, we design periodic silicene and germanene sheets with (288 atoms) with a dimension (6.74 × 2.447) nm for silicene and of (6.74 × 2.447) nm for germanene as shown in Figure 2(1,2).

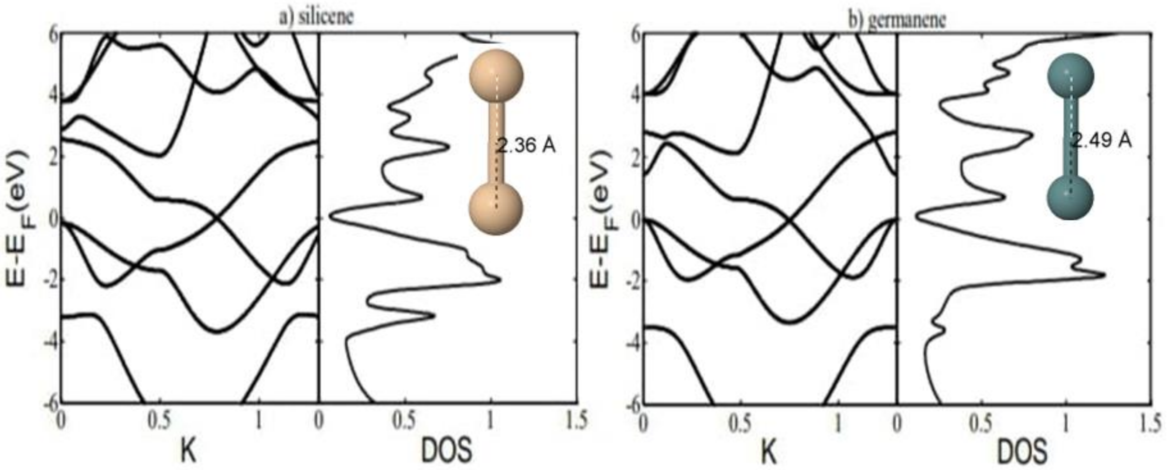

Figure 1. The optimum band structure and state density It's either a) Silicene or b) Germanene. Band energy relative to Fermi energy

