Interaction between graphene and the surface of SiO\(_2\)

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Abstract

The interaction between graphene and a SiO\(_2\) surface has been analyzed with first-principles DFT calculations by constructing the different configurations based on α-quartz and cristobalite structures. The fact that single-layer graphene can stay stably on a SiO\(_2\) surface is explained based on a general consideration of the configuration structures of the SiO\(_2\) surface. It is found that the oxygen defect in a SiO\(_2\) surface can shift the Fermi level of graphene down which opens up the mechanism of the hole-doping effect of graphene adsorbed on a SiO\(_2\) surface observed in a lot of experiments.

(Some figures may appear in colour only in the online journal)

1. Introduction

Graphene, which is a monolayer of carbon atoms with a honeycomb lattice [1], has attracted enormous attention [2] due to its fascinating physical properties [3], such as abnormal quantum Hall effects [4] and massless Dirac fermions [5], which are ascribed to the linear dispersion near Dirac points in the \(k\) space. In addition, with an extremely high mobility of carriers, graphene is expected to be the core material in the next generation of carbon-based nanoelectronics [6–8]. However, the prominent electronic properties of graphene are very sensitive to a change of external conditions [8–10]. The electronic states near Dirac points are modulated easily due to the adsorption of some molecules [11, 12], structural corrugation [13–15] and interaction with substrate surfaces [16–19]. Obviously, this issue is critical to wider electronic-device applications, such as field effect transistors. With the view of two-dimensional materials as transport layers in switching devices, the interaction between graphene and the dielectric layer is important. The change of structural and electronic properties of graphene due to the interaction deserves to be analyzed.

In recent research, two surfaces (SiC and SiO\(_2\)) have drawn a great deal of attention. Graphene can be grown epitaxially on SiC substrate by high-temperature annealing. Therefore, the interaction between graphene and a SiC surface has been intensively investigated [17, 20–22]. The other surface is the SiO\(_2\) surface which is the thin oxide layer of a Si substrate and is widely used as an insulating medium for Si-based device design [4, 5, 8, 9, 23]. Since graphene was discovered on SiO\(_2\) surfaces by optical measurement, various experiments on graphene sheets and nanoribbons [24], including device fabrication and the measurement of fundamental properties, have been undertaken on SiO\(_2\) substrates [4, 5, 8, 9, 23]. The possibility of the properties of graphene adsorbed on SiO\(_2\) being modulated has been reported by many experiments [4, 8, 25, 26]. The stable gate-controlled conduction has proven that few-layer graphene can be stable on a SiO\(_2\) surface [23]. In an early paper by Novoselov et al, electronic measurement showed that single-layer graphene on a SiO\(_2\) surface can be doped chemically [5]. In the experiment of Tomero et al, the graphene was found to be initially p-type and changed to n-type after annealing at 200 °C in vacuum for graphene devices fabricated on a Si/SiO\(_2\) substrate [27]. Using scanning...
probe microscopy, Ishigami et al found that the graphene sheet was only conformed partially to the SiO$_2$ substrate [25]. Raman spectroscopy has been used to observe the spatially inhomogeneous doping effect of graphene supported by a SiO$_2$ substrate [26]. It has been found that coupling between the graphene and the SiO$_2$ surface can be induced by thermal annealing and the adsorbed oxygen can be activated to accept the charge from the graphene [28, 29]. Theoretical calculations will play an important role in elucidating the micro-mechanism of the interaction between graphene and SiO$_2$ and help to explain the different phenomena in the experiments.

Kang et al considered that graphene stayed on O-polar, Si-polar and partially hydrogenated Si-polar α-quartz (0001) surfaces [30]. They found that free-standing graphene could stay on a Si-terminated surface. The electronic properties of graphene near Dirac points were modified obviously on O-polar and partially hydrogenated Si-polar surfaces. Shemella et al analyzed the O-polar surface and found that the π electronic properties of graphene were destroyed fully [31]. With hydrogen termination, graphene can freely stand on the surface. Hossain et al found that graphene was adsorbed on specific sites of the O-terminated surface and the charge transferred from the graphene to the Si- (or O)-terminated surface [32]. Interestingly, Nguyen et al found that the O-terminated surface could be reconstructed and thus graphene could stand freely on the O-polar surface [33]. The linear dispersion of π electrons was retained with a small band gap at the Dirac point and charge transfer was not found. Evidently, although many theoretical calculations have been performed to consider the interaction between graphene and SiO$_2$ surfaces, the results from different theoretical studies seem to not be fully consistent [34]. There is not an explicit conclusion that can give a clear physical insight into the interaction and explain the experimental phenomena.

