Density functional theory based study of graphene and dielectric oxide interfaces

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Abstract

We study the effects of insulating oxides in their crystalline forms on the energy band structure of monolayer and bilayer graphene using a first principles density functional theory based electronic structure method and a local density approximation. We consider the dielectric oxides SiO$_2$ ($\alpha$-quartz) and Al$_2$O$_3$ (alumina or $\alpha$-sapphire), each with two surface terminations. Our study suggests that atomic relaxations and resulting equilibrium separations play a critical role in perturbing the linear band structure of graphene in contrast to the less critical role played by dangling bonds that result from cleaving the crystal in a particular direction. For Si-terminated quartz a Dirac cone is retained while it is restored on adding a second graphene layer for O-terminated quartz. Alumina needs more than two graphene layers to preserve the Dirac cone. Our results are, at best, semi-quantitative for the common amorphous forms of the oxides considered.

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

1. Introduction

Recent advances in large area graphene films on metal substrates and understanding the morphology of their domains [1], deposition of dielectrics [2], making metal contacts [3] and designing novel electronic switches [4] are making graphene-based electronics more likely. Theoretical efforts have played a crucial role in this development, often elucidating the complex interplay of substrates and dielectrics with graphene. Notable among these efforts is the understanding of the role of interface and substrate charge inhomogeneity in degrading the carrier mobilities [5]. Density functional theory (DFT)-based electronic structure methods, used in some of these studies, have provided inputs for optimization of various processes used in graphene electronics. A crucial obstacle in graphene electronics research has been the need to improve the substrate quality to maintain the novel intrinsic graphene properties. In this paper we address the interface electronic structure of graphene with two crystalline oxides, namely quartz (SiO$_2$) and alumina (Al$_2$O$_3$), using an ab initio DFT-based numerical method. Crystalline substrates/dielectrics provide a compelling alternative to amorphous substrates/dielectrics.

Our studies have implications for the interpretation of future experiments with crystalline oxides.

The atomic structure of graphene on amorphous insulating substrates has been explored in some experimental studies [6] using nanometer scale microscopic techniques such as scanning tunneling microscopy and atomic force microscopy. These studies suggest that graphene conforms to the structural inhomogeneity of the underlying substrate. In addition, a study using Raman spectroscopy examined the role of amorphous oxides on phonon dispersion, indirectly hinting at the change in the electronic spectrum of graphene due to the presence of oxide substrates [7]. We are aware of two recent DFT studies of monolayer graphene on a crystalline SiO$_2$ [8, 9], which discuss perturbations to the linear band structure due to the presence of oxides, the role of dangling bonds and their passivation in influencing the linear band structure. There is another recent study of hydrogenated graphene on an O-terminated silicon-dioxide substrate [23] which reports breaking of spin degeneracy in zigzag nanoribbons due to charge imbalance in the substrate.

Our paper is organized as follows. In section 2, we discuss the computational method and convergence parameters used for this study, followed by the motivation and procedure used to build surface models from their bulk counterparts. The
Four oxide bulk unit cells were chosen to represent the thin surfaces we constructed surface models of both quartz and alumina. Using these optimized lattice parameters, we found these values to be very close to the experimental values, differing by less than 1% (table 1). Using these optimized lattice parameters, we constructed surface models of both quartz and alumina.

| Bulk quartz         | \(d(C-x) \ (x = Si, Al, O)\) | \(E^{\text{bind}}\) C | \(E^{\text{bind}}\) O | \(E^{\text{bind}}\) H |
|---------------------|-------------------------------|------------------------|------------------------|------------------------|
| This work           | 4.914 (5.408)                 | 10.061                 | 4.00                   | 7.81                   | 1.02                   |
| Expt. [13, 14]      | 4.913 (5.405)                 |                        |                        |                        |                        |
| Si-terminated       | 3.0 [1.89] [15]               |                        |                        |                        |                        |
| O-terminated        | 1.76 [1.3] [16]               | –0.581                 | 3.48                   | 7.96                   | 1.97                   |

| Bulk alumina        | \(d(C-x) \ (x = Si, Al, O)\) | \(E^{\text{bind}}\) C | \(E^{\text{bind}}\) O | \(E^{\text{bind}}\) H |
|---------------------|-------------------------------|------------------------|------------------------|------------------------|
| This work           | 4.907 (4.908)                 | –1.017                 | 4.09                   | 8.00                   | 1.44                   |
| Expt. [19, 17]      | 4.943 (4.907)                 |                        |                        |                        |                        |
| Al-terminated       | 2.7 [1.89–2.19] [18]          | –0.689                 | 3.88                   | 7.95                   | 1.69                   |
| O-terminated        | 2.15                           |                        |                        |                        |                        |