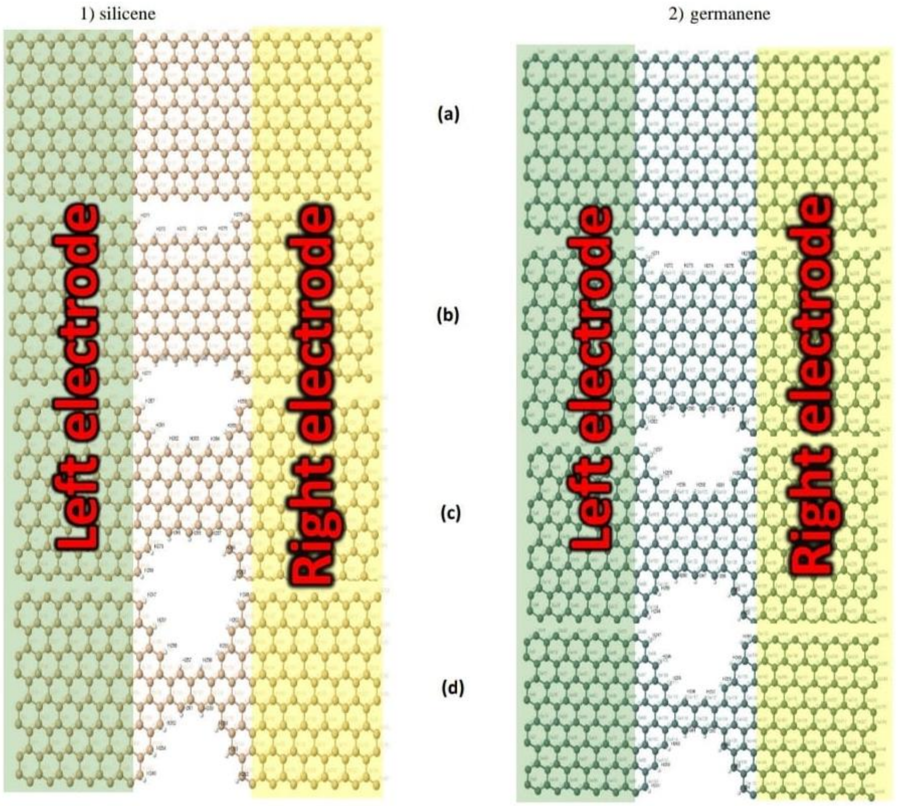

Figure2. Division of the crystal structure of silicene and germanene to calculate electrical and thermal properties: ***a) perfect crystalline, b) one-layer etching, c) two-layer etching, d) three-layer etching***

In this study, we designed silicene and germanene nanoelectronic devices, the two electrodes are used from the same structure (Si and Ge) with a scattering region in the middle of the system. In Fig. 2 the left panel represents the silicene structure with different etching scattering regions, the same thing is repeated for the germanene structure (right panel). To investigate the properties of each system and compared both we designed four different structures by removing a layer of atoms from the top and bottom of the scattering region as shown in Figure 2(b-c) for both silicene and germanene, as we can see from Fig. 3 the transmission coefficient decreases with an increase in the etching step, it is clear from this figure that the germanene is less affected than silicene for the same steps, T(E) is calculated for each system. As we can see from Fig. 3, the T(E) of the fully crystalline silicene–germanene sheet is two open channels (black line), which is in good agreement with the band structure and DOS calculation. It is clear that T(E) decreases with increasing drilling depth (Fig. 3 red, blue, and green line), as the value of T(E) decreased in silicene from (2 to 2.51 $\times 10^{-3}$) and in germanene from (2 to 4.38 $\times 10^{-2}$). As well as, the silicene transmission shifted to the low energy by (0.11 eV) for all systems (solid and dash line). This technique is useful for the transition from metals to semi-metals.

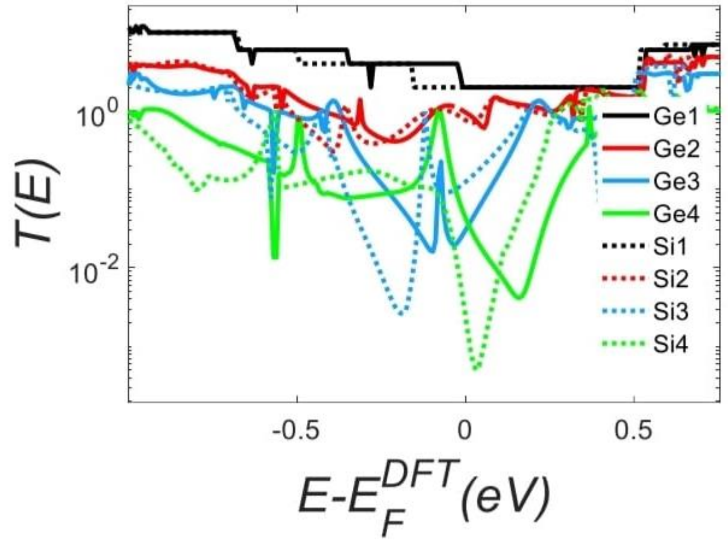

Figure 3 Fermi energy-dependent transport coefficients in silicene and germanene

From the following equation, the electrical conductivity can be calculated [33]:

$$G = \frac{1}{v} = G_0 \int_{-\infty}^{\infty} dET\,(E) \left(\frac{df(E)}{d(E)}\right) \qquad (1)$$

Whare $f(E)$ is the fermi dirac distribution and G_0 is the conductance quantum which is equal to $(2e^2/h)$, (e) is the electron charge, and (h) is Planck constant.

The electrical conductivity value of the four silicene and germanene structures is shown in Fig. 4, where the graph shows the value of conductivity LOG (G/Go) versus energy. The conductance varied from (0.26 to -1.82) for Si1 and Si4 respectively near the Fermi level (EF = 0 eV). The germanene conductivity is generally higher than silicene conductivity, to compare each color we can see that the minimum value for the silicene (dash line) is lower than the minimum value of the germanene (solid line).

