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Effect of Shear Deformation on Electrical and Optical Properties of Graphene Adsorbed Si Atom

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Research Article

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ABSTRACT

The first-principles method based on the density functional theory (DFT) studies the electrical and optical properties of the graphene-adsorption Si atom system by shear deformation. Including adsorption energy, energy band, charge transfer, light absorption coefficient and reflectivity. The results of the study show that when the Si atom is adsorbed on the graphene B site, the absolute value of the adsorption energy is the largest and the system is the most stable. The stability of graphene-adsorption Si atoms increases with shear deformation. The degree of shear has little effect on the stability of the system. Adsorption of Si atom can open the graphene band gap, which changes graphene from a metal to a semiconductor. When the shear deformation is greater than 3%, the graphene geometry is distorted. The band gap of the adsorption system first increases and then decreases as the shear deformation increases. The adsorption systems are all indirect band gaps with band gap values less than 0.3 eV, corresponding to narrow band gap semiconductors. The number of charge populations indicates that covalent bonds and ionic bonds coexist in the adsorption system. The adsorption of Si atom increases the charge transfer between Si and C, but the degree of shear has little effect on charge transfer. In the study of optical properties, the absorption coefficient and reflectance of the shear deformation-induced adsorption system were reduced compared with the shear-induced adsorption system, and the blue-shift phenomenon appeared with the increase of the shear deformation.

INTRODUCTION

Since the discovery of graphene by British scientists such as Novoselov et al. [1-4], it has caused widespread concern in scientific research. Graphene is a planar two-dimensional carbon structure with a unique sp^2 hybrid orbital and therefore has many special properties. Especially in terms of physical properties [5,6], such as high thermal conductivity, anomalous quantum Hall effect [7], electron mobility [8], massless Dirac fermions [9], and broad-band light absorption, etc. Promote the extensive application of graphene in the field of nanoelectronics and optical devices [10]. The two-dimensional planar structure of graphene has a large specific surface area and is almost completely transparent. It has great potential for development and research in the optical field [11-15].

Dai et al. [16] studied the adsorption of Si on graphene by vacancy on the basis of density functional theory. The results of the study indicate that Si atom interact with C atom when Si is adsorbed on vacant graphene. The spin properties of C atom in graphene changes, which increases the adsorption properties of graphene. Hu et al. [17] studied the effect of N, Al, and P doping on the adsorption of Si on graphene using a first-principle method. Al, P doping enhances the adsorption of Si on graphene. N doping has little effect on the adsorption of Si on graphene. The system of Si-adsorbed N-doped graphene and P-doped graphene has magnetic properties. The Si-adsorbed Al-doped graphene system has a magnetic moment of 0 and does not exhibit magnetic properties.

Since the adsorption of Si atoms can open the graphene bandgap and change its properties, such studies have been limited. In addition, the electrical and optical studies of graphene-adsorbed Si atom systems under shear deformation are also rarely reported. In this paper, Si atom was adsorbed on 4 × 4 graphene based on the first-principles method, and then shear deformation

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was applied to observe the structural stability, electronic structure and optical properties of the adsorption system.

Calculation method and physical model

In this paper, the CASTEP quantum mechanics module based on the first-principles DFT plane wave pseudopotential method in MS8.0 is used to simulate the shear deformation of Si atom system adsorbed on grapheme [18]. The energy exchange correlation function uses the Perdew-Burke-Ernzerhof (PBE) functional form in the generalized gradient approximation (GGA) [19,20]. In the inverted lattice space, the cutoff can be taken as 350 eV. The Monkhorst-Pack special K-point sampling method was used for integral calculation in the Brillouin zone. In order to reduce the number of planar wave base groups in the system, the Vanderbilt super soft potential is used [21,22]. The energy convergence accuracy is not less than 2.0×10^{-5} eV/atom. The self-consistent field convergence iteration accuracy is set to 2.0×10^{-6} eV. The K-point is set to 6 × 6 × 1 and the BFG Soptimization algorithm is used [23,24]. When calculating, the X, Y plane is in the graphene plane, and the Z direction is perpendicular to the graphene plane. The thickness of the vacuum layer is 15 Å. At this time, the interlayer interaction force is negligible.

