Orientation and strain modulated electronic structures in puckered arsenene nanoribbons

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Abstract

Orthorhombic arsenene was recently predicted as an indirect bandgap semiconductor. Here, we demonstrate that nanostructuring arsenene into nanoribbons can successfully transform the bandgap to be direct. It is found that direct bandgaps hold for narrow armchair but wide zigzag nanoribbons, which is dominated by the competition between the in-plane and out-of-plane bondings. Moreover, straining the nanoribbons also induces a direct bandgap and simultaneously modulates effectively the transport property. The gap energy is largely enhanced by applying tensile strains to the armchair structures. In the zigzag ones, a tensile strain makes the effective mass of holes much higher while a compressive strain cause it much lower than that of electrons. Our results are crucial to understand and engineer the electronic properties of two dimensional materials beyond the planar ones like graphene.

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I. INTRODUCTION

Graphene, an ideal two-dimensional (2D) material, has charmed materials researchers with its peculiar electronic properties that allow electrons to move freely within its surface at high speed \[1-4\]. But it lacks a natural bandgap, which is a mandatory feature to control the electric flow on and off. This largely undermines graphene’s usefulness as a replacement for the mainstream semiconductors in optoelectronics. Just recently, few-layer arsenic was demonstrated to be an alternative 2D semiconductor \[5-7\]. It has a sizable bandgap (around 1 eV) and simultaneously retains a considerable carrier mobility (several thousand square centimeters per volt-second). From the point of view of applications, nanodevices are expected to be fabricated by using a single atomic layer, wherein electron are strictly confined within the surface. In principle, this allows the fastest flow of carriers across the surface, like graphene. Unfortunately, the intrinsic bandgap of monolayer arsenic (arsenene) is indirect, which is not desired for realistic device applications.

Generally, fabricating nanoribbons of materials are expected to have large changes in electronic properties due to the edge and nanoscale size effect \[8-11\]. Along this perspective, a study on arsenene nanoribbons would be an interesting research topic. It is expected to modulate the electronic structures of arsenene and possibly to introduce an indirect-direct bandgap transition. On the other hand, in practical applications, especially in nano-devices, the involved materials are always thin strips with edges. In experiments, arsenene nanoribbons can be obtained either by cutting mechanically exfoliated arsenene, or by patterning epitaxially-grown arsenene. Especially, the technique of scanning tunneling microscope (STM) lithography allow producing any pattern, width and edge shape of nanoribbons \[12\]. In this respect, it is timely and crucial to thoroughly investigate the electronic properties of arsenene nanoribbons to extend their use in semiconducting industry. However, as far as our knowledge goes, there is no such study committed up to now.

In this work, two types of hydrogen passivated arsenene nanoribbons with armchair (aANRs) and zigzag (zANRs) edges are considered and their electronic structures are investigated by employing density functional theory (DFT) calculations. Our calculations demonstrate that indirect-direct bandgap transition is possible in both aANRs ad zANRs only by changing the ribbon width. Most interestingly, the indirect-direct bandgap transition holds for narrow aANRs but wide zANRs. Furthermore, straining the nanoribbons can
also transform the bandgap to be direct. At the same time, the effective masses of carriers can be largely modified under stains. All these properties make arsene as an appealing 2D materials for future applications in optoelectronics.

The rest of this paper is arranged as follows. In Sec. II, we briefly describe the method used in this work. Results and discussion are represented in Sec. III. Finally, we conclude our work in Sec. IV.

II. THEORETICAL METHOD

All the calculations in this work are performed with Vienna *ab initio* Simulation Package (VASP) [13, 14]. The generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) functional [15] is adopted to describe the exchange-correlation energy between electrons within the projector augmented wave (PAW) method [16]. The plane wave energy cutoff is set to 450 eV to ensure the convergence of total energy. Structural optimizations are applied by relaxing the positions of all the atoms until the convergence tolerance of force on each atom is less than 0.01 eV/Å. Periodic boundary condition is used to simulate the 2D infinite sheet. A vacuum space at least 10 Å is used to avoid the interaction between periodic images. The reciprocal space is sampled by a fine grid of Gamma-centered Monkhorst-Pack’s mesh $11 \times 1 \times 1$ in the Brillouin zone.

