

Surface functionalization of GeC monolayer with F and Cl: Electronic and optical properties

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ABSTRACT

In this work, we systematically investigate the electronic and optical properties of surface-functionalized GeC monolayer with F and Cl using density functional theory. Our calculations indicate that the surface functionalization of the GeC with F and C atoms leads to the disruption of the planar structure of the GeC monolayer and the surface-functionalized GeC monolayer has a low-buckling structure. At equilibrium, all four configurations of surface-functionalized GeC monolayer with F and Cl, i.e., F–GeC–F, F–GeC–Cl, Cl–GeC–F, and Cl–GeC–Cl, are direct semiconductors. Their band gaps vary from 2.839 eV to 3.175 eV which are calculated using Heyd–Scuseria–Ernzerhof (HSE) hybrid functional. Compared to the other configurations, the formation energy of F–GeC–F is the smallest, -9.097 eV, which implies that this configuration is the most likely to occur. We also used the Mulliken population analysis to estimate the internal charge distribution and transferred charge in the systems. The functionalization of the surface leads to the shifting the first optical gap of the material. The fully chlorination of GeC causes its absorption coefficient to increase significantly, up to 14.912×10^4 cm⁻¹ at the incident light energy of 13.173 eV. Besides, surface-functionalized GeC monolayer with F and Cl strongly absorbs light in the near ultraviolet region. Our calculation results provide detailed information on how to change the electronic and optical properties of monolayer GeC by surface functionalization, which has promising applications in opto-electronic devices.

1. Introduction

Since graphene was successfully exfoliated by the experiment in 2004, it has become one of the most concerned materials from the scientific community due to its excellent physical and chemical properties [1]. The success of graphene has created a revolution in

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the research and search of two-dimensional layer materials. In fact, after graphene, many two-dimensional (2D) materials have been discovered, such as silicene, phosphorene, monochalcogenides or transition metal dichalcogenides. A lot of scientists are interested in these new materials [2–10]. The biggest disadvantage of graphene is that it has zero energy. This causes many inconveniences in applying graphene in opto-electronic devices [11]. The most similar graphene-like materials of recent interest are germanene and silicene, they are semi-metals. The combination of these group IV elements can create many layer materials such as SiC, SiSe or GeC, which are expected to have many applications in new generation devices [12].

Germanium carbide (GeC) is a 2D layered material of germanene/graphene combination. In GeC, the carbon and germanium atoms are arranged in a planar hexagonal lattice (similar to a graphene sheet) with sp^2 hybridization. Monolayer GeC belongs to $P\bar{6}m2$ space group. While 2D honeycomb lattice of Ge is stable only in the low-buckling structure [13], GeC is stable in the planar hexagonal structure [14]. At equilibrium, monolayer GeC is a semiconductor with a large nature band gap of 3.370 eV [15] and one can control its band gap via strain engineering [16] or electric field [17]. Similar to other layered 2D materials, the electronic properties of GeC depend greatly on the thickness of the material, i.e., the number of layers [16].

To alter the properties seek more applicability of materials, one of the ways of recent interest is a chemically surface functionalization [18–20]. Electronic properties of the fully hydrogenated [21] and fluorinated [22] GeC monolayer have considered using first-principles calculations. They have been indicated that the surface functionalization greatly alters the electronic and magnetic properties of GeC [23]. Drissi and co-workers indicated that the full (or half) fluorination altered strongly the electronic properties, especially the band gap, of monolayer GeC [22]. Previous first-principles calculations have also shown that fully hydrogenation or fluorination significantly increases the band gap of monolayer GeC [21,22]. Previous calculations focused on structures of fully hydrogenated GeC [24] or fully fluorinated GeC [22]. There have not been many studies on structures of fully functionalization with Cl, especially, a mixture functionalization with F and Cl. Therefore, there are still many problems related to surface functionalization of monolayer GeC that need to be further studied. In the present work, we systematically investigate the electronic and optical properties of surface functionalization of monolayer GeC with F and Cl, including all four configurations of surface functionalization of F–GeC–F, F–GeC–Cl, Cl–GeC–F, and Cl–GeC–Cl, using density functional theory. We focus on changing the structural properties, energy gap, and optical properties of the monolayer GeC when it is chemically functionalized by F and Cl atoms. The charge distribution, charge transfer between atoms, and electron charge density of atoms in the surface-functionalized GeC monolayer are also investigated in this work.

