A two-dimensional SiGeO monolayer with high electron mobility and negative Poisson’s ratio

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Abstract. In this paper, we perform the first-principle calculations to explore the electronic and mechanical properties of two-dimensional SiGeO. SiGeO is an indirect band gap semiconductor with a gap of 1.29 eV and a high electron mobility of $1.70 \times 10^3$ cm$^2$V$^{-1}$s$^{-1}$. The uniaxial strain can trigger the indirect-to-direct band gap transition. Moreover, SiGeO exhibits an extraordinary auxetic property, and its in-plane negative Poisson’s ratio is three times larger than that of borophenes. These properties would endow two-dimensional SiGeO with great potential in the application of electromechanical devices.

1. Introduction

Two-dimensional (2D) material has aroused great attention since the discovery of graphene. The extraordinary electronic and mechanical properties render 2D materials a noteworthy candidate for the next generation nanodevices [1]. As the analog of graphene, silicene and germanene share similar honeycomb configuration and electronic properties [2]. Although they have competitive characteristics such as intrinsic high carrier mobility and good compatibility with modern silicon-based semiconductor industry, the zero-band gap of silicene and germanene has greatly limited their applications in microelectronic devices.

The electronic properties of 2D materials could be adjusted by introducing extra elements [3]. Recently, Wang et al. have investigated the electronic and mechanical properties of fully oxidized silicene (SiO) and germanene (GeO) [4]. SiO and GeO are proved to be semiconductors and possess unconventional auxetic behavior. The intriguing properties inspired us to study the materials relate to Si, Ge and O. In this work, we predict a new 2D SiGeO with an indirect band gap of 1.29 eV. The band would experience an indirect-to-direct band gap transition while the uniaxial compressive strain larger than 2%. Additionally, SiGeO monolayer possesses high electron mobility and in-plane negative Poisson’s ratio (NPR). These properties indicate that 2D SiGeO has potential application in nanoelectronic and nanomechanical devices.

2. Computational details

All calculations are carried out by using the CASTEP code based on the density functional theory (DFT) [5]. Exchange-correlation energies are described by the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) functional [6]. The energy cutoff for the plane waves is set to 1030 eV. All structures are fully relaxed until the forces are smaller than 0.01 eV/Å and the energy tolerances are less than $5 \times 10^{-7}$ eV per atom. A $10 \times 13 \times 1$ Monkhorst–Pack k-points is sampled. The vacuum spacing larger than 20 Å is applied to ensure that the interactions between the layers are...
negligible. The PBE functional is adopted to calculate the band structures. For the existence of heavy Ge atoms, the spin-orbit coupling (SOC) effect is also taken into consideration. The phonon dispersion is calculated by using the linear response method [7].

3. Results and discussion

3.1. Geometric Structures, cohesive energy and phonon dispersion

Figure 1a presents the top and side views of fully optimized structure of SiGeO in a 2×2 supercell. The primitive cell of SiGeO consists of two Si atoms, two Ge atoms and two O atoms. The corresponding lattice constants of \( a \) (armchair direction) and \( b \) (zigzag direction) are 5.114 Å and 3.932 Å, respectively. To evaluate the energetic stability of SiGeO, we calculated its cohesive energy by the formula: 

\[ E_{coh} = (mE_{Si} + nE_{Ge} + kE_{O} - E_{total})/(m+n+k) \]

where \( E_{Si} \) (\( E_{Ge} \), \( E_{O} \)) and \( E_{total} \) are the energy of an isolated Si (Ge, O) atom and a primitive SiGeO cell, respectively. \( m \), \( n \), \( k \) is the number of Si (Ge, O) atom in the primitive cell. The result shows that SiGeO has a cohesive energy of 5.73 eV/atom which is higher than that of silicene (3.72 eV/atom) [8] and germanene (3.19 eV/atom) [9], indicating the robust bond feature of SiGeO.

The phonon dispersions are calculated to determine the dynamical stability of SiGeO. As shown in Figure 1b, the absence of imaginary vibrational frequency indicates SiGeO monolayer is dynamically stable. Moreover, the highest phonon mode (819 cm\(^{-1}\)) is significantly larger than that of phosphorene (450 cm\(^{-1}\)) [10] and MoS\(_2\) (500 cm\(^{-1}\)) [11], suggesting the robustness of covalent bonding characteristic in SiGeO.

![Figure 1](image-url)

Figure 1. (a) Top and side views of the atomic structure of SiGeO in a 2×2 supercell. The dashed lines indicate a unit cell. (b) Phonon dispersion of SiGeO.

3.2. Electronic properties

As shown in Figure 2a, SiGeO is a semiconductor with an indirect band gap of 1.36 eV at the PBE level of theory. The conduction band minimum (CBM) locates at Γ-Y path, while the valence band maximum (VBM) locates at the A-B path. While the SOC effect is taken into consideration, the conduction bands around the A point will move down and become the CBM. Moreover, the VBM will shift to the B-Γ path due to the SOC effect. The partial density of states (PDOS) shows that the VBM is mainly contributed by the Si-p, Ge-p and O-p orbitals (Figure 2b). The band calculated by the PBE+SOC has a narrower gap of 1.29 eV, which is closer to that of bulk silicon (1.16 eV) [12], implying that SiGeO has the potential for photovoltaic applications.
Then we explore the electronic property of SiGeO under the external strain. As presented in Figure 2c, the band gap changes of SiGeO induced by the uniaxial or biaxial strain show a parabolic behavior. Additionally, SiGeO will turn to a direct band gap semiconductor when the uniaxial compressive strain along the x direction is larger than 2%.