III. RESULTS AND DISCUSSION

A. Geometric properties of arsene nanoribbons.

By cutting arsene sheet perpendicular to the zigzag and armchair directions, two types nanoribbons with armchair (aANRs) and zigzag (zANRs) edges are respectively generated. These aANRs and zANRs are further classified by the number of As-As rings ($N_r$) contained in the structure. Wherein, each As-As ring includes six As atoms, as illustrated in the planar view in Figs. 1(a) and 1(b). An aANR (zANR) with $N_r$ As-As rings is represented as $N_r$-aANR ($N_r$-zANR). Two structures of 4-aANR and 4-zANR ($N_r = 4$) are respectively given in Figs. 1(a) and 1(b) for examples. It should be noted that all the nanoribbons considered in our calculations are passivated with hydrogen. For an evaluation of the thermal stability,
the edge formation energy \( (\mathcal{E}_{\text{edge}}) \) is estimated as

\[
\mathcal{E}_{\text{edge}} = \frac{1}{2W_D} (E_{\text{ribbon}} - N_a E_a - \frac{N_H}{2} E_{H_2})
\]

where \( W_D \) is the width of the nanoribbon, \( E_{\text{ribbon}} \) is the total energy of the nanoribbon, \( N_a \) is the number of As atoms in the nanoribbon, \( E_a \) is the energy of arsenene per atom, \( N_H \) is the number of hydrogen atoms, and \( E_{H_2} \) is the energy of a H\(_2\) molecule. Our calculation results (see Fig. 1(c)) indicate that the formation of edges are slightly endothermic for both aANRs and zANRs, and the order of stability is zANRs > aANRs. Of the nanoribbons, the armchair ones are more easily to be stretched than to be compressed, with respect to that the total energy under stretching is much lower than that under compressing (see the left scale of Fig. 1(d)). Stretching and compressing the zigzag ones are revealed to be nearly equivalent (see the right scale of Fig. 1(d)). Additionally, a basic knowledge of the bonding feature of arsenene is necessary to understand the electronic properties. As illustrated in the inset of Fig. 1(c), each unit cell of arsenene includes four inequivalent As atoms. Wherein, the \( r_1 \) and \( \theta_1 \) describe mainly the in-plane bondings, and in contrast, the \( r_2 \) and \( \theta_2 \) represent primarily the out-of-plane bondings. Changes of these parameters will spark a huge effect on electronic structures, as discussed in the following parts.