Figure 1a is a 4 × 4 × 1 intrinsic graphene cell of 32 atoms in total. Three highly symmetrical adsorption sites are considered when graphene adsorbs Si atom, see **Figure 1b**. In the H position, Si atom is adsorbed in the center of the C ring. At the T site, the Si atom is adsorbed directly above the C atom. In position B, Si atom is adsorbed at the C-C bond center

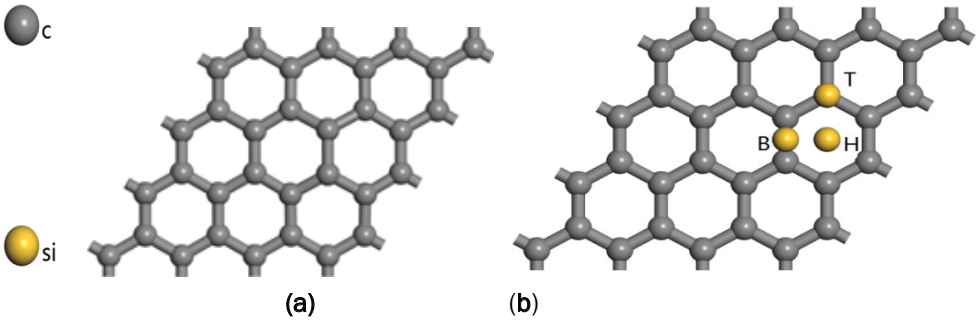

Figure 1. Graphene model: (**a**) Intrinsic graphene model; (**b**) Graphene adsorption Si atom model

Figure 2 shows the geometric optimization model of graphene after shear deformation. The degree of graphene shear is characterized herein as the ratio of lattice constants, ie, the distance that a row of atoms of a graphene cell moves relative to another row. Take 5% of the shear shape as an example. The specific operation is: move the blue chain to the right by 5%, fix it, and then move the yellow chain to the left by 5% and fix it to optimize the structure.

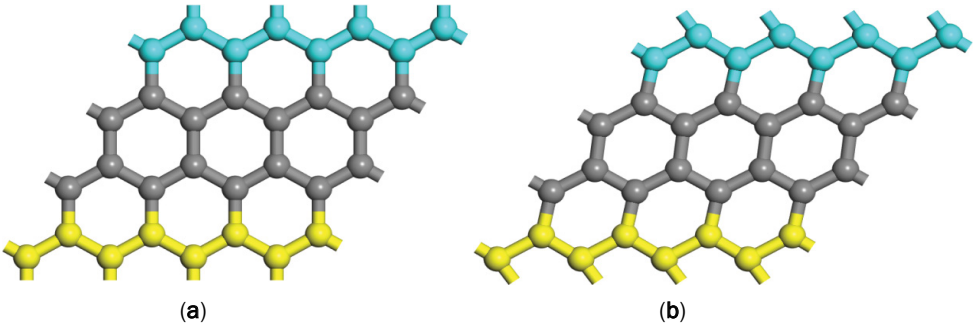

Figure 2. Shear model (**a**) 0% graphene model; (**b**) 5% shear model

Figure 2 In order to study the structural stability of Si-adsorbed graphene at different shear levels, the adsorption energy of different degree of shear deformation system was calculated. Given the definition of adsorption energy, as follows [24]:

$$E_{ad}=E_{gra\text{-}si}-E_{gra}-E_{si} \quad (1)$$

In the formula, E_{gra} is the energy of graphene or shear graphene, E_{si} is the energy of Si atom, and $E_{gra\text{-}si}$ is the energy of the adsorption system. According to the formula (1), the larger the absolute value of the adsorption energy, the more stable the structure.

RESULTS AND DISCUSSION

Structural optimization and structural stability

In this paper, the auto-optimization method is used to calculate the adsorption energy of three high-symmetry positions of graphene adsorbing Si atoms. It can be seen from **Table 1** that when Si atom is adsorbed to the B-site of graphene, the adsorption

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energy of the system is absolutely self-maximizing and the system is the most stable. The adsorption energy was calculated by the formula (1) to be -1.25 eV. At this time, the C-C bond length was 1.43 nm, and the C-Si bond length was 2.09 nm. The C-Si bond length is longer than the C-C bond length, indicating that the adsorption of Si atoms by the graphene leads to the interaction between the C atoms and the Si atoms in the graphene, so that the graphene structure undergoes a certain degree of change. As can be seen from **Figure 3**, the C atom adjacent to the Si atom is pulled up. Next, this paper will analyze the interaction between C and Si under shear deformation of graphene-adsorbed Si atom.