Figure 2. (a) Band structures of SiGeO monolayer calculated at PBE/PBE+SOC level of theory. The inset illustrate shows the Brillouin zone. (b) The PDOS calculated at the PBE+SOC level. (c) Band gap of SiGeO under the uniaxial and biaxial strain calculated at the PBE+SOC level.

To further understand the electrical properties of SiGeO monolayer, we calculated its carrier mobility. According to the deformation potential (DP) theory, the carrier mobility of 2D system can be calculated by the formula [13]:

\[
\mu = \frac{e \hbar C_{2D}}{k_B T m^* m_d E_1}
\]

where \(k_B\) is the Boltzmann constant, \(T\) (300K) is the temperature, \(m^*\) is the carrier effective mass along the transport direction, and \(m_d\) is the average effective mass calculated by \(m_d = \sqrt{m_x m_y}\). The term \(C_{2D}\) is the deformation potential constant defined as \(2(E - E_0)/S_0 = C_{2D}(\Delta l/l_0)\), where \(E_0\) (\(S_0\)) is the energy (area) of the optimized 2D structure, and \(\Delta l/l_0\) is the lattice dilation along the transport direction (Figure 3a). \(E_1\) represents the DP constant and defined as \(E_1 = \Delta V / (\Delta l/l_0)\), where \(\Delta V\) is the change of the energy of the band edge position (Figure 3b). As listed in Table 1, the electron (hole) mobilities along x and y directions are in the same order of magnitude. However, the electron mobilities are an order of magnitude larger than that of holes, mainly caused by the flat band around the VBM. The highest electron mobility is larger than that of phosphorene (1140 cm²V⁻¹s⁻¹) [14] and MoS₂ (200 cm²V⁻¹s⁻¹) [15], suggesting its potential application for nanoelectronics devices. Moreover, the great difference between the electron and hole mobility renders SiGeO is available for the electron–hole separation.
Figure 3. (a) The relationship between the energy difference and the applied strain along the x and y directions, respectively. (c) Shifts of conduction band and valence band under uniaxial strain.

Table 1. Carrier effective mass ($m^*$), DP constant ($E_1$), in-plane stiffness ($C_{2D}$) and carrier mobility ($\mu$) of SiGeO at 300K along the x and y directions, respectively. $m_0$ represents the mass of free electron.

| Direction | Carrier type | $m^*$ ($m_0$) | $E_1$ (eV) | $C_{2D}$ (N/m) | $\mu$ (cm$^2$V$^{-1}$s$^{-1}$) |
|-----------|-------------|--------------|-----------|----------------|-----------------------------|
| x         | Electron    | 0.18         | -5.00     | 79.58          | 1343.49                    |
|           | Hole        | 3.54         | 1.64      | 193.67         |                             |
| y         | Electron    | 0.47         | -2.20     | 51.79          | 1702.84                    |
|           | hole        | 0.24         | 4.08      | 301.31         |                             |

3.3. Poisson’s ratio

To evaluate the Poisson’s ratio of 2D SiGeO, we focus on the response of lattice parameters with the external uniaxial strain along x and y directions, respectively. The Poisson’s ratio can be obtained by fitting the relationship between the uniaxial strain $\varepsilon_s$ and the resultant strain $\varepsilon_{rs}$ as $\varepsilon_{rs} = -\nu_1\varepsilon_s + \nu_2\varepsilon_s^2 + \nu_3\varepsilon_s^3$, where $\nu_1$ can be viewed as the Poisson’s ratio. As Figure 4 shows, the thickness $d$ of SiGeO decreases linearly with the increment of lattice parameter of $a$ (x direction) and $b$ (y direction), respectively, suggesting an out-of-plane positive Poisson’s ratio. Yet, the in-plane parameter of $a$ (b) will increases gradually with increasing the parameter $b$ (a), suggesting an in-plane NPR. The NPR values along the x and y directions are -0.12 and -0.06, respectively, showing an anisotropic mechanical property. The largest NPR is two times of that of penta-graphene (-0.068) [16], three times of that of borophenes (-0.04) [17], and equivalent to that of Ag$_2$S (-0.12) [18].

Figure 4. The Poisson’s ratio as a function of uniaxial deformation along the (a) x and (b) y direction.

4. Conclusion

In summary, we have theoretically researched the structure, electronic and mechanical properties of 2D SiGeO. Dynamical stability of SiGeO is proved based on the phonon calculation. The band
calculation shows that SiGeO possesses an indirect band gap of 1.29 eV, and the indirect-to-direct band gap transition can be realized by the uniaxial strain. Moreover, SiGeO has high electron mobility up to $1.70 \times 10^3$ cm$^2$/V·s. Most notably, SiGeO is an auxetic material with large NPR that is higher than that of penta graphene and borophenes. We hope these properties could render SiGeO a useful material for the applications of nanodevices in the future.

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