Results from these calculations are discussed in section 3, which details the role of atomic relaxations, the resulting equilibrium distances and the role of unsaturated or dangling bonds of oxide surfaces in perturbing the linear band structure of graphene. We address the origin of change in linear band dispersions with the help of orbital and atom projected densities of states, charge densities and also present the energetics of our interface models. Finally, we summarize our results and present our conclusions.

2. Computational method and surface models

This section addresses the details of the computational method we used, followed by the procedure adopted to obtain the surface models of quartz and alumina from the bulk and the convergence parameters employed. We adopted a plane-wave based electronic structure method [10] using a local density approximation (LDA) [11] for exchange and correlation, and the projector augmented plane-wave potential for electron–ion interaction [12]. The bulk structures for both quartz and alumina are consistent with those mentioned in the literature [13] and the surface models built from the bulk structures conform to the widely accepted quartz and alumina structures [19] containing alternating cation and anion layers.

The unit cell of bulk quartz contains 27 atoms with three silicon planes and six oxygen planes, each plane comprising three atoms. The unit cell of alumina contains 30 atoms with four aluminum planes and six oxygen planes, again with each plane consisting of only three atoms. We used a \(7 \times 7 \times 5\) \(k\)-point mesh in the hexagonal Brillouin zone (BZ) and a kinetic energy cut-off of 612 eV. The results were carefully checked in comparison to a larger \(k\)-point set and higher energy cut-offs.

After optimization of atomic positions and the lattice constant for the bulk structures, we found these values to be very close to the experimental values, differing by less than 1% (table 1). Using these optimized lattice parameters, we constructed surface models of both quartz and alumina. Four oxide bulk unit cells were chosen to represent the thin surfaces by DFT is challenging, partly due to the inherent results from these calculations are discussed in section 3, which details the role of atomic relaxations, the resulting equilibrium distances and the role of unsaturated or dangling bonds of oxide surfaces in perturbing the linear band structure of graphene. We address the origin of change in linear band dispersions with the help of orbital and atom projected densities of states, charge densities and also present the energetics of our interface models. Finally, we summarize our results and present our conclusions.

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Figure 2. Energy band structures of monolayer graphene on (a) Si-terminated quartz, (b) O-terminated quartz and their respective total densities of states (c) and (d). The supercells were relaxed and oxide surfaces unpassivated. The Fermi energy is set at zero. The bands with a significant contribution from carbon are marked in red. The origin of occurrence of linear bands at the $\Gamma$-point instead of $K$-point of the supercell is explained in the text.

Figure 3. Energy band structures of monolayer graphene on (a) Al-terminated alumina, (b) O-terminated alumina and their respective total densities of states in (c) and (d). The oxide surfaces were unpassivated and the supercells were relaxed. The Fermi energy is set at zero.

complexity in generating the amorphous structures by DFT (the traditional melt and quench method) as well as the requirement of a relatively large size of the supercell to represent roughness, a computationally intensive task for DFT calculations. Moreover, crystalline structures have a larger number of dangling bonds than their amorphous
counterparts. Therefore, an additional constraint in using the crystalline substrates, besides treating surface roughness in an approximate way, is to saturate these dangling states for assessing the external effects on graphene electronic structure. To make the combined graphene and oxide thin film structure an isolated system, we used a vacuum region adjacent to the graphene layer in the stacking direction. The supercell was then repeated in all three crystallographic directions by imposing periodic boundary conditions on the crystal wavefunctions.

The dangling states at the bottom of the supercell were saturated with hydrogen atoms and the atoms within the top two unit cells of the oxide film and all the graphene atoms were allowed to relax while keeping the cell size fixed. We used the same energy cut-off value, as in the bulk calculations, but the \( \mathbf{k} \)-point mesh in the BZ was chosen to be \( 7 \times 7 \times 1 \). The convergence of results with respect to larger \( \mathbf{k} \)-mesh size, larger vacuum sizes and energy cut-off was also checked. For atomic relaxation, the total energy was assumed to have converged when all the components of the Hellman–Feynman forces were smaller than 0.01 eV Å\(^{-1}\).