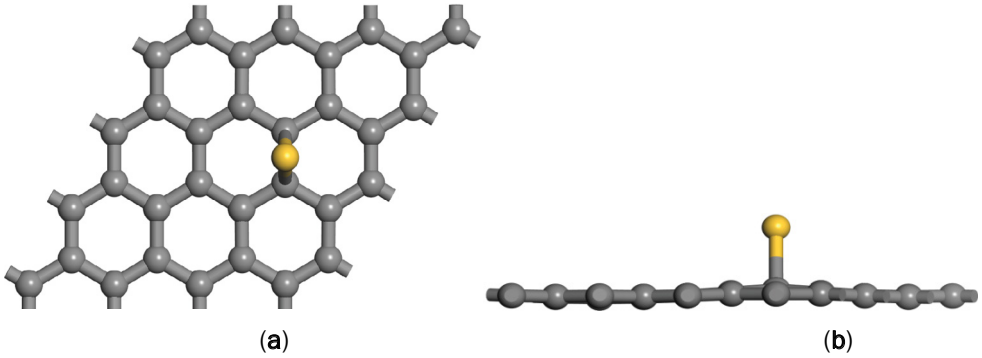

Figure 3. Optimized geometry of Si atom adsorbed on graphene (**a**) Top view; (**b**) Front view

Table 1. Adsorption energy of Si atoms adsorbed on graphene at different positions

Adsorption position	T position	B position	H position
Adsorption energy (eV)	-1.13	-0.65	-1.25

Table 2 shows the adsorption energy and adsorption height of Si atoms adsorbed on graphene under different shear deformations. When the shear deformation becomes 0%-1%, the adsorption energy of the adsorption system decreases as the shear deformation increases. When the shear deformation becomes 1%-5%, the adsorption energy of the adsorption system increases with the shear deformation. It can be seen that the stability of the adsorption system decreases first and then increases with the shear deformation. When the shear deformation is 1%, the adsorption energy of the system is at least -1.20 eV. When the shear deformation becomes 5%, the maximum adsorption energy of the system is -1.53 eV. Compared with the adsorption energy of un-sheared system -1.25 eV, there is no significant difference. With the increase of shear deformation, there is little difference between the adsorption height of the adsorption system. It can be concluded that the degree of shear has little effect on the stability of the atomic structure of Si adsorbed on graphene.

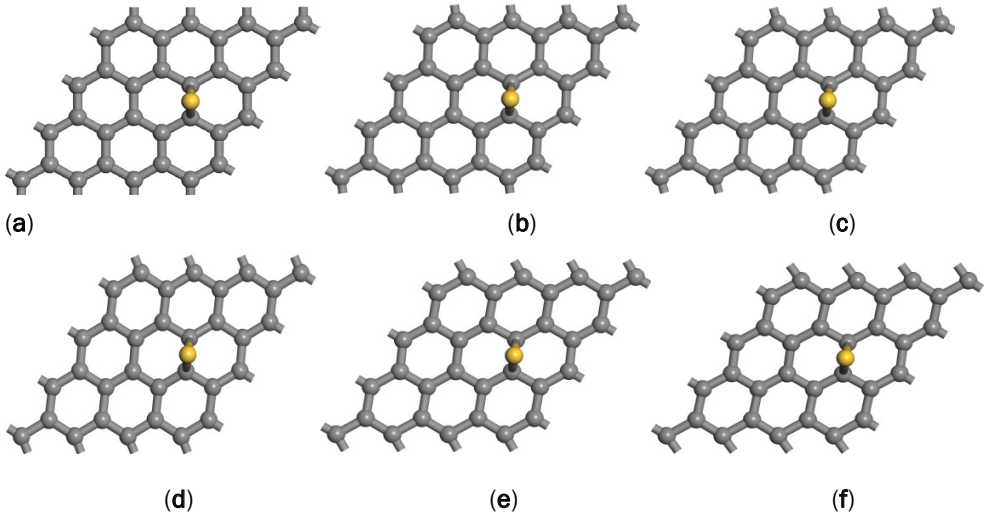

Figure 4. Geometrically optimized graphs **(a)-(f)** are top views of the graphene-adsorption Si system when the shear deformation becomes 0%, 1%, 2%, 3%, 4%, 5%

Figure 4 shows the structural optimization model for the adsorption of Si atoms on graphene at 0%, 1%, 2%, 3%, 4%, and 5% shear deformation. From **Figure 4**, it can be seen that when the shear deformation is less than 3%, the geometric structure of the adsorption system is not greatly distorted. When the shear deformation is greater than 3%, the geometric structure of the adsorption system is distorted, but the planar structure of the adsorption system is still hexagonal.