In this work, we analyze the interaction between graphene and a SiO$_2$ surface by constructing models based on α-quartz and cristobalite. The SiO$_2$ surface from Si/SiO$_2$ involves a large number of configurations due to its amorphous nature. This results in the atomic detail at the interface between the graphene and the SiO$_2$ being difficult to simulate. Thus, in order to consider the interaction at the interface, some typical local atomic configurations need to be analyzed to elucidate the micro-mechanism of the interaction. In the previous theoretical study, the different configurations were not considered in detail. We systematically considered the different cases for the interaction, including the Si-polar surface with two dangling bonds per surface Si atom, the Si-polar surface with one dangling bond per surface Si atom, the O-polar surface, the Si-adsorbed surface, the O-adsorbed surface, the reconstructed O-polar surface and a surface with defects. Based on the analysis of different configurations, we explain the reason why single-layer graphene can stand stably on a SiO$_2$ surface and the charge distribution of graphene adsorbed on SiO$_2$ is inhomogeneous. We also find that the oxygen defect in the SiO$_2$ surface results in the hole-doping phenomenon of graphene adsorbed on a SiO$_2$ surface.

2. Structures and method

2.1. Model structures

The interaction between graphene and SiO$_2$ surfaces is simulated using the repeated-slab model. In order to avoid the spurious vertical coupling effect, the vacuum separation is set to be more than 15 Å. In this work, both α-quartz and cristobalite are used to construct the surface of SiO$_2$. For the α-quartz structure, the (0001) surface is chosen to simulate the interaction. Seven layers of silicon dioxide with a H-passivated bottom surface are used in order to eliminate the effect of interaction of the surfaces. For the 1 × 1 surface of α-quartz, the 2 × 2 cell of graphene can be matched properly with a small difference of lattice constants. Thus, both oxygen (O)-terminated and silicon (Si)-terminated 1 × 1 surfaces are used to model the interaction with graphene. In order to simulate the case of oxygen (or silicon) adsorbed SiO$_2$ surfaces, the 2 × 2 supercell is constructed to interact with one layer of graphene with a 4 × 4 cell (32 carbon atoms). In order to simulate the other configurations of the SiO$_2$ surface, the (111) surface of cristobalite is adopted to model the interaction with the graphene layer, although cristobalite is a high-temperature polymorph of SiO$_2$. Like the α-quartz (0001) surface, the lattice constant of the 1 × 1 surface can match properly with that of the 2 × 2 cell of graphene. Twelve layers of silicon dioxide are used to eliminate the coupling effect of the surfaces. The 2 × 2 surface is also used to simulate the O- (or Si-, OH-, and SiH-) adsorbed SiO$_2$ surface.

2.2. Calculation details

In this work, all the calculations are performed using density functional theory [35]. The generalized gradient approximation (GGA) is used to express the exchange–correlation energy of interacting electrons by the parametrization of Perdew–Burke–Ernzerhof (PBE) [36]. With the accurate frozen-core full-potential projector augmented wave (PAW) method [37], the electron–core interaction is described as implemented in the VASP program package [38, 39]. The k-space integral and plane-wave basis, as detailed below, are tested to ensure that the total energy is converged at the 1 meV/atom level. A kinetic energy cutoff of 600 eV for the plane-wave expansion is found to be sufficient. For the 1 × 1 surface, the geometry is optimized with an 8 × 8 × 2 k mesh. The 2 × 2 surface is constructed based on the optimized 1 × 1 surface and then is optimized with a 2 × 2 × 1 k mesh. The self-consistent electronic structure calculations are performed with a 12 × 12 × 1 k mesh for the 1 × 1 surface and a 6 × 6 × 1 k mesh for the 2 × 2 surface. The dipolar correction is considered in the calculation [40]. In the configurations with physical adsorption of the graphene layer on the surface, the van der Waals (vdW) interaction is found to be important for the binding strength. The effect of the dispersion force is considered with the empirical correction scheme of Grimme (DFT + D/PBE) as implemented in the VASP code [41], which has been proved to be successful on graphene-based structures [42].
3. Results and discussion