3. Relaxed atomic positions, energy band dispersions, densities of states, charge densities and energetics

In this section, we discuss the effect of underlying oxide surfaces on the electronic band structure of graphene for different surface terminations. In particular we explore the impact of graphene–oxide distances, oxide dangling bonds and atomic relaxations on the band structure. With relaxations of atomic positions, we get the equilibrium oxide–graphene distances tabulated in table 1. All the distances are larger than the corresponding interatomic distances of the constituent atoms in bulk or molecular compound phases, suggesting that formation of compound phases at low temperature is unlikely. However, higher temperature effects may support formation of these phases.
We present detailed examination for the different structures beginning with Si-terminated quartz. After relaxation of the supercell we observe that graphene retains its planar hexagonal structure and the top few layers of Si and O in the oxide are pushed away from the graphene layer. In-plane rearrangement of Si and O atoms is negligible. Figure 2(a) shows the band structure, and figure 6(a) shows the charge density plot. The equilibrium distance between graphene and the oxide surface as well as average charges on C, O and H atoms are listed in table 1. As expected from the large equilibrium separation, there is no structural perturbation and no hybridization of C p with the oxide, and graphene retains its linear band structure. There is virtually no charge transfer out of the graphene sheet; however, there is some charge redistribution within the oxide. It is noteworthy that the linear crossing point of graphene bands in our supercell is at the Γ point of the Brillouin zone (BZ) and not the traditionally expected K point. This is due to the crystal symmetry of our supercell. Such an effect is also seen in calculations involving sub-monolayer alkali metal adsorption on graphene surfaces [21]. We explain the reason for this shift in the appendix. On O-terminated quartz, again the in-plane relaxations of Si and O atoms are negligible. However, the topmost O layer is pushed away from graphene whereas the immediate next O layer is pulled toward it, until both the layers are equally distant from the graphene layer, suggesting bonding between them. Si layers are pulled toward the graphene sheet which, in turn, shows significant structural distortion. There is considerable charge transfer away from graphene; however, the oxide surface next to graphene is as polar as the bulk. We can clearly see signs of bonding from the charge density plot (figure 6(b)) and hybridization of C p and O p orbitals (figure 5(a)). A similar conclusion was reached in a recent DFT-based calculation for monolayer graphene on O-terminated quartz [9].

For Al-terminated alumina, graphene after relaxation is not planar. Al and O atoms show considerable in-plane distortion and are generally pushed away from the C layer. The graphene layer as well as O atoms close to the surface tend to gain some charge (figure 6(c)). There is a lot of hybridization between C p, Al s and Al p (figure 5(b)) and, as such, we do not see graphene’s linear spectrum, rather a highly delocalized contribution of graphene to the band structure (figure 3(a)). In the case of O-terminated alumina, like Al-terminated alumina, Al and O atoms show considerable in-plane relaxation. However, like O-terminated quartz, the topmost O layer is pushed away from graphene while the immediate next O layer is pulled closer, until they are at almost the same distance. Again this hints at C–O bonding which is corroborated by the charge density plot (figure 6(d)) and DOS plot (figure 5(c)). We see charge transfer away from the C layer as well as the top O planes and significant hybridization between C p and O p orbitals.

In an attempt to regain the linear band structure of graphene we add a second carbon layer to O-terminated quartz and Al- and O-terminated alumina. For O-terminated quartz, we see that a second layer restores the linear band structure (figure 4(a)). However, for both terminations of alumina, linearity is not restored (figures 4(b) and (c)) as is explained by the considerable hybridization of C p orbitals with Al p and O p, in both cases.

