Electronic States of Silicene and Germanene on Amorphous Alumina

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Abstract

We investigated the optimized structures and electronic states of silicene and germanene adsorbed on amorphous Al₂O₃ surface by the first-principles calculations. We found that the silicene is adsorbed on amorphous Al₂O₃ stronger than the germanene. Accordingly, the electronic states of silicene are affected more than germanene. However, in both cases, the electronic states around K point are affected by the interactions with the surface atoms.

1. Introduction

Two-dimensional crystals consisting of group IV element heavier than carbon, such as silicene, germanene, and stanene, are supreme thin-film materials. They have been theoretically predicted to possess high carrier mobility and some intriguing functions such as band-gap control and topological insulator [1,2]. They have been recently synthesized on metallic substrate [3-6]. However, it has been reported that the electronic state of silicene on a metallic substrate are dramatically modified by the strong interactions with the surface atoms [7,8]. This indicates that one cannot utilize the intriguing electronic states inherent in two-dimensional crystals successfully and perfectly when they are placed on a metallic substrate. Therefore, toward the device fabrication utilizing the electronic states inherent in the two-dimensional crystals, it is prerequisite for understanding their properties on insulating substrates. In this study, we investigate the electronic states of silicene and germanene adsorbed on amorphous Al₂O₃ surface by the first-principles calculations.

2. Method and Model

The calculations were performed using the VASP (Vienna ab-initio simulation package) code [9,10], which is based on the density functional theory (DFT). The projected-augmented-wave potential was used to describe the interactions between ionic core and valence electrons [11]. We employed the exchange-correlation functional of Perdew-Burke-Ernzerhof-type generalized gradient approximation [12]. All atomic configurations were relaxed until the Hellmann-Feynman force becomes smaller than 5 meV/Å. The atomic configurations were drawn by VESTA (visualization for electronic and structural analysis) [13].

A typical calculation model and the corresponding effective potential are shown in Fig.1(a) and (b), respectively. The primitive translation vectors of the unit cell are $a_1 = 3(a/2, -\sqrt{3}a/2, 0)$, $a_2 = 3(a/2, \sqrt{3}a/2, 0)$, $a_3 = (0, 0, c)$, where a = 3.87Å and c = 50.0Å for 3×3 silicene and

 $a = 4.06\text{\AA}$ and $c = 50.0\text{\AA}$ for 3×3 germanene on amorphous Al₂O₃. The amorphous Al₂O₃ surface was simulated by the slab model. In this study, a silicene or germanene was adsorbed only on one surface. In general, an artificial dipole field is induced in vacuum of such a slab model. In order to remove the artificial field, we utilized the dipole correction scheme [14]. It is observed in Fig.1(b) that there is no electric field in vacuum except for the switching point of the dipole correction.

3. Results

The optimized atomic configurations of silicene and germanene on amorphous Al_2O_3 are shown in Fig.2(a) and (b), respectively. We can see from Fig.2 that silicene on amorphous Al_2O_3 is distorted moderately and germanene on amorphous Al_2O_3 keeps clear honeycomb structure. This means that the silicene is adsorbed on amorphous Al_2O_3 stronger than the germanene, within the generalized gradient approximation.

Figure 3 represents the electronic band structures of (a) silicene and (b) germanene on amorphous Al_2O_3 , respectively. The red dots indicate the band structures of freestanding ones. We find from Fig.3(a) that the electronic states of silicene are clearly affected due to the interactions with the surface atoms, especially around K point. In addition, we can see from the electronic states around K point that the electrons of the silicene were transferred to the surface. On the other hand, the electronic states of germanene are unchanged from the free-standing one except for the electronic states at K point, as seen in Fig.3(b). The band gap opens at K point owing to the interactions with the surface atoms, as well as the silicene case. However, in both cases, a state remains in the gap.

4. Summary

The optimized structures and the electronic states of silicene and germanene adsorbed on amorphous Al_2O_3 surface were investigated by the first-principles calculations. We found that silicene has larger interactions with amorphous Al_2O_3 surface than germanene. In our presentation, we will discuss the details about the electronic states in relation to the surface adsorptions.

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Fig. 1 (a) A slab model for silicene on amorphous Al₂O₃ surface. The small (red), middle (blue), and large (sky blue) circles correspond to oxygen, silicon and aluminum atoms, respectively. The periodic boundary conditions are imposed on any directions. The vacuum length is about 25Å. (b) The effective potential Veff of (a). The origin is set to the Fermi energy.

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Fig. 2 The optimized atomic configurations of (a) silicene and (b) germanene on amorphous Al_2O_3 . The blue circles in (a) and the purple circles in (b) correspond to silicon and germanium atoms, respectively. In both (a) and (b), the left panel is the side view and the right panel is the top view.



Fig. 3 Electronic band structures (blue dots) of (a) silicene and (b) germanene on amorphous Al₂O₃ surface. The red dots indicate the band structures of freestanding silicene and germanene. The energy origin is set to the Fermi energy. The vasp_unfold code [15] was used to draw the unfolded band structures.