2. Computational method

All calculations of this study were performed based on density functional theory (DFT) using the Quantum Espresso package [25] with generalized gradient approximation (GGA) of the Perdew–Burke–Ernzerhof (PBE) functional [26,27] and a semi-empirical DFT-D2 approach by Grimme [28] was used to consider correctly the weak van der Waals interactions which exist in material. The projector augmented-wave method was used to treat the ion–electron interaction. The energy cut-off of 500 eV is used for a plane-wave basis. The Brillouin zone is sampled by a $(15 \times 15 \times 1)$ k -mesh for simulations of electronic properties of monolayers GeC and H–GeC–H. All geometry structures were fully relaxed with the criteria for energy and force convergence is respectively 10^{-6} eV and 10^{-3} eV/Å. A vacuum space of 20 Å along a vertical direction of the monolayer surface is used to eliminate interactions between neighbour slabs.

It is well-known that PBE functional underestimates the energy gap values of insulators and semiconductors [29]. However, GW approximation [30] or Heyd–Scuseria–Ernzerhof (HSE06) hybrid functional [31] was considered as a suitable approach to solve this problem. Therefore, to accurately estimate the energy gap of the surface-functionalized GeC monolayer, in this study we use also the HSE06 hybrid functional to calculate its electronic structure.

3. Results and discussion

Monolayer GeC at equilibrium consists of two elements of Ge and C in the planar honeycomb lattice, the buckling constant $\Delta_h = 0$ and the lattice constant of pure GeC at equilibrium is 3.253 Å. In this work, we consider four configurations of surface functionalization of GeC with F and Cl. These are F–GeC–F, F–GeC–Cl, Cl–GeC–F, and Cl–GeC–Cl. Optimized atomic structures of pure GeC monolayer and surface functionalized GeC are shown in Fig. 1. Our calculations demonstrated that surface functionalization has caused the planar structure (similar to graphene) of GeC monolayer to be broken. At the equilibrium, all four configurations of surface functionalization of GeC monolayer with F and Cl have a low-buckled structure with a buckling constant Δ_h varying from 0.489 Å to 0.627 Å. Our calculated results are well consistent with previous DFT results [22]. Compared to pure GeC monolayer, surface functionalization leads an increase in the lattice constant of GeC. In four configurations of surface-functionalized GeC with F and Cl, the lattice constant of the Cl–GeC–Cl is largest, 3.395 Å. Besides, the Ge–C bond length in monolayer GeC is significantly changed when the surface is chemically functionalized. The structural parameters of configurations of GeC with surface functionalization are also listed in Table 1. As shown in Table 1, structurally, the Ge–C bond length in the F–GeC–F is the shortest compared to the other configurations. Besides the lengths of the bond between Ge (or C) and F atoms is smaller than that of the bond between Ge (or C) and Cl atoms. Also, the $d_{\text{Ge-Cl}}$ is much larger than $d_{\text{Ge-F}}$ in all configurations.

To check the possibility of adsorption F and Cl atoms on the GeC monolayer, we calculated the formation energy via the following expression

$$E_{ads} = E_{\text{X1-GeC-X2}} - (E_{\text{GeC}} + E_{\text{X1}} + E_{\text{X2}}), \quad (1)$$

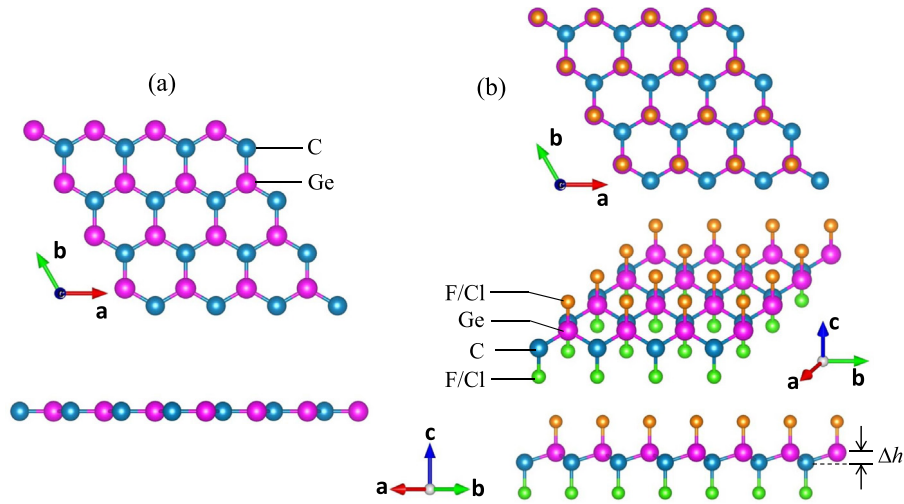


Fig. 1. Different views of optimized atomic structure of (4 × 4) GeC (a) and surface-functionalized GeC monolayer with F and Cl (b).