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Table 2. Adsorption energy and adsorption height of Si atom system adsorbed by graphene under different shear deformations.

Shear deformation	0%	1%	2%	3%	4%	5%
Adsorption energy (eV)	-1.25	-1.2	-1.23	-1.28	-1.38	-1.53
Adsorption height (Å)						
	2.09	2.08	2.07	2.06	2.09	2.07

Graphene adsorption Si atom system electronic structure

Charge population: In order to analyze the type of bonding between C and Si atoms and the bonding strength, **Table 3** shows the charge population of the system.

Table 3: Atomic populations of C and Si atoms under different shear deformations

Shear deformation		0%	1%	2%	3%	4%
C	Max	0	0.01	0.02	0.01	0
	Min	-0.18	-0.18	-0.19	-0.19	-0.16
Si		0.48	0.49	0.5	0.5	0.52

It can be seen from **Table 3** that the intrinsic graphene has no charge on the C atom. After applying shear deformation to the Si atom-absorbing graphene system, the Si atoms lose their electrons and carry a positive charge of 0.48-0.59. The charge on the C atom has both positive and negative charges. Electrons are transferred from Si atoms to C atoms. The nuclear electronic arrangement of atoms is C1s22s22p2, Si1s22s22p63s23p2, respectively. Atomic to full-shell structure, Si atom volatile electrons, C atom can lose electrons and electrons. Intrinsic graphene systems have only covalent bonds between C atoms. The adsorption of Si atom by graphene increases the charge transfer between the atoms in the graphene, resulting in the formation of an ionic bond between the C atom and the Si atom in the system, ie, the covalent bond and the ionic bond coexist in the graphene-adsorbed Si atom system. After the shear deformation is applied, the electron transfer between the C and Si atoms fluctuates insignificantly, which is consistent with the fact that the shear degree mentioned above has a weak influence on the stability of the adsorption system.

Effect of shear deformation on the atomic band structure of graphite-adsorption si

In this paper, the energy bands of intrinsic graphene and graphene adsorption Si atom systems are calculated and analyzed using the CASTEP module in MS8.0. From **Figure 5**, it can be seen that the Fermi level of the intrinsic graphene passes through the Dirac point. Graphene corresponds to metalloid properties. After the graphene adsorbs Si atoms, the bandgap is opened because the adsorption of Si atoms increases the electron transfer between the C atom and the Si atom. At this time, the electrons jump from the valence band to the conduction band, resulting in high energy in the conduction band. In the valence band, a bandgap is formed and the graphene is changed from a metalloid to a semiconductor.

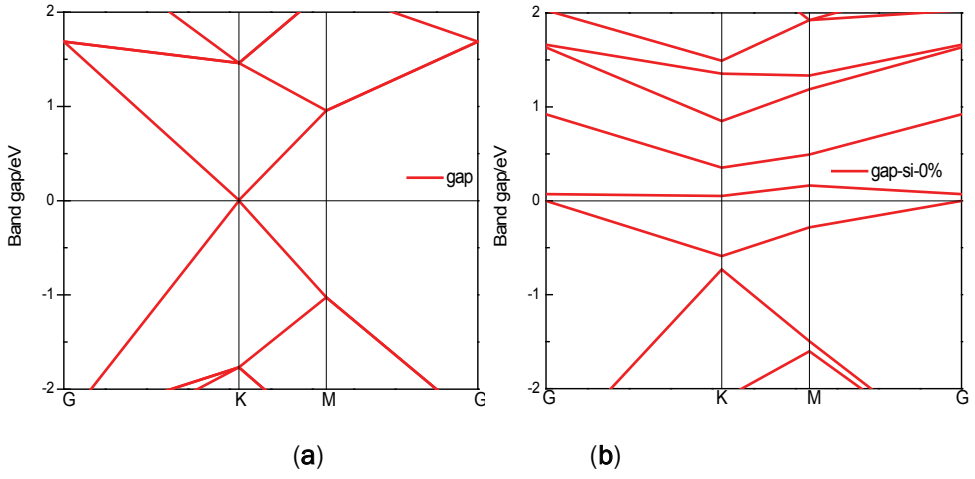

Figure 5: (**a**) Intrinsic graphene band; (**b**) Graphene adsorption Si atomic band