3.1. Electronic properties of the bulk and surface

Before starting the calculation for the surface, the structural and electronic properties of the bulk are investigated. The calculated lattice constants $a$ (4.848 Å) and $c$ (5.371 Å) are similar to the experimental lattice parameters (4.913 Å and 5.405 Å), for the $\alpha$-quartz structure with symmetry group P3121. For the cristobalite structure with symmetry group FD-3M, the obtained lattice constant is 7.363 Å. By consideration of the [111] direction, the hexagonal cell with lattice constants $a$ (5.20 Å) and $c$ (12.75 Å) is employed. The calculated lattice constant of $1 \times 1$ graphene (primitive unit cell) is 2.464 Å. For the (0001) surface of $\alpha$-quartz, $2 \times 2$ graphene placed on it has a lattice mismatch of $\sim 3\%$. The mismatch between the lattice constant of $2 \times 2$ graphene and that of the cristobalite (111) surface is about $\sim 5\%$. When the lattice of $2 \times 2$ graphene is changed to match that of both surfaces, the strain effect on the electron properties of graphene can be ignored.

After the optimization of structure, the electronic properties of $\alpha$-quartz and cristobalite are obtained. The calculated bands are plotted versus the high-symmetry lines in the hexagonal-symmetry Brillouin zone. As shown in figure 1, cristobalite and $\alpha$-quartz have similar band gaps. Their large band gaps demonstrate their insulating property which is consistent with previous calculations [43, 44]. The difference is that the valence band edge and conduction band edge of cristobalite are at the same point (the $\Gamma$ point). The valence band edge of $\alpha$-quartz is not at the $\Gamma$ point. As mentioned in the previous study [45], the band gap is underestimated by DFT-GGA calculations. An exact estimation needs to perform a quasiparticle band structure calculation [45]. However, this does not affect the analysis of the electronic properties of the mixed system of graphene and a SiO$_2$ surface, as stated in the next part.

It is well known that the SiO$_2$ surface in most experiments has an amorphous structure. For amorphous SiO$_2$, the bond lengths and bond angles have a continuous distribution [43] without a periodic cell which makes it difficult to simulate the surface with DFT. However, the local structures of some crystal forms of SiO$_2$ are similar to that of amorphous SiO$_2$. The crystal SiO$_2$ structures, such as $\alpha$-quartz and cristobalite, have local structures of fourfold tetrahedral bonds for Si and twofold bridging bonds for O. For $\alpha$-quartz, the calculated Si–O bond length and the bond angle of Si–O–Si are about 1.590 Å and 143.05°, respectively. For cristobalite, the bond length and the bond angle are about 1.594 Å and 180°, respectively. The similar local structures result in similar electronic insulating properties. In addition, the different bond angles of $\alpha$-quartz and cristobalite can form the different surface configurations. Therefore, it is appropriate to use the surfaces of $\alpha$-quartz and cristobalite to simulate that of amorphous SiO$_2$, since the local structures of the amorphous surface with different dangling bonds can be simulated by the different surfaces of $\alpha$-quartz and cristobalite.

Now we analyze some basic configurations of the SiO$_2$ surface. If the top surface is the oxygen or hydroxyl (OH), the Si atoms of the bottom surface are passivated by hydrogen.
If the top surface is silicon or SiH, the oxygen atoms of the bottom surface are also passivated by hydrogen. In figure 2, seven configurations of the surface are demonstrated, based on \(\alpha\)-quartz and cristobalite. For the Si-polar surface as a local stable configuration, the Si atom can have two dangling bonds (figure 2(A)), one dangling bond (figures 2(B) and (C)), or no dangling bond if the silicon atom is passivated by two hydrogen atoms. For the O-polar surface as a local stable configuration, the oxygen atom can have one dangling bond (figure 2(F)), or no dangling bond if the oxygen atom is passivated by one hydrogen atom. It is noticed that each oxygen pair is bonded with one silicon atom (figure 2(D)) for the \(\alpha\)-quartz (0001) surface as a simple cleaved surface. The oxygen pair may be unstable and reconstruct the surface by removing one of the oxygen atoms (figure 2(G)) or be passivated by partial hydrogenation (figure 2(E)) or full hydrogenation.