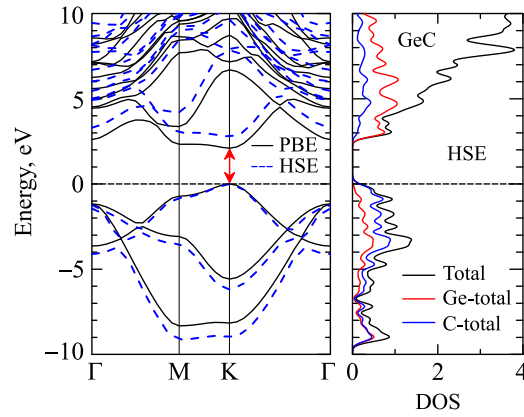


Fig. 2. Band structure and density of states (DOS) of pure GeC monolayer.

Table 1

Lattice constants a (in Å), bond lengths between atoms d (in Å), buckling constant Δh (in Å), formation energy E_{ads} (in eV), and band gaps by PBE functional E_g^{PBE} and HSE06 hybrid functional E_g^{HSE} (in eV) of surface functionalized GeC with F and Cl at equilibrium.

| Configuration | a | d_{Ge-C} | d_{Ge-F} | d_{Ge-Cl} | d_{C-F} | d_{C-Cl} | Δh | E_{ads} | E_g^{PBE} | E_g^{HSE} |
|---------------|-------|------------|------------|-------------|-----------|------------|------------|-----------|-------------|-------------|
| GeC | 3.253 | 1.878 | – | – | – | – | 0 | – | 2.095 | 2.761 |
| F–GeC–F | 3.260 | 1.952 | 1.684 | – | 1.420 | – | 0.516 | –9.097 | 1.645 | 2.839 |
| F–GeC–Cl | 3.279 | 1.955 | 1.696 | – | – | 1.821 | 0.489 | –7.089 | 2.024 | 3.175 |
| Cl–GeC–F | 3.298 | 2.005 | – | 2.148 | 1.428 | – | 0.627 | –7.021 | 1.909 | 3.046 |
| Cl–GeC–Cl | 3.395 | 2.052 | – | 2.155 | – | 1.828 | 0.606 | –5.448 | 1.885 | 2.926 |

where X1 and X2 stand for F or Cl atoms (X1 = F, Cl; X2 = F, Cl), E_{GeC} and $E_{X1-GeC-X2}$ are respectively the energies of pure GeC and surface functionalized GeC with X1 and/or X2 atoms. E_{X1} and E_{X2} are energies of X1 and X2 atoms which is estimated in the gas form. Our calculated results for the formation energy E_{ads} of all four configurations of GeC with surface functionalization are also shown in Table 1. From Table 1 we can see that the formation energies of all four configurations are negative. This implies that the adsorption of F and Cl atoms on the GeC monolayer is chemically possible for all four configurations. However, the formation energy for different configurations is different. The formation energy of the F–GeC–F is the lowest. This proves that chemical adsorption on F–GeC–F configuration is most likely to occur.

We next investigate the electronic properties of the surface-functionalized GeC. Firstly, we calculate the band structure and density of states (DOS) of pure GeC monolayer at PBE and HSE06 level as shown in Fig. 2. At equilibrium, monolayer GeC is a semiconductor with a direct gap opening at K-point of the Brillouin zone. The calculated band gap of pure GeC is 2.095 eV at the PBE level. It has been shown that by using the HSE06 hybrid functional, we can get the value of the energy gap more