To understand the distance-dependent electronic structure of the combined graphene and oxide system, we manually adjusted the interface distances both below and above the calculated equilibrium distances. The atomic positions were not relaxed while other computational parameters kept the same as those used in the self-consistent runs discussed above. We demonstrate our calculations by using Si-terminated quartz as an example. We chose two representative distances 2 Å and 4 Å which are, respectively, below and above the equilibrium distance of 3 Å (table 1). The Dirac cone is preserved for the 4 Å case (figure 7(a)) but not for the 2 Å case (figure 7(b)), suggesting a strong dependence of band structure on the interfacial distance. We have performed

![Diagram](image-url)
Figure 6. Charge density plots for monolayer graphene on (a) Si-terminated quartz, (b) O-terminated quartz, (c) Al-terminated alumina and (d) O-terminated alumina. The oxide surfaces were unpassivated and the supercells were relaxed.

these tests with other surface terminations and found that the interfacial distance dictates whether the Dirac cone can be preserved or not. The equilibrium distance after relaxation is thus quite important in determining graphene’s properties.

Table 1 shows the binding energy values for graphene on the four surface terminations considered in this study. The binding energy values are obtained by using the following definition:

\[
E_{\text{bind}} = E(\text{supercell}) - E(\text{Gr}) - E(\text{oxide})
\]

where \(E(\text{supercell})\) denotes the total energy of the supercell containing the oxide and a graphene layer. \(E(\text{Gr})\) and \(E(\text{oxide})\) denote, respectively, the total energies of isolated graphene and isolated oxide in the same supercell set-up, with the same energy cut-off and k-point mesh as that of the combined graphene and oxide calculations. It is interesting to note that while graphene on Si-terminated quartz has a large positive binding energy, the other three cases have small negative binding energies. This suggests that graphene tends to be repelled from the surface of Si-terminated quartz, which is also why we see a large equilibrium distance between graphene and the substrate and no perturbation to graphene’s band structure. On the other hand, in the other three cases, graphene tends to bind to the oxide surface. We must take note, however, that these calculations do not include the van der Waals force which might ultimately lead to stabilization of the graphene on Si-terminated quartz structure.

To assess the importance of dangling bond saturations on graphene’s electronic spectrum, we performed a calculation with the top oxide surface saturated with hydrogen atoms. This calculation was undertaken only for the O-terminated surface of quartz since the Si-terminated surface already preserves the Dirac cone without surface passivation. Both Al- and O-terminated surfaces of alumina, even in the initial structures, show non-trivial stoichiometry; as a result passivation of dangling bonds is avoided. Two separate calculations were performed with equilibrium O–C interfacial distance in O-terminated quartz: one with unrelaxed and unpassivated oxide surfaces, and another with unrelaxed passivated oxide surface with graphene on top of it. We find that on unpassivated surfaces, there is no effect on graphene’s band structure except for some doping effects (figure 8). This hints at the non-critical role played by dangling bond states. To check the effect of relaxation of the unpassivated surfaces in all four terminations without the graphene layer, we performed additional calculations which show that both Al- and Si-terminated surfaces are inherently stable, compared to the initial surface model we built from the corresponding bulk structures as well as the final relaxed unpassivated structures. The interatomic and interplanar distances were found to be no different from the unrelaxed initial and relaxed final structures and the
surface atomic configurations were similar. This situation corresponds to the configuration adopted by the Si and Al surface terminations in experiments immediately after cleaving from the bulk crystals. Therefore, our initial surface models with graphene on the top of these surfaces and the corresponding interfacial distances in table 1 obtained upon relaxing these combined structures without performing the intermediate step relaxing the unpassivated oxide surfaces, are valid. The situation is not same with O-terminated surfaces of quartz and alumina. Both surfaces show large relaxations of in-plane surface atoms. However, they are all displaced by the same amount. To a first order approximation, this uniform displacement is equivalent to displacing the graphene layer in-plane with respect to the oxide surface. Since our graphene position is an independent variable, this displacement would not matter. We believe all second-order effects of relative in-plane movement between substrate layers are taken care of in the relaxations of the combined structures that we perform.

4. Summary and conclusion

In summary, we have studied, using a first principles DFT method, the effect of two crystalline insulating oxides, quartz and alumina, on the electronic structure of monolayer graphene. Si-terminated quartz retains the graphene band structure on non-passivated surface with atomic relaxations. O-terminated quartz and both alumina terminations perturb the linear bands of graphene. The graphene and oxide interface distance is critical in determining the extent of disturbance to graphene. By comparison, the effect of dangling bond states on the oxide surface is not very crucial. Bilayer graphene on O-terminated quartz retrieves its linear band structure while graphene on alumina terminations (Al or O) perhaps needs additional graphene layers. Our studies are relevant in situations where a crystalline dielectric is used either as a template for growth or as a substrate/dielectric for exfoliated graphene experiments. Recent use of crystalline BN as a substrate/dielectric for graphene experiments is a promising step in this direction, and we believe more experiments with crystalline oxides should be conducted in future, which make DFT-based studies useful for interpreting experiments.