Figure 6 shows the atomic energy band structure of Si adsorbed on graphene with 0%, 1%, 2%, 3%, 4%, and 5% shear strain. **Table 3** shows the bandgap values of Si atom adsorbed on intrinsic graphene and graphene at different shear deformations. From **Figure 6 and Table 3**, it can be seen that when the shear shape changes to 0%, the graphene-adsorbed Si atom can generate a tiny band gap with a bandgap value of 0.051 eV. When the shear deformation becomes 0%-4%, the bandgap of the adsorption system increases with the shear deformation. When the shearing deformation is 4%, the band gap value of the adsorption system is a maximum of 0.293 eV. The bandgap of the intrinsic system increases with the increase of the shear deformation when the shear deformation is in the range of 0%-4%. When the shear deformation becomes 4%, the band gap of the intrinsic system is a maximum of 0.707 eV. Compared with the intrinsic system, the adsorption system can be seen that the Si atom adsorption can

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inhibit the shear deformation and open the graphene bandgap. When the shear deformation becomes 5%, the bandgap of the adsorption system decreases, which indicates that the shear deformation can affect the interaction between C and Si atoms in the adsorption system. It can be seen from **Table 4** that the band gap values of the adsorption systems are all less than 0.3 eV, and therefore correspond to narrow band gap semiconductors.