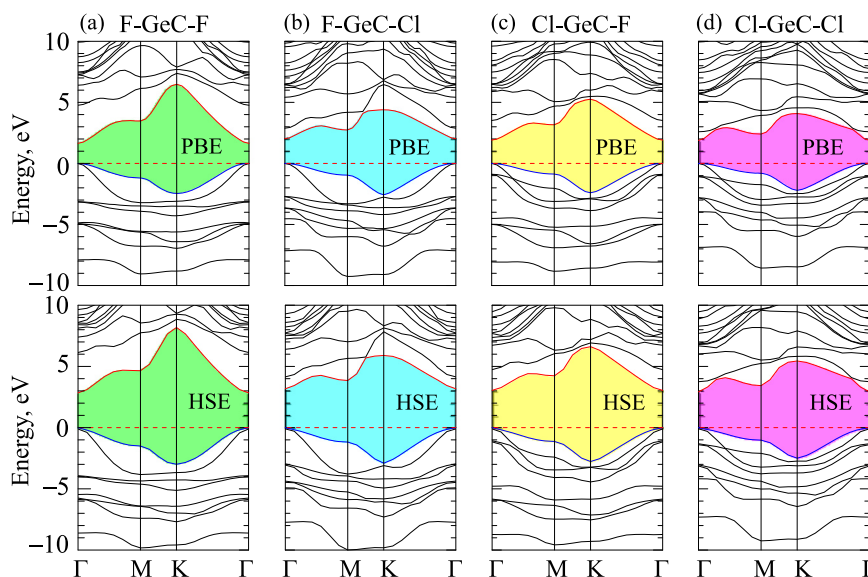


Fig. 3. Band structure of surface functionalized GeC monolayer: (a) F-GeC-F, (b) F-GeC-Cl, (c) Cl-GeC-F, and (d) Cl-GeC-Cl.

accurately. The band gap of pure GeC at HSE06 level is 2.761 eV, which is larger than that by using PBE functional. From Fig. 2, we see that the only significant difference when calculating at PBE and HSE06 level is the band gap value. The DOS calculation results show that while the orbital of Ge atom has a large contribution to the formation of the conduction band, the contribution to the valence band of orbitals of C atoms is somewhat more prominent than that of orbitals of Ge atoms. The electronic band structures of four configurations of surface-functionalized GeC with F and Cl are shown in Fig. 3. Our calculated results indicate that monolayer GeC with surface functionalization of all four configurations are semiconductors with a direct band gap. However, surface functionalization significantly changes the band structure of the GeC monolayer. In the pure GeC monolayer, the valence band maximum (VBM) and the conduction band minimum (CBM) are located at the point K. Surface functionalization causes both the VBM and CBM to move from the K-point (in the pure GeC monolayer) to Γ -point G in the Brillouin zone.

The surface functionalization alters the band structure of all four configurations. The consequence of this is that the band gap also changes. In all our calculations, the Fermi level is set at zero, $E_F = 0$. Interestingly, the VBM of all configurations is very close to the Fermi level. Then, the band gap is determined by the energy value of the CBM. In four configurations of surface-functionalized GeC, the band gap of F-GeC-Cl is largest. The band gaps of surface-functionalized GeC monolayer with F and Cl atoms are shown in Fig. 4. Our HSE06 calculations indicate that the band gap of configurations with functionalization with both F and Cl atoms (i.e., F-GeC-Cl or Cl-GeC-F) is larger than that of fully fluorinated F-GeC-F or fully chlorinated Cl-GeC-Cl.

Focusing on the contribution of atomic orbitals to electronic bands, we calculate the partial density of states (PDOS) as shown in Fig. 5. Our calculated results demonstrate that p - and s -orbitals of F and Cl atoms from both sides of functionalized GeC have a significant contribution to the conduction band in all configurations. However, the contribution of these orbitals to the valence band is quite small. Also, the electronic bands of surface-functionalized GeC monolayer are mainly contributed from C- p , Ge- s , and Ge- p orbitals.