**B. Electronic structures of aANRs**

Usually, nanostructuring a semiconducting material into nanoribbons can modulate effectively the gap value \( (\mathcal{E}_{g}) \) due to the quantum confinement effect \([11, 17, 18]\). It is true in our case. As can be found in Fig. 2, the amplitude of bandgap in aANRs gradually increases when it goes from 8-aANR to 2-aANR. The gap value scales inversely with the ribbon’s width of \( W_D \), as listed in Tab. 1. The \( \mathcal{E}_{g} \) increases from 0.79 eV to 1.15 eV with \( W_D \) changing from 31.7 Å to 9.5 Å. Besides, it is found that the nature of the bandgap (i.e., direct or indirect) largely depends on the ribbon’s width. An indirect-direct bandgap transition takes place when reducing the ribbon’s width. As shown in Figs. 2(a)-2(c), 2-aANR, 3-aANR and 4-aANR exhibit direct bandgaps. Both the conduction band minimum (CBM) and valence band maximum (VBM) locate at the same crystal point \( \Gamma \). While in 5-aANR (Fig. 2(d)), 6-aANR (Fig. 2(e)), 7-aANR (Fig. 2(f)) and 8-aANR (Fig. 2(g)), the bandgaps appear as indirect. The CBM is still located at the \( \Gamma \) point while the VBM rises along the
Γ-X line and close to the X point. Among the aANRs, direct bandgaps are grasped by the narrower ones with $W_D \leq 16.9 \, \text{Å}$. Indeed, such an indirect-direct bandgap transition reflects the structural modifications when arsenene is cut into nanoribbon structures. From inspection of Tab. I, one should have noticed that along with reducing the ribbon’s width, the lattice constant along the infinite direction (denoted as ‘$a$’ in Tab. I) decreases. This consequently affects the bond lengths of $r_1$ and $r_2$ and the bond angles of $\theta_1$ and $\theta_2$. When the ribbon’s width is reduced, $r_1$ increases while $r_2$ decreases (Fig. 4(a)); $\theta_1$ increases in contrast to $\theta_2$ decreasing (Fig. 4(b)). As it is found, the increase in one of the bond lengths (or angles) leads to decrease in the other bond length (or angle). At narrower width, both $r_2$ and $\theta_2$ are more decreased. As a result, the out-of-plane bondings, mainly $p_z$-orbital alike, is strengthened. An decrease in energy is a natural consequence. This effect is clearly demonstrated from the orbital-resolved density of states (DOS), as displayed in the bottom panels in Fig. 2. In the narrower structures, such as 2-aANR (Fig. 2(a)), 3-aANR (Fig. 2(b)) and 4-aANR (Fig. 2(c)), the $p_z$ orbitals occupy a lower energy in the valence band (VB) and the VBM is dominated by the $p_y$ orbitals of in-plane bondings. While in the wider ones from 5-aANR to 8-aANR (see Figs. 2(d)-2(g)), the case is converse. The $p_z$ orbitals rise in energy and predominate the VBM. Such a competition between the in-plane and the out-of-plane bondings manipulate the energy gap to be direct or indirect.

By using the nearly free electron model, the effective mass of holes at the VBM ($m^*_h$) and of electrons at the CBM ($m^*_e$) are calculated using $m^* = \hbar^2/(\partial^2 E/\partial k^2)$. In this work, we only concern the $m^*_h$ and $m^*_e$ at the Γ point in direct bandgaps. We find that $m^*_h$ and $m^*_e$ are comparable in aANRs. In 16.96 Å wide 4-aANR, $m^*_h = 0.24m_0$ and $m^*_e = 0.30m_0$ ($m_0$ is the static electron mass). Nanostructuring modifies these values slightly, for example, in the narrowest 9.53 Å wide 2-aANR, $m^*_h = 0.37m_0$ and $m^*_e = 0.45m_0$.

C. Electronic structures of zANRs

Now, we switch our attention to zANRs. The quantum confinement effect is obviously observed in zANRs. The $E_g$ increases from 1.06 eV to 1.87 eV by decreasing the $W_D$ from 37.7 Å to 8.9 Å (see Tab. I). Strikingly different from the case of aANRs, in zANRs, the indirect-direct bandgap transition happens when increasing the ribbon’s width of $W_D$. As
displayed in Figs. 3(a)-3(d), the bandgaps are indirect in \( N_r \)-zANR with \( N_r \leq 5 \) (\( W_D \leq 23.4 \ \text{Å} \)). The CBM occurs at the \( \Gamma \) point while the VBM lies along the \( \Gamma \)-X line and close to the \( \Gamma \) point. As the ribbon width is increased up to \( \sim 28.2 \ \text{Å} \), the bandgap turns to be direct with both the CBM and VBM located at the \( \Gamma \) point. Therefore, direct bandgaps hold for the relatively wider zigzag nanoribbons. In contrast to that in aANRs, the values of \( m_h^* \) and \( m_e^* \) in zANRs are relatively larger. In 6-zANR, \( m_h^* = 5.96m_0 \) and \( m_e^* = 5.09m_0 \). While in 8-zANR, \( m_h^* = 1.63m_0 \) and \( m_e^* = 1.25m_0 \).