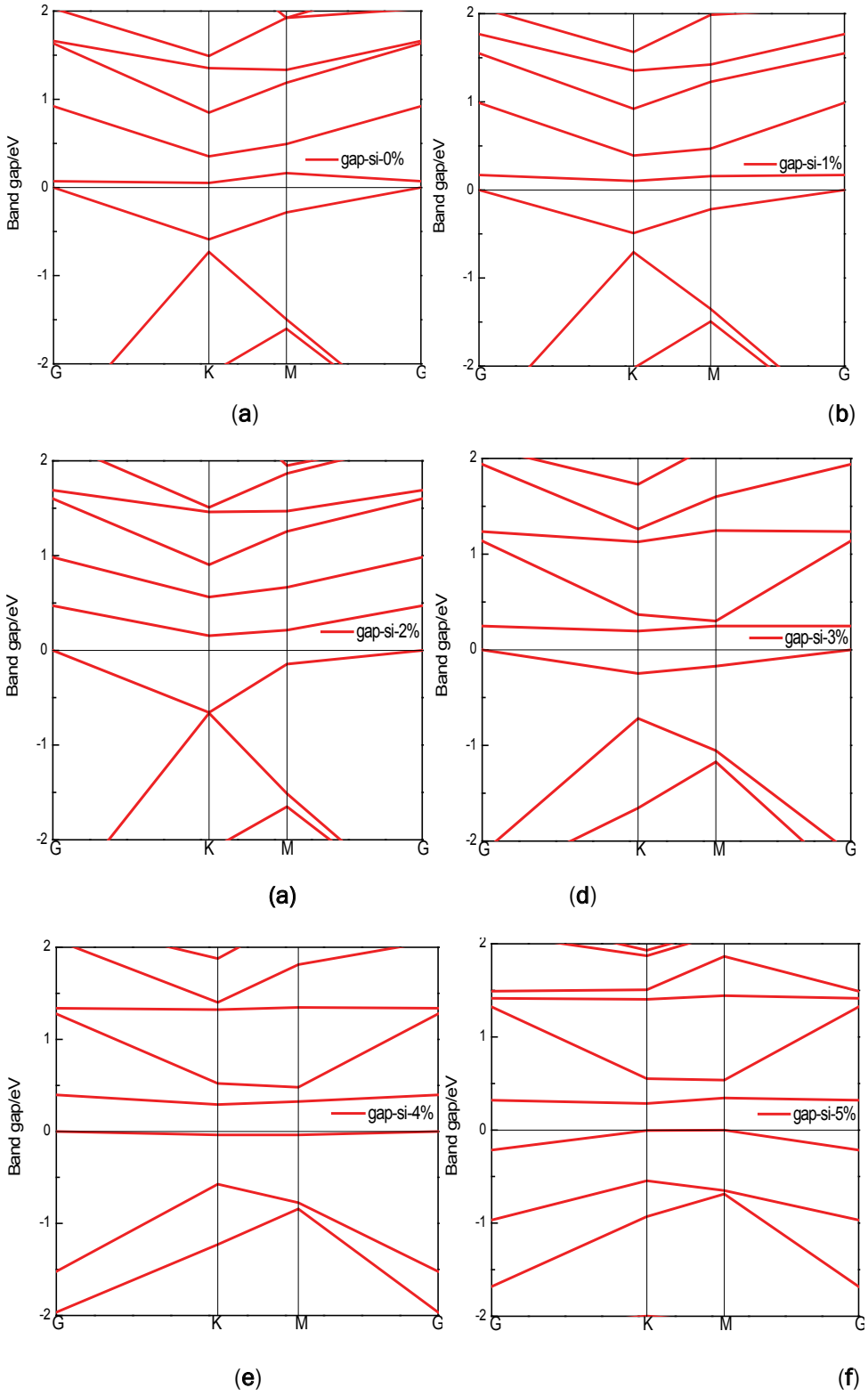

Figure 6: (a-f) Shear deformation of 0%, 1%, 2%, 3%, 4%, 5% of graphene adsorption Si atom band structure

Table 4: Band gap values of Si atom adsorbed on intrinsic graphene and graphene at different shear deformations

Shear deformation	0%	1%	2%	3%	4%	5%
Intrinsic band gap (eV)	0	0.15	0.332	0.504	0.707	0.452
Adsorptive band gap (eV)	0.05	0.102	0.153	0.196	0.293	0.285

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Figure 7 is a graph showing the band gap values of intrinsic graphene and graphene-adsorbed Si atom systems as a function of shear deformation. It can be seen from the figure that the bandgap of intrinsic graphene increases substantially linearly when the shear shape becomes 0%-4%. The intrinsic graphene decreases linearly when the shear deformation is 4%-5%. For the adsorption system, when the shear deformation is 0%-4%, the bandgap of the adsorption system increases with the shear deformation. When the shear deformation is about 0.5%, the band gap value of the adsorption system is equal to the band gap value of the intrinsic system. When the shear shape changes to 0%-0.5%, the band gap value of the adsorption system is larger than the band gap value of the intrinsic system. When the shear deformation is changed to 0.5%-5%, the band gap of the intrinsic system is always larger than the band gap of the adsorption system.

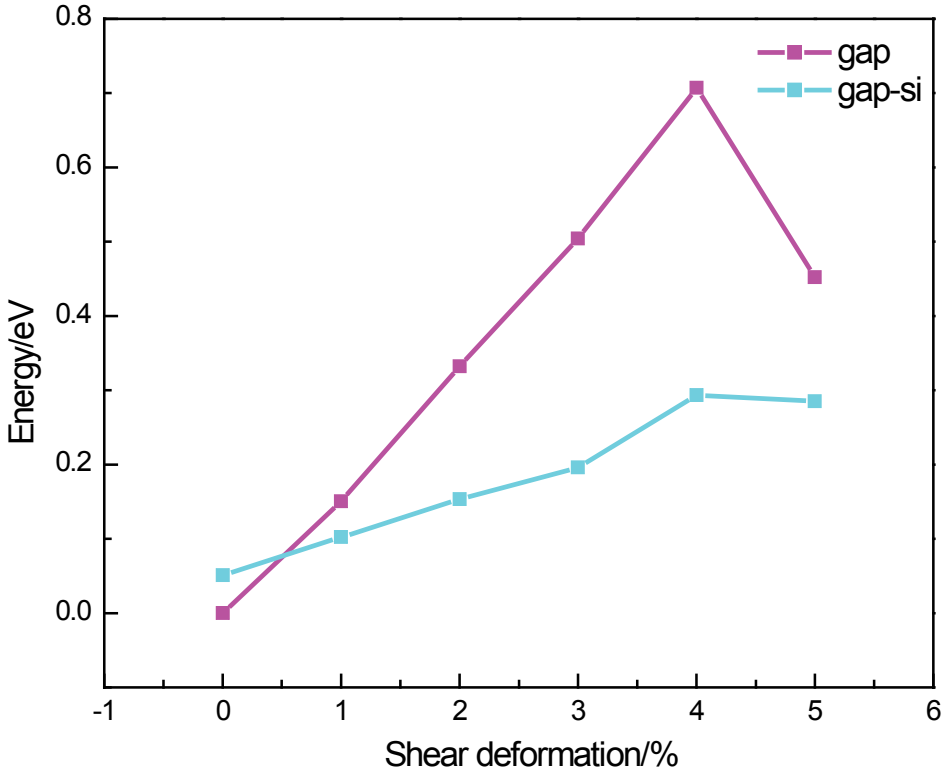

Figure 7: The intrinsic graphene (purple line) and graphene adsorb Si atom (blue line) change with shear deformation