Mulliken population analysis [32] was used to estimate the internal charge distribution and transferred charge between monolayer GeC and functionalization species in the surface-functionalized GeC monolayer. We estimated the charge distribution for both pure GeC monolayer and all four configurations of surface-functionalized GeC monolayer as listed in Table 2. From Table 2 we can see that in all four configurations, the charge has transferred from the monolayer GeC to the atoms of functionalization species F and/or Cl. The maximum transferred charge from monolayer GeC to the functionalization species is +0.95 ($\sim 0.59e$) in the case of fully fluorinated GeC monolayer F-GeC-F. Although the charge is transferred from monolayer GeC to the functionalization species, the amount of charge transferred from Ge and C to the functionalization species is different, even in the cases of fully fluorinated F-GeC-F or fully chlorinated Cl-GeC-Cl. Our calculations show that the total charges of Ge and C in F-GeC-F are +1.54 and -0.59 , respectively. This means that the amount of transferred charge from Ge to the functionalization species is less than that from C to the functionalization species. In contrast, in F-GeC-Cl, the functionalization species gets more charge from Ge atom than from C atom. More specifically, in the Cl-GeC-F and Cl-GeC-Cl configurations, while a large amount of charge is transferred from C to the functionalization species, a small amount of charge is transferred to Ge atom. However, in both cases, the charge is still transferred from the monolayer GeC to the functionalization species as above-mentioned. The difference in the charge transfer process between atoms in the surface-functionalized GeC monolayer is explained by the difference in electronegativity of the atoms, especially the electronegativity of germanium is lower than that of carbon. The charge transfer between the GeC monolayer and the functionalization species in the case of the surface-functionalized GeC monolayer with F and Cl is quite different from the case of fully hydrogenated GeC monolayer, where the charge is transferred from hydrogen atoms to monolayer GeC [24].

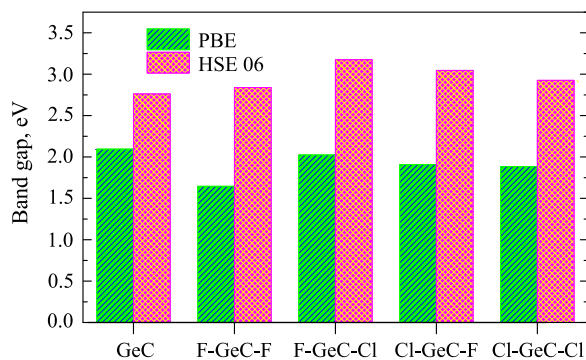


Fig. 4. Calculated band gap of surface functionalized GeC monolayer at the PBE and HSE06 levels.

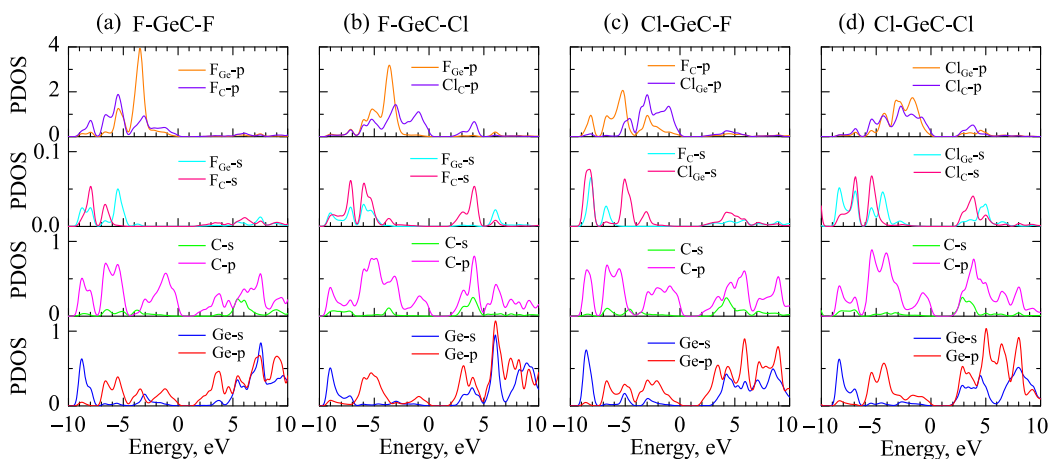


Fig. 5. Partial density of states (PDOS) of surface functionalized GeC monolayer: (a) F-GeC-F, (b) F-GeC-Cl, (c) Cl-GeC-F, and (d) Cl-GeC-Cl. $F(Cl)_{Ge}$ and $F(Cl)_C$ stand for F(Cl) bonded directly to Ge atom and C atom, respectively.