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Appendix

Quartz, alumina and the graphene layer all have a hexagonal unit cell. Let \( \mathbf{A}_1, \mathbf{A}_2 \) and \( \mathbf{A}_3 \) be the lattice vectors of the entire graphene and oxide system and \( \mathbf{B}_1, \mathbf{B}_2, \) and \( \mathbf{B}_3 \) be the corresponding reciprocal lattice vectors. Similarly, let \( (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3) \) and \( (\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3) \) be the triad of primitive and reciprocal lattice vectors of the graphene layer alone.

We note that the lattice structure of the graphene plus oxide system is a \( (2\sqrt{3}) \times (2\sqrt{3}) \) reconstruction of the lattice structure of the graphene layer alone. Thus \( A = 2\sqrt{3}a \) where \( A \) is the lattice constant of the entire system and \( a \) is the lattice constant of the two-dimensional graphene layer. Since both unit cells are hexagonal this implies that the reciprocal lattice structure of the graphene layer on top is a \( (2\sqrt{3}) \times (2\sqrt{3}) \) reconstruction of the reciprocal lattice structure of the graphene plus oxide system below. Taking \( \mathbf{a}_1 \) to be along \( \hat{x} \),

\[
\mathbf{a}_1 = a\hat{x}
\]  

\[
\mathbf{a}_2 = a\left(\frac{1}{2}\hat{x} + \frac{\sqrt{3}}{2}\hat{y}\right)
\]  

\[
\mathbf{a}_3 = a\left(\frac{\sqrt{3}}{2}\hat{x} + \frac{1}{2}\hat{y}\right)
\]  

The reciprocal lattice vectors are,

\[
\mathbf{b}_1 = \frac{2\pi}{a}\left(\hat{x} - \frac{1}{\sqrt{3}}\hat{y}\right)
\]  

\[
\mathbf{b}_2 = \frac{2\pi}{a}\left(-\frac{1}{2}\hat{x} + \frac{\sqrt{3}}{2}\hat{y}\right)
\]  

\[
\mathbf{b}_3 = \frac{2\pi}{a}\left(-\frac{\sqrt{3}}{2}\hat{x} - \frac{1}{2}\hat{y}\right)
\]  

\[
\mathbf{b}_4 = \frac{2\pi}{a}\left(-\frac{1}{2}\hat{x} - \frac{\sqrt{3}}{2}\hat{y}\right)
\]

\[
\mathbf{b}_5 = \frac{2\pi}{a}\left(-\frac{\sqrt{3}}{2}\hat{x} + \frac{1}{2}\hat{y}\right)
\]

\[
\mathbf{b}_6 = \frac{2\pi}{a}\left(\hat{y}\right)
\]
This means that the K vector lies on the reciprocal lattice vector \( \mathbf{b}_1 \) of the supercell. The overlap is due to the symmetry reasons and is explained in the text.

\[ \tilde{\mathbf{b}}_2 = \frac{2\pi}{a} \left( \frac{2}{\sqrt{3}} \hat{y} \right) \quad (A.7) \]

\[ \tilde{\mathbf{B}}_1 = \frac{2\pi}{2\sqrt{3}a} \left( \frac{2}{\sqrt{3}} \hat{x} \right) \quad (A.8) \]

\[ \tilde{\mathbf{B}}_2 = \frac{2\pi}{2\sqrt{3}a} \left( -\frac{1}{\sqrt{3}} \hat{x} + \hat{y} \right) \quad (A.9) \]

Figure A.1 shows the BZ set-up with these vectors using equations (A.6)–(A.9).

Now if we take the same \( \Gamma \) point as the center of both the BZs and draw the reciprocal unit cell of both the structures, we realize that the \( \mathbf{K} \) point of only the graphene layer lies on the reciprocal lattice vector \( \mathbf{\tilde{B}}_1 \) of the graphene plus oxide system (as shown in figure). This means that the \( \mathbf{K} \) point of graphene layer folds in by symmetry onto the \( \Gamma \) point of the entire system.

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