Before investigating the interaction between the graphene and the different configurations, we calculate the electronic properties of the different surfaces. As shown in figure 3(A), we can find that the dangling bonds of the surface Si atom introduce two localized bands in the region of the band gap. Since there are two isolated electrons for the surface Si atom, one of the bands is occupied fully leaving one vacant band near the conduction band edge. Therefore, it is possible for it to not be activated. If one electron is paired by the introduction of hydrogen, the residual electron will form one typical dangling bond. This case is similar to that of the Si atom in the cristobalite (111) surface. There is one localized state in the center of the band gap and the state is half occupied (figures 3(B) and (C)). In figure 3(D), we show the band structure of an O-polar surface with one oxygen pair. It is well known that each oxygen atom has one orbital with one isolated electron. The two orbitals from two oxygen atoms will interact with each other and form two separated bands in the center of the band gap and one of the bands will be occupied. However, this case may be different from that of the Si atom of the surface in figure 3(A), since the two electrons do not form a stable pair due to the large distance. If one of the oxygen atoms is passivated by hydrogen, we can find that the localized state is shifted to the top of the valence band and is half occupied (figure 3(E)). This case is a little different from the case of the cristobalite (111) surface. As shown in figure 3(F), there are two localized bands which are almost degenerate.

### 3.2. Adsorption of graphene on different surface configurations

We first consider that the graphene layer is adsorbed on the O-polar surface. Figures 4(A)–(E) show the optimized geometric structures for different adsorption sites of the surface. It is found that the graphene layer keeps its planar hexagonal network for all these cases with physical adsorption, except the chemical adsorption site in the potential curve (figure 4(G)) for the paired oxygen configuration (figure 4(B)). For the reconstructed surface (figure 4(A)), the result is similar to the previous experimental and theoretical studies [33, 46, 47]. The difference is that the adsorption energy is smaller (about 12 meV/unit cell). With the correlation of the vdW energy, the adsorption is increased to 210 meV/unit cell. From the equilibrium position of the potential curve in figure 4(F), we can find that the distance between the carbon and the oxygen is about 3.8 Å. The change of distance is very small after the correlation of the vdW force. This demonstrates that the reconstructed surface...
Figure 3. The band structures of the surface models of α-quartz and cristobalite: Si-polar (0001) α-quartz surface (A), Si-polar (0001) α-quartz surface with one dangling bond per surface Si atom (B), Si-polar (111) cristobalite surface (C), O-polar (0001) α-quartz surface (D), O-polar (0001) α-quartz surface with one H-terminated oxygen (E) and O-polar (111) cristobalite surface (F).

Figure 4. Top views of optimized structures of graphene on the O-polar surface including the bridge site of the reconstructed α-quartz surface (A), the top site of the (0001) α-quartz surface with paired oxygen (B) and the top (C), bridge (D) and hexagonal center sites (E) of the (111) cristobalite surface, and potential-energy curves as a function of the distance of the surface oxygen atom and the nearest-neighbor carbon atom of graphene including curve (F) for configuration (A), curve (G) for configuration (B) and curves (H) for configurations (C)–(E). The surface unit cell is shown by the dashed lines.
Figure 5. Top views of the optimized structures of graphene on the Si-polar surface including the bridge (A) and hexagonal center sites of the (0001) α-quartz surface and the hexagonal center (C), top (D) and bridge (E) sites of the (111) cristobalite surface, and potential-energy curves as a function of the oxygen atom of the surface and the nearest-neighbor carbon atom of the graphene including curve (F) for configuration (A), curve (G) for configuration (B) and curves (H) for configurations (C)–(E). The surface unit cell is shown by the dashed lines.

Figure 6. The band structures of the mixed systems of graphene adsorbed on a SiO$_2$ surface: the O-polar (0001) α-quartz surface with paired oxygen due to physical adsorption on the top site (A), the O-polar (111) cristobalite surface with a bridge site (B), the H-terminated O-polar (111) cristobalite surface with a bridge site (C), the Si-polar (0001) α-quartz surface with a bridge site (D), the Si-polar (111) cristobalite surface with a hexagonal center site (E) and the H-terminated Si-polar (111) cristobalite surface with a top site.