Table 2

Mulliken population analysis of the internal charge distribution in pure monolayer GeC and surface functionalized GeC monolayer. The charge transfer between GeC and species is shown in the last column. $F(Cl)_{Ge}$ and $F(Cl)_C$ stand for F(Cl) bonded directly to Ge atom and C atom, respectively.

| Configuration | | s | p | Total | Charge | Transferred charge |
|---------------|-----------|------|------|-------|--------|--------------------|
| GeC | Ge | 1.06 | 1.79 | 2.85 | +1.15 | – |
| | C | 1.42 | 3.72 | 5.15 | –1.15 | |
| F-GeC-F | F_{Ge} | 1.97 | 5.62 | 7.58 | –0.58 | +0.95 |
| | Ge | 1.02 | 1.44 | 2.46 | +1.54 | |
| | C | 1.38 | 3.21 | 4.59 | –0.59 | |
| | F_C | 1.95 | 5.42 | 7.37 | –0.37 | |
| F-GeC-Cl | F_{Ge} | 1.97 | 5.6 | 7.57 | –0.57 | +0.64 |
| | Ge | 1.00 | 1.44 | 2.45 | +1.55 | |
| | C | 1.46 | 3.45 | 4.91 | –0.91 | |
| | Cl_C | 1.93 | 5.14 | 7.07 | –0.07 | |
| Cl-GeC-F | Cl_{Ge} | 1.95 | 5.36 | 7.31 | –0.31 | +0.66 |
| | Ge | 1.16 | 1.73 | 2.88 | +1.12 | |
| | C | 1.37 | 3.09 | 4.46 | –0.46 | |
| | F_C | 1.95 | 5.40 | 7.35 | –0.35 | |
| Cl-GeC-Cl | Cl_{Ge} | 1.95 | 5.36 | 7.30 | –0.30 | +0.36 |
| | Ge | 1.18 | 1.70 | 2.88 | +1.12 | |
| | C | 1.47 | 3.29 | 4.76 | –0.76 | |
| | Cl_C | 1.93 | 5.12 | 7.05 | –0.06 | |

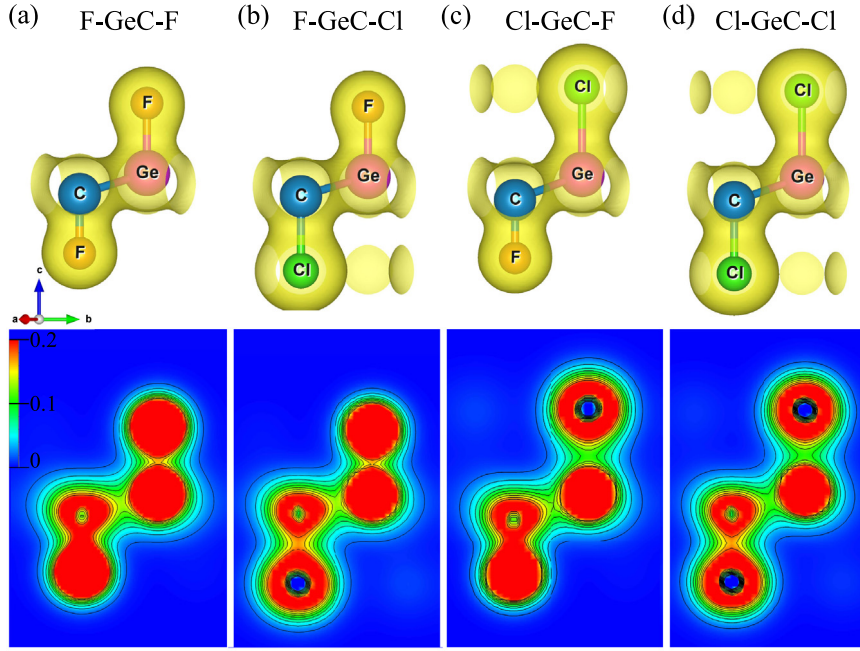


Fig. 6. Charge density in surface functionalized GeC monolayer with F and Cl atoms: (a) F-GeC-F, (b) F-GeC-Cl, (c) Cl-GeC-F, and (d) Cl-GeC-Cl. The electron densities in contour form (bottom panel) is in e/Bohr^3 unit.