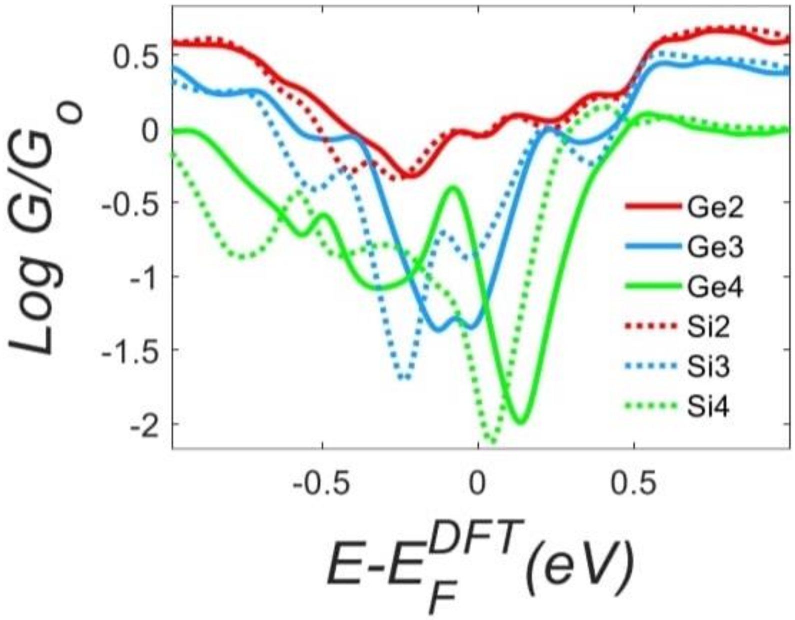

Figure 4. Electrical conductivity values due to energy at room temperature in silicene and germanene

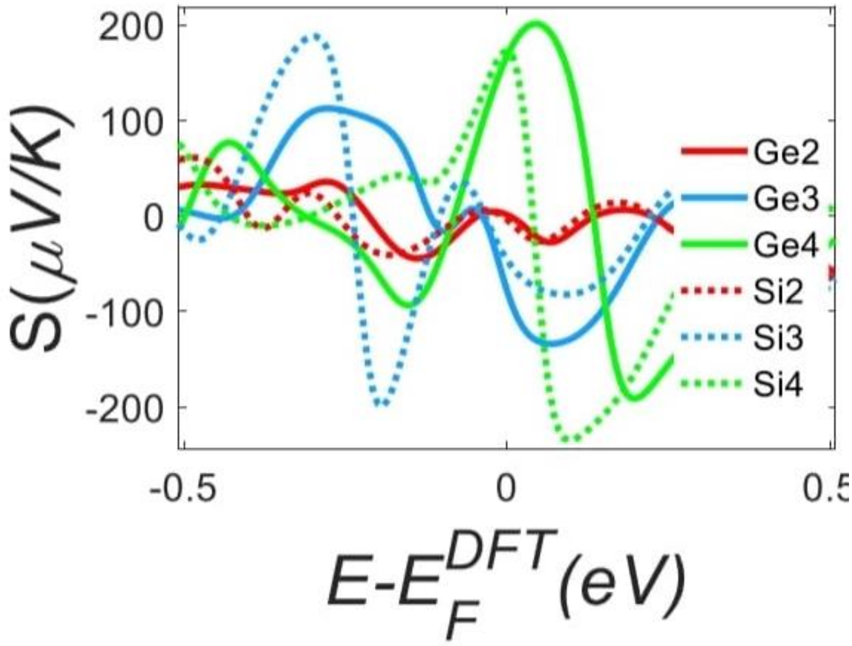

Figure 5. Seebeck's coefficient (S) for the Fermi energy in silicene and germanene