Similar with that in aANRs, the indirect-direct bandgap transition in zANRs is closely related to the structural changes, as illustrated in Figs. 4(c) and 4(d). By widening the ribbon’s width, the lattice constant along the infinite direction (represented as ‘\( b \)’ in Tab. I) increases. As a result, the values of \( r_2 \) and \( \theta_2 \) keep almost unchanged; whereas, \( r_1 \) and \( \theta_1 \) are increased. The increase in \( r_1 \) and \( \theta_1 \) will weaken the in-plane covalent bondings and give rise to an energy increase correspondingly. This is why the VBM in the wider structures are predominated by the in-plane \( p_y \) orbitals (from 6-zANR to 8-zANR, see Figs. 3(e)-3(g)). Oppositely, the VBM is occupied by the \( p_z \) orbitals in the narrower ones from 2-zANR to 5-zANR (see Figs. 3(a)-3(d)). Here also we clearly see the indirect-direct bandgap transition is controlled by a competition between the in-plane and out-of-plane bondings. The mechanism is the same as that discussed above in aANRs. It is that, contracted in-plane bonding parameters (\( r_1 \) and \( \theta_1 \)) stabilize the \( p_y \) orbitals in the VB; shrunked out-of-plane bonding parameters (\( r_2 \) and \( \theta_2 \)) stabilize the \( p_z \) orbitals. The relatively higher energy states ultimately dictate the VBM. We should note that these structural changes occur naturally at different ribbon’s widths. Further reducing the parameters by external fields, such as straining, will cause an energy increase, discussed as below.

Based on the above discussion, it is highly expected to achieve direct bandgaps by manufacturing narrow armchair or wide zigzag arsenene nanoribbons. Our results are insightful in consideration of the following two aspects. First, an intrinsic direct bandgap make arsenene applicable in optoelectronics devices. Also, it would be of great interest for valleytronic applications via achieving degenerate energy valleys at different \( k \)-points \cite{19,22}. Second, the indirect-direct bandgap transition observed in arsenene nanoribbons provides researchers with solid evidence to engineer the bandgap properties of similarly puckered structures or other non-planar structures. Future experiments can test our proposal directly.

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D. Electronic structures of aANRs at strains

To further understand the effects of structural changes and engineer the electronic properties of the nanoribbons, strain is applied along the infinite direction of each type of nanoribbons. The magnitude of the strains are employed up to a magnitude of ±10%, which is physically realizable considering that it is much lower than the theoretical ultimate strain of the puckered structure [7, 23]. We assign the positive (negative) values of \( \varepsilon \) for tensile (compressive) strains, respectively. Here, we present the results for 5-aANR and 5-zANR only but similar trends hold for other ribbon widths.

As illustrated in Fig. 5, the armchair structure is particularly sensitive to tensile strains. Although 5-aANR possesses an intrinsic indirect bandgap, a very low tensile strain of \( \varepsilon = +1\% \) successfully induce a direct bandgap. By contrast, a much higher compressive strain of \( \varepsilon = -10\% \) is required to make the transition happen. Additionally, tensile strains apparently enhance the bandgap width. As strain is applied between \( \varepsilon = +1\% \) and \( \varepsilon = +10\% \), the bandgap increases from 0.94 eV to 1.12 eV (see Tab. II). In contrast, compressive strain reduces the energy gap. Straining the structure at \( \varepsilon = -1\% \) and \( \varepsilon = -10\% \) corresponds to the gap values of 0.86eV and 0.61 eV, respectively.