is stable and the interaction between the graphene and the surface is weak, as Nguyen et al stated [33]. There is no charge transfer between the graphene and the reconstructed surface and the surface only weakly disturbs the electronic state of the graphene at the Dirac points to result in a small gap which can even be ignored. For the (111) cristobalite surface, the distances between the carbon and the oxygen (about 3.0 Å) are similar at different adsorption sites (figures (C)–(E)). The hexagonal center is the stabllest site with an adsorption energy of about 470 meV/unit cell, as shown in figure 4(H).
After considering the correlation of the vdW energy, the adsorption energies are 654.6, 573.2 and 547.0 meV/unit cell for the configurations of adsorption with a hexagonal center site (figure 4(E)), top site (figure 4(C)) and bridge site (figure 4(D)), respectively. For the top site of the (0001) α-quartz surface with paired oxygen, the physical adsorption has an equilibrium distance of 3.4 Å and an adsorption energy of 112 meV/unit cell (301 meV/unit cell with the vdW correlation). However, after hopping a potential barrier of about 260 meV, the chemical adsorption is formed with a distance between the carbon and the oxygen of 1.55 Å, as shown in figure 4(G). For the chemical adsorption, the carbon has a trend to drop down in order to form a chemical bond with the oxygen atom of the surface. The adsorbed carbon atom deviates away from the graphene plane to result in a large strain energy due to the localization of the adsorption site. As a consequence, it is possible for chemical adsorption at the top site of the (111) cristobalite surface to form. However, the adsorption is unstable due to the large strain energy (figure 4(H)). The same applies for the partly hydrogenated O-polar surface on which the graphene just forms the physical adsorption. Of course, for the fully hydrogenated O-polar surface, the interaction between the graphene and the surface is weak, since there is no active site for chemical adsorption or strong physical adsorption as other authors have stated.

For the Si-polar surface, the optimized geometric structures for the different adsorption sites of the surface are shown in figures 5(A)–(E). For all the cases, the graphene is adsorbed physically on the surface and the graphene layer keeps its planar hexagonal network. The binding energy is smaller than that of the adsorption on the O-polar surface. For the (0001) α-quartz surface, the adsorption energy is about 13 meV/unit cell with an equilibrium distance of about 4.3 Å. With the correlation of the vdW energy, the adsorption energy is about 96 meV/unit cell. For the (111) cristobalite surface, the binding energies (top and bridge: 18.5 meV/unit cell; hexagonal center: 24 meV/unit cell) are a little larger than those of the (0001) α-quartz surface. After the correlation of the vdW energy, the binding energies are obviously enhanced (top site with 165 mev/unit cell, bridge site with 160 meV/unit cell and hexagonal center with 204 meV/unit cell). This may be attributed to the activity of the silicon atom with one dangling bond for the (111) cristobalite surface. For both surfaces, the hexagonal center is the stabllest site, similarly to the case of the O-polar surface. The reason is that the charge repulsion between the graphene and the surface of SiO$_2$ is weak due to the space separation of the carbons and the surface atoms. In addition, on the top site of the (111) cristobalite surface, it is possible for the graphene to form chemical adsorption due to the activity of the dangling bond of the silicon atom, as shown in figure 5(H). This case is similar to the configuration of silicon with one dangling bond on the (0001) α-quartz surface due to H termination, as stated by Kang et al. [30]. Of course, for the fully hydrogenated Si-polar surface, the adsorption is physical. In general, as the above discussion suggests, the graphene layer can be adsorbed freely on SiO$_2$, except for special cases. The interaction between them is weak and it is possible for the electronic properties of the graphene to be changed weakly.

3.3. Electronic properties of interfaces without/with defects

In figure 6, the band structures of some typical configurations of graphene adsorbed on surfaces are demonstrated. As
figure 6(A) shows, when a graphene layer is adsorbed physically on an O-polar (0001) α-quartz surface with paired oxygen, the band structure of the graphene is not changed obviously. It is found that the vacant band from the pair is occupied partly, the Fermi level is pinned at that band and an electron is transferred from the graphene layer to the surface to result in p-doping of the graphene, as shown in figures 8(A) and (B). If the graphene is adsorbed chemically on the surface after jumping the energy barrier, the band structure of the graphene is broken strongly with a large band gap (about 2.7 eV), as previously reported [30]. If there is an isolated oxygen on the surface, the localized band from the oxygen will result in a shift of the Fermi level, as shown in figure 6(B). The band structure of the graphene is not changed when it is adsorbed on a bridge site of an O-polar (111) cristobalite surface. The results from the top and hexagonal sites are similar to that for the bridge site. For a Si-polar surface, the charge transfer between the graphene and the surface is very small, as shown in figures 6(D) and (E). Whether there is a nonactive Si atom with two free electrons or an active Si atom with a single dangling bond on the surface, the shift of the Fermi level (in figures 8(C) and (D)) can be ignored, compared with the O-polar surface. This may be attributed to the similar electronegativity of silicon on the SiO$_2$ surface and the carbon of the graphene. If the surface (O-polar or Si-polar) is passivated by hydrogen, the bands from the π electrons of the graphene mostly stay in the large band gap of the surface and the electronic properties of the graphene are not affected by the surface, as shown in figures 6(C) and (F).