The negative slope of (ln T(E)) correlates with the Seebeck coefficient S. The following equations can be used to determine the thermoelectric properties of Seebeck coefficient (S), thermal conductance (K), and figure of merit (ZT) [34,35] :

$$S(T) = -\frac{1 L_1}{eT L_0} \qquad (2)$$

$$K = \frac{2}{h}\frac{1}{T}\left(L_2 - \frac{L_1^2}{L_0}\right) \qquad (3)$$

$$ZT = \frac{GTS^2}{K} \qquad (4)$$

Where $Li = \int_{-\infty}^{\infty} dEF(E)\,(E - E_F)^i$

The Integral $L0$, $L1$, $L2$ are obtained at (i = 0, 1, 2) respectively. Fig. 5 shows the Seebeck coefficient of silicene and germanene. The Seebeck coefficient fluctuated between positive and negative values at fermi level (EF = 0). The highest value of S is for the structure Si4 and Ge4 which is (173 and 167 µV/k) respectively.

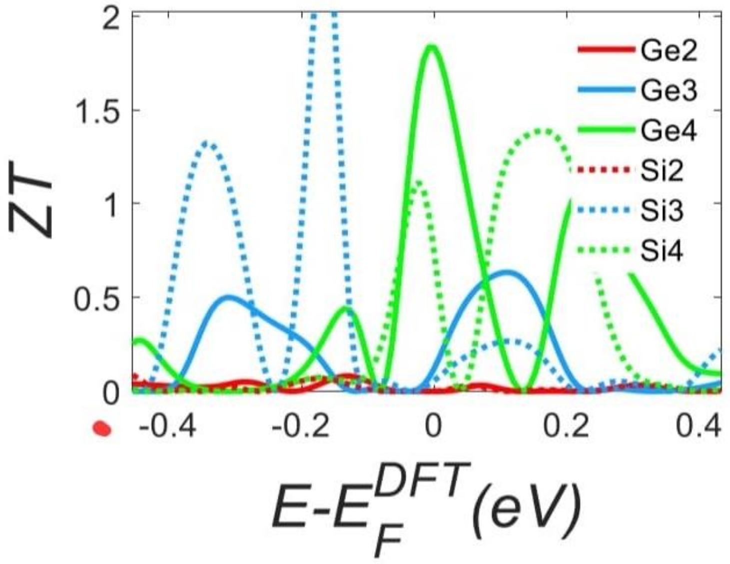

Figure 6. ZT as a function of the Fermi energy in silicene and germanene at room temperature 300 K

ZT is the figure of merit which expresses the performance of the refractory material. The dimensionless figure of merit (ZT) is used to determine how effective a thermoelectric power system is. The above equation (4) is used to calculate a figure of merit (ZT) [36]:

Figure 6 shows how the ZT of silicene and germanene changes with energy. The most that ZT can be worth is (1.8) for the structure Ge4. All values are summarized in Table 1 for all structures in this study. Seebeck's (S) and (ZT) values at EF = 0 and 300 °C thermal conductivity (k) values are listed in Table 1.

Table 1. conductance, Seebeck coefficient and quantum efficiency of all systems

Mol.	LOG(G/Go)	S(µV/K)	ZT	Mol.	LOG(G/Go)	S(µV/K)	ZT
Si 1	0.3	1.561	$8.9\text{x}10^{-5}$	Ge 1	0.4	41.21	0.06
Si 2	-0.05	-4.076	0.0006	Ge 2	-0.045	1.08	$4.3\text{x}10^{-5}$
Si 3	-0.8	-46.62	0.056	Ge 3	-1.3	-78.87	0.12
Si 4	-1.8	173.01	0.73	Ge 4	-0.9	167.7	1.83

Conclusion

In this study, we compared the electrical and thermoelectric properties of different sizes of silicene and germanene scattering regions. The result shows that the conductance are decreasing with an increase in the etching scattering region. Also the Seebeck coefficient are increasing with the increase in the etching as well. Moreover, the ZT increase with the increase in the drilling and the highest value is for Ge4 which equals (1.83), this structure is a candidate to be the best for nanoelectronic device.

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