In Fig. 6, we show the calculated results for the electron charge densities of atoms in surface-functionalized GeC monolayer with F and Cl atoms. Our calculations indicate that, in F-GeC-F as shown in Fig. 6(a), the spatial ranges between the atom pairs of Ge-F, Ge-C and C-F correspond to the electron density of $0.16 e/\text{Bohr}^3$, $0.12 e/\text{Bohr}^3$, and $0.18 e/\text{Bohr}^3$, respectively. In the second configuration of F-GeC-Cl, the electron densities corresponding to Ge-F, Ge-C atom pairs is equal to the electron densities for those atom pairs in the case of F-GeC-Cl configuration, i.e., $0.12 e/\text{Bohr}^3$ for Ge-F pair and $0.18 e/\text{Bohr}^3$ for C-Cl pair. The electron densities for the C-Cl atom pair in the F-GeC-Cl is $0.16 e/\text{Bohr}^3$. The electron densities for the Ge-Cl and Ge-C in the Cl-GeC-F and Cl-GeC-Cl are the same, they are both equal to $0.1 e/\text{Bohr}^3$. The electron densities for C-F atom pair in the Cl-GeC-F and form C-Cl atom pair in the Cl-GeC-Cl are $0.18 e/\text{Bohr}^3$ and $0.16 e/\text{Bohr}^3$, respectively. These spatial ranges are created by the orbital overlap of Ge and C atoms with F and Cl atoms that depict the covalent constituent of the Ge-C, Ge-F(Cl), and C-F(Cl) bonds in F(Cl)-GeC-F(Cl) crystal. As shown in Fig. 6, Ge(C) and F(Cl) atoms are joined by the charge distribution, which is a common particularity of a covalent bond.

For optical properties, we concentrate to the dielectric function $\epsilon(\omega)$ of materials which can be expressed as $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$. The imaginary part $\epsilon_2(\omega)$ is usually estimated first by sum of the occupied-unoccupied transitions. After that, we can receive the real part $\epsilon_1(\omega)$ through the Kramer-Kronig transformation [33,34]. The imaginary part $\epsilon_2(\omega)$ of the dielectric function $\epsilon(\omega)$ can be expressed as the following [33,34]:

$$\epsilon_2^{ij}(\omega) = \frac{4\pi^2 e^2}{Vm^2\omega^2} \sum_{\mathbf{k}n\sigma} \langle \mathbf{k}n\sigma | p_i | \mathbf{k}n'\sigma \rangle \langle \mathbf{k}n'\sigma | p_j | \mathbf{k}n\sigma \rangle \times f_{\mathbf{k}n}(1 - f_{\mathbf{k}n'})\delta(E_{\mathbf{k}n'} - E_{\mathbf{k}n} - \hbar\omega), \quad (2)$$

where ω is the angular frequency of the electromagnetic irradiation, $m(e)$ is the mass (charge) of electron, \mathbf{p} is the momentum operator, $|\mathbf{k}n\sigma\rangle$ term stands for the wave function of the crystal corresponding to energy $E_{\mathbf{k}n}$. \mathbf{k} is the wavevector and $f_{\mathbf{k}n}$ is the Fermi distribution. The absorption coefficient $\alpha(\omega)$ can be calculated via the dielectric function $\epsilon(\omega)$ as the followings [34]

$$\alpha(\omega) = \frac{\sqrt{2}\omega}{c} \left[\sqrt{\epsilon_1^2(\omega) + \epsilon_2^2(\omega)} - \epsilon_1(\omega) \right]^{1/2}. \quad (3)$$

Calculated dielectric function of surface-functionalized GeC monolayer with F and Cl atoms is shown in Fig. 7. We consider the optical characteristics of functionalized GeC under parallel polarization incident light with energy from 0 to 30 eV. Noted that the imaginary part of the dielectric function is correlated to the absorption coefficient $\alpha(\omega)$ directly. Our calculations show that the first optical gap of pure GeC is at 2.872 eV. The surface functionalization significantly changes the optical characteristics of the monolayer GeC. Fig. 7(b) demonstrate that while only first optical gap of the F-GeC-F moved to a low energy region (the first optical gap of F-GeC-F is at 2.136 eV), the rest of the configurations moved to a high energy domain when the monolayer is functionalized with F and Cl atoms. The first optical gap of F-GeC-Cl, Cl-GeC-F, and Cl-GeC-Cl configurations is at 4.021 eV, 5.275 eV, and 3.441 eV,

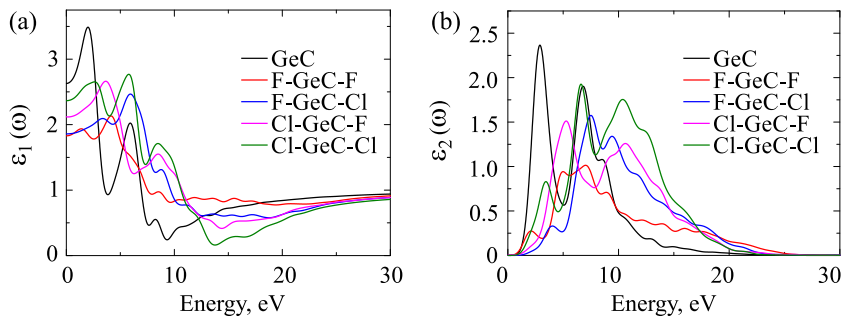


Fig. 7. Real part $\varepsilon_1(\omega)$ (a) and imaginary part $\varepsilon_2(\omega)$ (b) of dielectric function of surface functionalized GeC monolayer.