From the above analysis, the interaction between the graphene and the surface is mostly by the physical adsorption. The weak interaction does not break the band structure of the graphene as reported in a lot of experiments. However, it is also possible to form chemical adsorption on special configurations, such as the configuration of an oxygen pair on an O-polar surface. However, the previous studies have shown that it is easy for the cleaved SiO$_2$ to be reconstructed or hydroxylated (or hydrogenated) to eliminate the dangling bonds. Therefore, it seems to be impossible that there is a large region of active surface with dangling bonds, while it
is possible for oxygen and silicon defects with dangling bond to appear on the surface. In figure 7, we give an analysis of some typical SiO$_2$ surfaces with defects. For oxygen defects (figures 7(A) and (B)) and a silicon defect with one dangling bond (figure 7(D)) in the H-passivated (O-polar or Si-polar) surface, the graphene layer will still be adsorbed physically on the surface and the active defect will not interact chemically with the carbon atoms of the graphene. However, the oxygen defects introduce localized energy levels at the top of the valence band and result in the Fermi level of the graphene being shifted down, as shown in figure 8(F). The charge transfer evidently induces hole-doping of the graphene. For a silicon defect, there is no charge transfer and the electronic properties do not change. The defect just induces one localized energy level near the Dirac points. However, the electronic scattering from the defect will affect the mobility of carriers in the graphene layer. Therefore, the defects result in a spatially inhomogeneous distribution of charge in the graphene plane. In some special cases, it is possible for raised defects to appear on the surface. In figures 7(C) and (E), these kinds of oxygen and silicon defects are demonstrated, respectively. It is found that the raised defects can form a chemical interaction with the graphene layer by dropping the carbon atom down to form a C–O bond or C–Si bond. Such defects strongly disturb the electronic properties of the graphene near the Dirac points (in figure 8(E)) and a band gap is obviously opened. An oxygen defect results in down-shift of the Fermi level of graphene and a silicon defect results in up-shift of the Fermi level. One energy level from the defect is coupled with the bands from the Dirac cone and the Dirac cone is broken near the coupling region.

4. Conclusion

The interaction between graphene and a SiO$_2$ surface has been studied systematically by first-principles DFT calculations. Different configurations of the SiO$_2$ surface are considered, based on α-quartz and cristobalite. It is found that the graphene layer is mostly adsorbed physically on the surface and the hexagonal center site is the stablest site for both O-polar and Si-polar surfaces. This may be attributed to the largest spatial separation of charges to reduce the Coulomb repulsion when the graphene layer approaches the region of the surface due to the van der Waals interactions and possible charge transfer. It is found that the adsorption on the O-polar surface is stronger than that on the Si-polar surface. It is ascribed to the effect of charge transfer on the O-polar surface which increases the electrostatic interaction between the graphene and the surface. Due to the charge transfer, it is found that the graphene adsorbed on the O-polar surface is hole-doped, as observed in experiments.

H-passivated surfaces do not affect the electronic properties of the graphene whether they are O-polar surfaces or Si-polar surfaces, whereas surfaces with defects have a strong effect on the electronic properties of graphene. It is found that an oxygen defect in the surface can result in hole-doping of graphene. The raised atom defects will interact chemically with the graphene layer and disturb the band structure of the π electrons. Raised oxygen results in down-shift of the Fermi level of graphene and raised silicon results in up-shift of the Fermi level. Therefore, we suggest that a SiO$_2$ surface which is used as a substrate for fabrication of a graphene device should be cleaved with an atomic level of planeness and then be passivated by hydrogen.

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