Optical properties

In order to study the influence of different shear deformations on the optical properties of Si atom adsorbed on graphene, the absorption coefficient and reflectance of the system were calculated. From **Figure 8a**, it can be seen that the shear shape becomes 0%, and 1%, 2% of the adsorption system stops the absorption of light at a wavelength of about 7500 nm. The shear deformation became 4%, and the 5% adsorption system stopped the absorption of light at a wavelength of approximately 7800 nm. From **Figure 8b** it can be seen that all of the adsorption systems begin to absorb light at a wavelength of about 47 nm. From **Figure 8c**, it can be seen that the adsorption system with a 3% shear shape shows a maximum absorption peak at a wavelength of about 210 nm. The adsorption system with shearing deformation of 4% and 5% exhibited the maximum absorption peak at a wavelength of approximately 230 nm. The adsorption system with a shear deformation of 2% exhibits a maximum absorption peak at a wavelength of about 250 nm. The adsorption system with a 3% shear profile shows a maximum absorption peak at a wavelength of about 270 nm. The adsorption system with the shear shape of 0% exhibits the maximum absorption peak at a wavelength of about 290 nm. The absorption peaks were reduced to 3%, 1%, 0% (2%), 4%, and 5% in the order of shearing, resulting in blue shift. The blue shift of the absorption peak may be due to the energy band change induced by structural deformation during continuous shearing. Adsorption of the Si atom lifts the C atom and the C-C bond becomes longer. Under relatively small shear deformation, as the shear deformation increases, the C-C bond length becomes longer, which will weaken the C-C interaction and make the electronic energy levels become isolated, so that the absorption peak shifts blue and the peak value increases.

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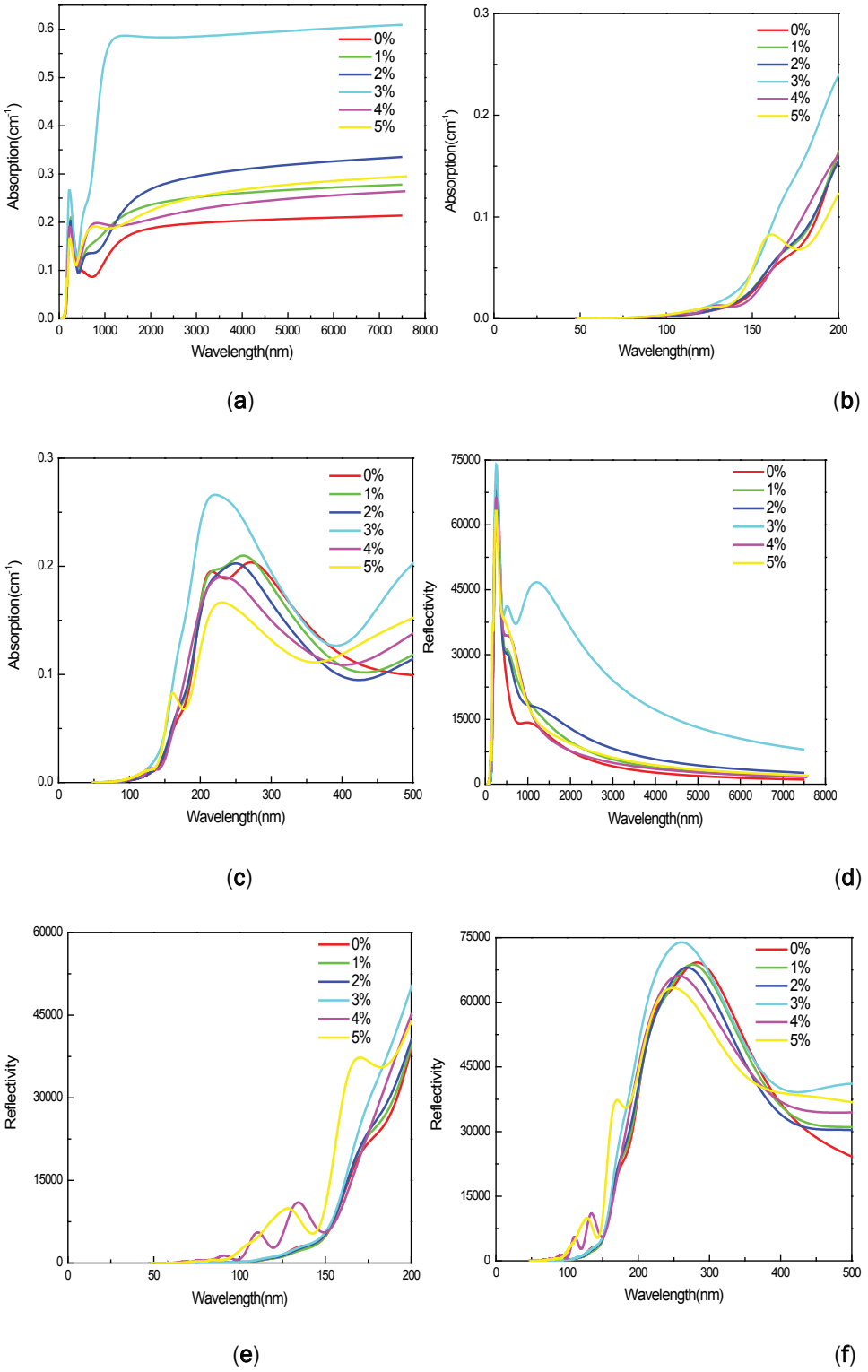