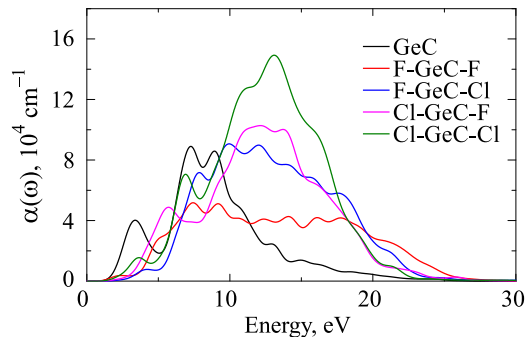


Fig. 8. Absorption coefficient $\alpha(\omega)$ of surface functionalized GeC monolayer.

respectively. Hence, only the F-GeC-F monolayer possesses the first optical gap in the visible light range. Absorption coefficient $\alpha(\omega)$ of surface-functionalized GeC monolayer is shown in Fig. 8. Our calculations demonstrate that, compared to the pure GeC monolayer, the full functionalization of GeC monolayer with F greatly reduces the absorption coefficient of the monolayer. The maximum of the absorption coefficient of pure GeC monolayer is $\alpha(\omega)_{max}^{GeC} = 8.900 \times 10^4 \text{ cm}^{-1}$ at incident light energy of 7.272 eV which compared to maximum of the absorption coefficient of the F-GeC-F monolayer being $\alpha(\omega)_{max}^{F-GeC-F} = 5.170 \times 10^4 \text{ cm}^{-1}$ at the incident light energy of 7.374 eV. In contrast, the fully functionalization by Cl (Cl-GeC-Cl) significantly increases the absorption coefficient of the monolayer. The maximum of the absorption coefficient of the Cl-GeC-Cl monolayer is $\alpha(\omega)_{max}^{Cl-GeC-Cl} = 14.912 \times 10^4 \text{ cm}^{-1}$ at the incident light energy of 13.173 eV. From Fig. 8 we see that the surface-functionalized GeC monolayer strongly absorbs light with energies from about 7 eV to 16 eV, i.e., light in the near-ultraviolet region.

4. Conclusion

We have systematically considered the electronic and optical properties of surface-functionalized GeC monolayer with F and Cl using density functional theory. Our DFT calculations indicated that the formation energies of all configurations of monolayer GeC chemically functionalized with F and Cl are negative, which implies that all configurations can occur. At equilibrium, all four configurations of surface functionalization of monolayer GeC with F and Cl are direct semiconductors. Using Milliken population analysis, our calculations indicated that, in all four configurations of surface-functionalized GeC monolayer with F and Cl, the charge transfer from the monolayer GeC to the functionalization species was observed. The amount of transferred charge between atoms is different because they have different electronegativity. Surface functionalization significantly changes the energy gap of the GeC monolayer and increases the absorption coefficient in some configurations. With a large band gap and sand able to highly absorb the light in the near ultraviolet region, monolayer GeC chemically functionalized with F and Cl, especially F-GeC-F, maybe a potential candidate for applications in optoelectronic devices, such as ultraviolet photodetectors.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

Tuan V. Vu: Conceptualization, Methodology, Software, Investigation, Formal analysis, Funding acquisition. **Nguyen Thi Tuyet Anh:** Conceptualization, Methodology, Software, Investigation, Formal analysis. **Duy Phu Tran:** Investigation, Validation. **D.M. Hoat:** Investigation, Validation. **Nguyen T.T. Binh:** Methodology, Writing — review & editing, Supervision. **Hien D. Tong:** Investigation, Validation. **Bui D. Hoi:** Methodology, Writing — review & editing. **Chuong V. Nguyen:** Conceptualization, Methodology, Software, Investigation, Formal analysis, Writing — review & editing. **Huynh V. Phuc:** Methodology, Writing — review & editing. **Nguyen N. Hieu:** Investigation, Validation, Supervision, Writing — review & editing.

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