An analysis of the geometric structures is necessary to understand the band structures changes. The analysis results are plotted in Figs. 7(a) and 7(b). Both the bond length \((r_1\text{ and } r_2)\) and bond angle \((\theta_1\text{ and } \theta_2)\) change linearly with the amount of strain. When straining is applied from \( \varepsilon = -10\% \) to \( \varepsilon = +10\% \), \( r_1 \) and \( \theta_1 \) decrease while \( r_2 \) and \( \theta_2 \) increase. A closer look at the orbital-resolved DOS plots in Fig. 5 reveals that such structural changes makes the VBM is first dominated mainly by \( p_x \) and \( p_z \) orbitals (from \( \varepsilon = -10\% \) to \( \varepsilon = +2\% \)), then by \( p_y \) and \( p_z \) orbitals (from \( \varepsilon = +5\% \) to \( \varepsilon = +7\% \)), and finally by only the \( p_y \) orbitals (\( \varepsilon = +10\% \)). As discussed previously, the VBM of 5-aANR under zero strain is comprised of \( p_x \) and \( p_z \) orbitals (see Fig. 2(d)). Stretching this armchair structure along the armchair direction seems to be capable of stabilizing the \( p_x \) and \( p_z \) orbitals. Hence, the \( p_x \) and \( p_z \) orbitals occupy the relative lower energy and the \( p_y \) orbitals dominate the VBM. Similar phenomenon was observed in the similar structure of armchair puckered phosphorene nanoribbons [11]. In addition, at stretching strains, both \( m_h^* \) and \( m_e^* \) is lowered slightly in comparison with the case of no strain (see Tab. II). However, this does not affect the carrier transport property much since the ratio \( m_h^*/m_e^* \) keeps almost unchanged.
E. Electronic structures of zANRs at strains

The calculated band structures of 5-zANR at various strains are presented in Fig. 6. We can see that, at a low tensile or compressive strain of $|\varepsilon| < 5\%$, the bandgap remains as indirect. In a contrast, more strengthened stretching ($\varepsilon > +5\%$) or compressing ($\varepsilon < -5\%$) make the bandgap transfer from indirect to direct. In addition to this, in contrast to that in aANRs, both tensile and compressive strains result in decreased bandgaps in 5-zANR (see Tab. II). The gap energy decreases from 1.21 eV to 0.24 eV when straining is increased from $\varepsilon = 0$ to $\varepsilon = +10\%$. The value changes from 1.21 eV to 0.32 eV when strain is applied from $\varepsilon = 0$ to $\varepsilon = -10\%$.

The structural changes of 5-zANR at various strains are plotted in Figs. 7(c) and 7(d). Both the bond length ($r_1$ and $r_2$) and bond angle ($\theta_1$ and $\theta_2$) change linearly with the amount of strain. As the strain varies from $\varepsilon = -10\%$ to $\varepsilon = +10\%$, $r_1$ and $\theta_1$ increase while $r_2$ and $\theta_2$ decrease. This consequently imposes an influence on the electronic states near the VBM. At compressive strains, the VBM is composed mainly with the in-plane bondings of $p_x$ orbitals (from $\varepsilon = -10\%$ to $\varepsilon = -7\%$) and of $p_y$ orbitals (from $\varepsilon = -5\%$ to $\varepsilon = -1\%$). By comparison, at all tensile strains from $\varepsilon = +1\%$ to $\varepsilon = +10\%$, the VBM is predominated by the out-of-plane bondings of $p_x$ orbitals. This is because that, around the optimized structures, reducing the $r_1$ and $\theta_1$ causes an energy increase of the in-plane bondings of $p_x$ and $p_y$ orbitals; decreasing the $r_2$ and $\theta_2$ lead to the energy increase of the out-of-plane bondings of $p_x$ orbitals, sharing the same mechanism as that in strained aANRs. In addition, straining effectively tune the $m^*_h$ and $m^*_e$, especially the ratio of $m^*_h/m^*_e$ (see Tab. II). At strains of $\varepsilon > 0$, $m^*_h$ is much larger than $m^*_e$. The ratio of $m^*_h/m^*_e$ is around 3.7-6.5. In a sharp contrast, at strains of $\varepsilon < 0$, $m^*_h$ is much smaller than $m^*_e$ with the ration of $m^*_h/m^*_e = 0.1-0.2$.

IV. CONCLUSION

In summary, two types of arsenene nanoribbons are constructed and modeled. An indirect-direct bandgap transition is successfully realized by cutting narrow aANRs and wide zANRs. The indirect-direct bandgap transition is dominated by the competition between the in-plane and out-of-plane bondings. The energy gap of these nanoribbons can be modulated over a wide range by varying the ribbon’s width. Placing aANRs and zANRs
under strains significantly modifies the band structures as well as the carrier transport properties. Either stretching or compressing the nanoribbons with an appropriate strength can implement an indirect-direct bandgap transition in both aANRs and zANRs. In addition, in aANRs, the energy gap can be largely enhanced by applying tensile strains. In zANRs, tensile strain results in $m_h^*$ much larger than $m_e^*$ while compressive strain makes $m_h^*$ much smaller than $m_e^*$. Our results demonstrate the wide possibilities to tune the electronic properties of two dimensional puckered structures. Further experimental investigations of these structures would be of great interest.

