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Hydrogen Concentration and Electric Field Dependent on Electronic Properties of Germanene

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Abstract. Electronic properties of the pristine/hydrogenated germanene are investigated by means of first principles calculations. Our calculation shows interesting results where the electronic properties of the hydrogenated germanene exhibit semiconductor with a direct band gap. It is interesting because pristine germanene (germanium analogue to graphene) has semi-metal properties with zero band gap. We also obtained that the band gap of hydrogenated germanene was influenced by the hydrogen (H) concentration, it is decreasing non-linearly as the H concentration decreased. As 100 percent concentration of H applied on top and bottom layer of germanene, the band gap is 1.41 eV. The pairing of the p_z-orbital of Ge with the *s*-orbital of H gave contribution to the band gap of hydrogenated germanene. External electrical field is also can be applied to open the band gap. The band gap increasing linearly when the external electrical field increased on pristine germanene. The external electrical field no longer effect the band gap when it applied to the hydrogenated germanene.

INTRODUCTION

Two-dimensional honeycomb structure materials has attracted many researchers in order to investigate its properties and also to develop its applications. As pioneer in this kind of material, graphene (which is carbon based two-dimensional honeycomb structure material) has applied in many applications. Carbon based material, however, has compatibility problem when incorporate with silicon based technology, which has been used in electronic industry [1]. Since silicon and germanium, which are elements in the same group on the periodic table with carbon, have highly promising compatibility with silicon nano technology, so that many researchers attracted to looking for an opportunity to solve the inhibition [2].

Previously, silicon analogue to graphene (silicene) with buckled structure not only has been theoretically studied [3,4], but also has successfully grown over Ag [5,6] in experimental studies. The potentials of silicene have attracted many researchers to explore its advantages for many applications: new silicon based devices, hydrogen storage, solar cell, or gas sensor [7]. Inspired by graphene and silicene, germanene as germanium analogue to silicene also attracted to be investigated by theoretical studies [8,9]. According to previous work [8], germanene is a semiconductor with zero band gap (gapless) with linear energy dispersion near K-points. However, it would be limits germanene to be applied in electronics or photonics. Therefore, opening the band gap of germanene is highly desirable.

Generally, there are two mechanisms in order to open the band gap. The first mechanism is transforming germanium hybridization from sp^2 to sp^3. Basically, germanene has one unpaired orbital, so that valence electron can be freely move. In this present work, hydrogen atom was placed above and/or below germanium atom in boatlike configuration. Number of additional hydrogen relative to number of germanium atom was investigated in order to find the dependency of hydrogen consentration to the band gap of the system. The second mechanism is breaking the equivalence of two sublattice of germanene. In this work, external electric field which is perpendicular to germanene surface, was chosen to break the equivalence. In this work, computational method was performed in order to investigate electronical properties of germanene system for each mechanism.

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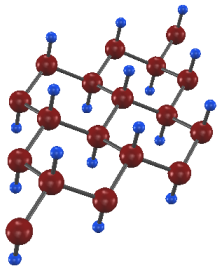

FIGURE 1. Full hydrogenated germanene with boatlike configuration: RED (germanium) BLUE (hydrogen).

COMPUTATIONAL DETAIL

Ab initio calculation based density functional theory (DFT) was performed with GGA Perdew-Burke-Ernzerhof (GGA-PPA) as exchange correlation functional. The energy cut off of the plane wave basis sets is 150 Ry. The surface of Brillouin zone was sampled by using a uniform grid (21×21×1) *k* points for SCF calculation. In density of state (DOS) calculation (15×15×1) was chosen to obtain smooth enough result, To prevent undesired interaction among the surfaces, the distance between two germanene surface sets to 40 Angstrom. (3×3×1) unit cells with 18 atoms was used as a pristine (pure) germanene. All calculation are carried out using program package called OpenMX[1].

RESULTS AND DISCUSSION

Hydrogenated Germanene

As mention earlier, to open the band gap, the hydrogen atom with *s*-orbital was placed in boatlike configuration (shown in Figure 1). Hydrogen and germanium would be bounded with *sp*-bond. As initial step, after relaxed atom position, the full hydrogenated germanene was calculated and the band gap opened in 1.41 eV. This result shows good agreement with other work [10] Next, by removing hydrogen atom one by one randomly, density of state for each hydrogenated system was calculated in order to check the band gap energy for each concentration hydrogen. As shown in Figure 2, the band gap decrease non-linearly when hydrogen was removed one by one. The result shows similar form with other work for hydrogenated graphene [11]. By fitting with third order polinomial, relationship for band gap energy (E_{gap} in eV) versus hidrogen consentration (x in %) in range between 60-100 % can be written as:

$$E_{gap} = 0.0005x^3 - 0.012x^2 + 1.025x - 28.13$$

As shown in Figure 3, some graphics of DOS has midstate. It comes from single hydrogen vacancy when removed from the system. Due to randomly removal, it possible to found single vacancy of hydrogen in the system. According to Gao *et. al.* [11], it can be handled by paired H vacancies.

