First principles many-body calculations of electronic structure and optical properties of SiC nanoribbons

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Received 27 October 2015, revised 28 December 2015
Accepted for publication 7 January 2016
Published 8 February 2016

Abstract
A first principles many-body approach is employed to calculate the band structure and optical response of nanometer-sized ribbons of SiC. Many-body effects are incorporated using the GW approximation, and excitonic effects are included using the Bethe–Salpeter equation. Both unpassivated and hydrogen-passivated armchair SiC nanoribbons are studied. As a consequence of low dimensionality, large quasiparticle corrections are seen to the Kohn–Sham energy gaps. In both cases quasiparticle band gaps are increased by up to 2 eV, as compared to their Kohn–Sham energy values. Inclusion of electron–hole interactions modifies the absorption spectra significantly, giving rise to strongly bound excitonic peaks in these systems. The results suggest that hydrogen passivated armchair SiC nanoribbons have the potential to be used in optoelectronic devices operating in the UV-Vis region of the spectrum. We also compute the formation energies of these nanoribbons as a function of their widths, and conclude that hydrogen-saturated ribbons will be much more stable as compared to bare ones.

Keywords: SiC, nanoribbons, GW approach, optical absorption, band structure, excitonic effects

(Some figures may appear in colour only in the online journal)
Just like carbon, it is well known that bulk SiC has several allotropes, although a layered graphitic one has not been experimentally realized so far. However, theoretical calculations have shown that graphitic SiC can be realized by using the technique of ‘extreme hole injection’ [13]. Therefore, it is conceivable that it can also be isolated in monolayer form, similar to graphene [14, 15]. Because of the fact that the basic unit of SiC contains two different atoms, a corresponding monolayer will exhibit a finite band gap. Similarly, it may be possible to synthesize SiC-based nanosstructures such as nanoribbons, nanotubes and nanodisks, etc [14, 15]. From an applications point of view, SiC nanostructures will have the advantage that their integration into the present Si-based technology will be relatively easier. Keeping this in mind, in this work we undertake a systematic electronic structure study of SiC nanoribbons (SiCNRs). Next, we briefly review the existing studies of SiC and related structures.

Consistent with intuition, various electronic structure studies have predicted SiC monolayer to be a semiconductor with a band gap of 2.5 eV [16–25]. Although, SiC monolayer has not been realized in the laboratory as yet, ultrathin graphitic SiC, which exhibits light-emitting properties, has recently been synthesized [26]. SiC microribbons [27], crystalline 3C–SiC nanobelts [28], bicrystalline SiC nanobelts [29] and crystalline SiCNRs [30] have been successfully synthesized. Nanowires of SiC have been synthesized by reacting SiO with carbon nanotubes at different temperatures [31]. First principles calculations have shown that hydrogenation of graphitic SiC can lead to the formation of stable SiC nanotubes [32].

As far as theory is concerned, SiCNRs have been studied extensively using a density-functional theory (DFT)-based first-principles methodology [17, 18, 33–41]. Sun et al [17] studied hydrogen-passivated SiCNRs using the Perdew–Wang functional (PW91) under the generalized-gradient approximation (GGA) exchange correlation scheme. They found that hydrogen passivated armchair SiCNRs (ASiCNRs) are semiconducting with a direct bandgap, which oscillates and exhibits a gradual overall increase with width. For the nanoribbons studied, they reported Kohn–Sham band gaps in the range 2.3–2.4 eV [17]. Sun et al [17] also found that unlike their graphene counterparts, hydrogen-passivated zigzag SiCNRs (ZSiCNRs) have nondegenerate spins, and were near half metallic, with the smaller gap being a few meVs, while the larger one being close to 0.6 eV. The ferrimagnetic state was reported to be most stable, with an antiparallel spin orientation between the two edges [17]. Bekaroglu et al [18] based upon their first-principles DFT-GGA calculations, reported that bare ASiCNRs have indirect band gaps in the range 1.3–1.7 eV. The same authors [18] as well as Morbec et al [41] studied the influence of vacancies on the electronic structure of SiCNRs using the DFT-GGA approach, and found that single (Si and C) vacancies induce magnetism in nonmagnetic ASiCNRs, and double (Si and C) vacancies induce magnetism in ZSiCNRs. Tang et al [40] studied bare-edge and half bare-edge ZSiCNRs using the DFT-GGA approach and reported that the bare-edge ZSiCNRs exhibit magnetic metallic behavior, while half bare edge ZSiCNRs are magnetic semiconductors with small band gap.

2. Computational details

In earlier works from our group we studied the optoelectronic properties of graphene nanoribbons using a semi-empirical
3. Results and discussion

In this section we present the results of our calculations on the quasiparticle band structure and optical absorption spectra of ASiCNRs. Before that, however, we use the same methodology to compute the band structure of the 2D SiC sheet at the GW level in order to validate our approach.