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FIG. 1: (color online) The planar views of arsenene nanoribbons with edges of (a) armchair and (b) zigzag. The edges are passivated with hydrogen atoms represented by small blue balls. Both the structures contain four As-As rings in width and hence are denoted as (a) 4-aANR and (b) 4-zANR. Each As-As ring includes six As atoms, indicated by blue rectangles. (c) The calculated edge formation energy ($E_{\text{edge}}$) for aANRs (black cubics) and zANRs (red circles) depending on the number of As-As rings ($N_r$). The inset of the (c) displays the constructing unit of arsenene. The $r_1$ and $\theta_1$ describe mainly the in-plane bondings, and the $r_2$ and $\theta_2$ represent primarily the out-of-plane bondings. (d) The total energy changes under straining in 4-aANR (black cubics, left scale) and 4-zANR (red circles, right scale). The positive (negative) values stand for tensile (compressive) strains, respectively.
FIG. 2: (color online) Top panels: band structures for $N_r$-aANR with (a) $N_r = 2$, (b) $N_r = 3$, (c) $N_r = 4$, (d) $N_r = 5$, (e) $N_r = 6$, (f) $N_r = 7$ and (g) $N_r = 8$. Vertical blue arrows indicate direct bandgaps and tilted red arrows represent indirect bandgaps. The valence band maxima for the indirect bandgaps are marked with vertical dotted lines. The horizontal dotted lines represent the Fermi energy level ($E_F$). Bottom panels: orbital-resolved density of states (DOS) for the corresponding band structures. The vertical dotted lines in the DOS plots represent the $E_F$ levels.
FIG. 3: (color online) Top panels: band structures for $N_r$-zANR with (a) $N_r = 2$, (b) $N_r = 3$, (c) $N_r = 4$, (d) $N_r = 5$, (e) $N_r = 6$, (f) $N_r = 7$ and (g) $N_r = 8$. Tilted red arrows represent indirect bandgaps and vertical blue arrows indicate direct bandgaps. The valence band maxima for the indirect bandgaps are marked with vertical dotted lines. The horizontal dotted lines represent the Fermi energy level ($E_F$). Bottom panels: orbital-resolved density of states (DOS) for the corresponding band structures. The vertical dotted lines in the DOS plots represent the $E_F$ levels.
FIG. 4: (color online) The distributions of the bond lengths of $r_1$ (black cubics) and $r_2$ (red circles) depending on the number of As-As rings ($N_r$) in (a) aANRs and (c) zANRs. The changes in the bond angles of $\theta_1$ (black cubics) and $\theta_2$ (red circles) with the $N_r$ in (b) aANRs and (d) zANRs.
FIG. 5: (color online) The band structures of 5-aANR at strains between $\varepsilon = -10\%$ to $\varepsilon = +10\%$. Vertical blue arrows indicate direct bandgaps. Tilted red arrows represent indirect bandgaps. The valence band maxima for the indirect bandgaps are marked with vertical dotted lines. The horizontal dotted lines represent the Fermi energy level ($E_F$). The corresponding orbital-resolved density of states (DOS) are displayed in the right panels for each of the band structures. The dotted lines in the DOS plots represent the $E_F$ levels.
FIG. 6: (color online) The band structures of 5-zANR at strains between $\varepsilon = -10\%$ to $\varepsilon = +10\%$. Vertical blue arrows indicate direct bandgaps. Tilted red arrows represent indirect bandgaps. The valence band maxima for the indirect bandgaps are marked with vertical dotted lines. The horizontal dotted lines represent the Fermi energy level ($E_F$). The calculated orbital-resolved density of states (DOS) are displayed in the right panels for the corresponding band structures. The dotted lines in the DOS plots represent the $E_F$ levels.
FIG. 7: (color online) The dependence of bond lengths of $r_1$ (black cubics) and $r_2$ (red circles) on various strains in (a) aANRs and (c) zANRs. The changes of bond angles of $\theta_1$ (black cubics) and $\theta_2$ (red circles) with various strains in (b) aANRs and (d) zANRs.
TABLE I: Number of As-As rings \((N_r)\), nanoribbon widths \((W_D, \text{ in unit of } \text{Å})\), lattice constants \((a \text{ for aANR and } b \text{ for zANRs, in unit of } \text{Å})\) and bandgap energy \((E_g, \text{ in unit of } \text{eV})\) for aANRs and zANRs. The subscript ‘d’ marks a direct bandgap and ‘i’ denotes an indirect bandgap.