Pristine/Hydrogenated Germanene Under External Electrical Field

In this part, the second mechanism of opening band gap is used by applying external electric field perpendicular to germanene surface. External electric field affects the linearity of the energy bands around the Fermi energy of germanene. From Dirac-like Hamiltonian:

$$\hat{H} = \begin{pmatrix} \Delta & \hbar v_f (k_x - ik_y) \\ \hbar v_f (k_x - ik_y) & \Delta \end{pmatrix}$$

where, Δ is onsite energy difference between the nearest sublattice. In full symmetrical condition, this difference should be zero, so that $E(k)=\pm\hbar v_f k$. This is the origin of linearity of energy with k closed to zero. Yet, under the

[1] http://www.openmx-square.org

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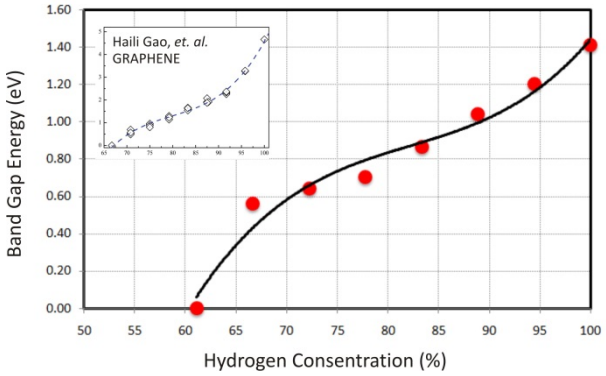

FIGURE 2. Relationship between hydrogen consentration and band gap energy.

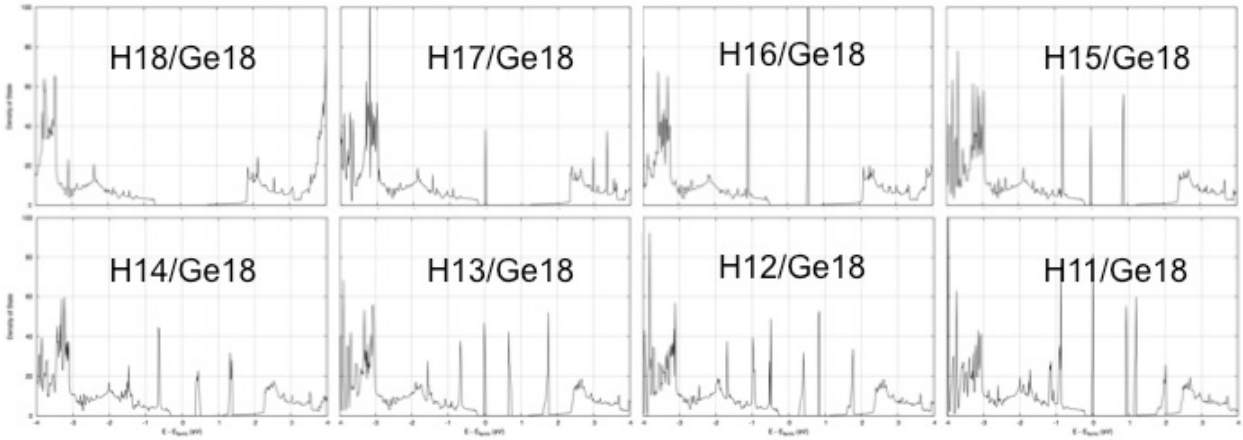

FIGURE 3. Density of state for each hydrogen consentration of hydrogenated germanene.

external electrical field, Δ is no longer zero. The energy can be written as $E(k)=\pm(\hbar v_f k+\Delta^2)^{1/2}$. For k closed to zero, $E(k)=\pm\Delta$. Thus, the band gap energy can be written as $E_{gap}=2\Delta$. Figure 4 shows good agreement with this derivation. External electrical field can be used to break the symmetry of sublattice. Effect of external electric field was also checked for hydrogenated germanene. The flat result in Figure 5 shows that the system keep the structure eventhough under various external electrical field.

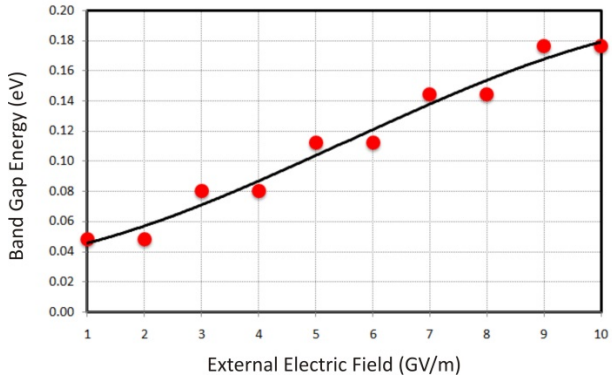

FIGURE 4. Relationship between external electrical field and band gap energy on pristine germanene.

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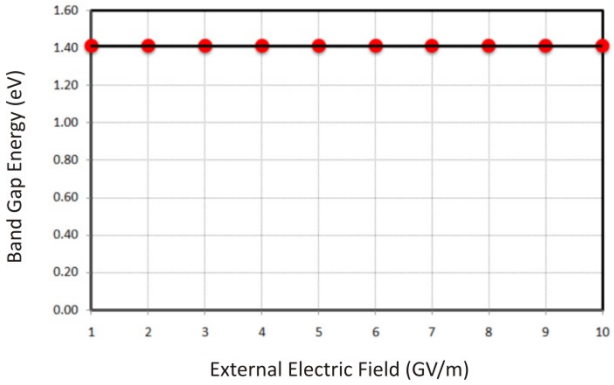

FIGURE 5. Relationship between external electrical field and band gap energy on full hydrogenated germanene

SUMMARY

Density functional theory has been applied to investigate hydrogen consentration and external electrical field effects for opening band gap of pristine/hydrogenated germanene. Band gap energy is appear in range 60-100 percent hydrogen consentration. The results was comparable with others work which is non-linearly decrease while the hydrogen consentration is decresing. External electrical field is also can be used to open the band gap. The band gap increasing linearly when the external electrical field increased. The external electrical field no longer effect the band gap when it applied to the hydrogenated germanene.

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