Figure 8: Optical absorption coefficient and reflectivity of graphene-adsorption Si atom system at 0%, 1%, 2%, 3%, 4%, 5% shear deformation: **(b),(c)** the enlarged view of **(a)** at the different wavelength; **(e),(f)** the enlarged view of **(d)** at different wavelength

From **Figure 8d**, it can be seen that the shear shape changes to 0%, 1%, 2%, and 3% of the adsorption system stops the reflection of light at a wavelength of about 7500 nm. The shear shape was changed to 4%, and the 5% adsorption system stopped the reflection of light at a wavelength of about 7700 nm. From **Figure 8e**, it can be seen that all adsorption systems begin to reflect light at a wavelength of approximately 47 nm. As can be seen from **Figure 8f**, the adsorption system in which the shear shape becomes 3% exhibits a maximum reflection peak at a wavelength of about 250 nm. The adsorption system with a shear deformation of 4% exhibits a maximum reflection peak at a wavelength of approximately 260 nm. The adsorption system with a shear deformation of 3% exhibits a maximum reflection peak at a wavelength of about 270 nm. The adsorption system with a shear deformation of 2% exhibits a maximum reflection peak at a wavelength of approximately 280 nm. The adsorption system with a shear deformation of 1% shows the maximum reflection peak at a wavelength of about 290 nm. The adsorption system with

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the shear shape of 0% shows the maximum reflection peak at a wavelength of about 310 nm. The reflection peaks decreased in the order of 3%, 0%, 1%, 2%, 4%, and 5%, resulting in blue shift.

Conclusions

Based on the first-principles method, the structural stability, electronic structure and optical properties of graphene-adsorbed Si atom system under different shear degrees were studied. The charge transfer, band gap, system metal type and semiconductor type transition relationship, light absorption coefficient and reflectivity of the system were analyzed. The results show that shear deformation can affect the structural stability of graphene, but the degree of shear has little effect on structural stability. The adsorption of Si atom can open the graphene band gap. After shear deformation, the band gap value of the adsorption system decreases with the increase of shear deformation, and the band gap value is less than 0.3eV, corresponding to the narrow band gap semiconductor. Graphene adsorbs Si atom so that graphene changes from metal to semiconductor. The ionic bond and the covalent bond coexist in the graphene-adsorbed Si atom system. Adsorption of Si atom increases the charge transfer between C and Si atoms. The graphene-adsorbed Si atom system subjected to shear deformation has a blue shift compared with the adsorption system in which the shear shape is changed to 3%, both the reflectance of light and the absorption coefficient of light decrease.

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