| \(N_r\) | \(W_D\) | \(a\) | \(E_g\) | \(W_D\) | \(b\) | \(E_g\) |
|--------|--------|------|--------|--------|------|--------|
| 2      | 9.5    | 4.39 | 1.15\(^d\) | 8.9    | 3.63 | 1.87\(^i\) |
| 3      | 13.3   | 4.51 | 0.99\(^d\) | 13.7   | 3.64 | 1.48\(^i\) |
| 4      | 16.9   | 4.57 | 0.94\(^d\) | 18.6   | 3.65 | 1.33\(^i\) |
| 5      | 20.6   | 4.60 | 0.90\(^i\) | 23.4   | 3.66 | 1.21\(^i\) |
| 6      | 24.3   | 4.63 | 0.85\(^i\) | 28.2   | 3.66 | 1.15\(^d\) |
| 7      | 28.1   | 4.65 | 0.80\(^i\) | 32.9   | 3.66 | 1.07\(^d\) |
| 8      | 31.7   | 4.66 | 0.79\(^i\) | 37.7   | 3.67 | 1.06\(^d\) |

\(18\) (February 6, 2015)
TABLE II: Bandgaps and effective masses of carriers with respect to strains in 5-aANR and 5-zANR. The bandgap energy is represented by $E_g$ (in unit of eV). The subscript ‘d’ denotes a direct bandgap and ‘i’ represents an indirect bandgap. The effective masses of holes ($m_h^*$) and of electrons ($m_e^*$) are calculated for direct bandgaps and those for indirect bandgaps are neglected with ‘N/A’.

|       | 5-aANR     | 5-zANR     |
|-------|------------|------------|
| $\epsilon$ | $E_g$ (eV) | $m_h^*/m_0$ | $m_e^*/m_0$ | $E_g$ (eV) | $m_h^*/m_0$ | $m_e^*/m_0$ |
| +10%  | 1.12$^d$  | 0.19       | 0.21       | 0.24$^d$  | 0.41       | 0.11       |
| +7%   | 1.07$^d$  | 0.20       | 0.23       | 0.51$^d$  | 0.53       | 0.10       |
| +5%   | 1.03$^d$  | 0.20       | 0.24       | 0.71$^d$  | 0.65       | 0.10       |
| +3%   | 0.96$^d$  | 0.21       | 0.26       | 1.13$^i$  | N/A        | N/A        |
| +1%   | 0.94$^d$  | 0.22       | 0.27       | 1.17$^i$  | N/A        | N/A        |
| 0     | 0.90$^i$  | N/A        | N/A        | 1.21$^i$  | N/A        | N/A        |
| -1%   | 0.86$^i$  | N/A        | N/A        | 1.19$^i$  | N/A        | N/A        |
| -3%   | 0.82$^i$  | N/A        | N/A        | 1.20$^i$  | N/A        | N/A        |
| -5%   | 0.77$^i$  | N/A        | N/A        | 1.20$^d$  | 0.13       | 1.24       |
| -7%   | 0.70$^i$  | N/A        | N/A        | 0.92$^d$  | 0.12       | 1.23       |
| -10%  | 0.61$^i$  | 0.31       | 0.42       | 0.32$^d$  | 0.19       | 1.20       |