3.1. SiC monolayer

Because the calculations presented here are the first reported GW calculations on ASiCNRs, it is important to benchmark the underlying approach. Therefore, we first use the same methodology to compute the quasiparticle band structure of monolayer SiC for which GW calculations had been reported earlier by Louie and coworkers [21]. The honeycomb structure adopted for the infinite SiC sheet is shown in figure 1(a), while its calculated GW band structure is presented in figure 1(b). We obtain a direct band gap of 3.4 eV located at the K point of the Brillouin zone at the GW level, which is 0.9 eV greater than our DFT-GGA band gap of 2.5 eV. Our GW result is found to be in very good quantitative agreement with the GW value of 3.6 eV, also located at the K point, reported by the Louie group [21]. Furthermore, we also calculated the excitonic binding energy of the 2D SiC sheet using the GW+BSE approach. Figure 1(c) shows the optical absorption spectra of the sheet, with (red curve) and without (blue curve) electron–hole interactions. The difference between the two prominent peaks of these two curves gives a binding energy of 1.5 eV, which is 0.3 eV more than the value 1.2 eV reported by Louie and coworkers [21]. This agreement between the GW and BSE calculations performed using two different packages assures us of the quality of our calculations.

3.2. Quasiparticle energies of hydrogenated armchair SiC nanoribbons

First we present and discuss the results of hydrogen-passivated ASiCNRs (H-ASiCNRs), for which three different families of width—that is, \( \text{Na}_1 \), \( \text{Na}_2 \), and \( \text{Na}_3 \)—have been studied, with \( \text{Na}_p \) an integer. In the H-ASiCNRs, for \( \text{Na}_p = 6 \), is located at the K point, reported by the Louie group [21]. Furthermore, we also calculated the excitonic binding energy of the 2D SiC sheet using the GW+BSE approach. Figure 1(c) shows the optical absorption spectra of the sheet, with (red curve) and without (blue curve) electron–hole interactions. The difference between the two prominent peaks of these two curves gives a binding energy of 1.5 eV, which is 0.3 eV more than the value 1.2 eV reported by Louie and coworkers [21]. This agreement between the GW and BSE calculations performed using two different packages assures us of the quality of our calculations.

3.2. Quasiparticle energies of hydrogenated armchair SiC nanoribbons

First we present and discuss the results of hydrogen-passivated ASiCNRs (H-ASiCNRs), for which three different families of width—that is, \( \text{Na}_1 = 3p \), \( \text{Na}_2 = 3p + 1 \), and \( \text{Na}_3 = 3p + 2 \) (\( p \) an integer)—have been studied, with \( \text{Na}_p \) ranging from 4–12. The geometrical structure of H-ASiCNRs for \( \text{Na}_p = 6 \) is shown in figure 1(d), for which our optimized average Si–C bond length is 1.78 Å, while Si–H and C–H bond lengths are 1.49 Å and 1.09 Å, respectively. Table 1 presents the band gaps at the GGA and GW levels, and the exciton binding energies for \( \text{Na}_p = 6, 7, 8 \). The GW self-energy corrections increase their band gaps by 1.6–1.8 eV when compared to their GGA values. Thus, the magnitude of the increase in band gaps for H-ASiCNRs due to electron correlation effects is significantly greater than the 1 eV increase observed in the monolayer discussed in the previous section, and for the increase reported for bulk SiC [21]. The larger correction observed for nanoribbons is a consequence of enhanced Coulomb interaction effects, and reduced screening in lower dimensions.

Next, we specifically discuss the case of 6-H-ASiCNR (notation \( \text{Na}_p = 6 \)), because the other two studied H-ASiCNRs exhibit similar behavior. In figures 2(a) and (b), we present our calculated GGA and GW quasiparticle band structures of 6-H-ASiCNR, from where it is clear that the hydrogen-passivated ASiCNRs are direct band gap semiconductors as their valence band maximum (VBM) and conduction band minimum (CBM) occur at the high symmetrical point \( \Gamma \) in the Brillouin zone. Partial charge density plots for VBM and CBM of 6-H-ASiCNRs are shown in the left-hand panel of figure 2(a). These plots reveal that the main contribution to the
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VBM charge density is from electrons distributed around the carbon atoms, while electrons from both Si and C atoms contribute to the CBM charge density. Figure 2(c) shows the atom projected density of states (PDOS) of 6-H-ASiCNR. The PDOS has been plotted both for internal atoms as well as the ones located on the edges. It clearly shows that edge and internal C atoms contribute mainly to the states near to the VBM, while internal Si atoms contribute dominantly to form the states close to the CBM. The contribution of hydrogen atoms appears in the conduction band states far away from the CBM. The self-energy corrections to various bands are plotted in figure 3(a), and are dependent on their nature. The $\pi$ band states associated with the $p_z$ orbitals are perpendicular to the ribbon plane, extending into the vacuum region. As a result, the many-body interactions for the $\pi$ states are less screened, and lead to large quasiparticle corrections. On the other hand, the $\sigma$ band states lie in the plane of the ribbon, and experience greater screening. Thus, the quasiparticle corrections for the $\sigma$ states are smaller than the $\pi$ states. In H-ASiCNRs, the bands around the Fermi energy comprise only of the $\pi$ states, which exhibit corrections which are mostly linear as a function of the energy. A few points (encircled, see figure 3(a)) which deviate from the main linear region correspond to the nearly free electron states which are loosely bound to the ribbon, and have weak many-body interactions resulting in smaller quasiparticle corrections [47]. Compared to their GGA shapes, the bands not only shift but also stretch by an average 30%–40%, and even cross due to the non-uniform quasiparticle corrections resulting from the GW calculations. The family behavior of the band gaps is preserved at the GW level, as the correction is roughly proportional to the GGA band gap. Figure 3(b) shows the band gap as a function of the ribbon width in the GGA and GW approximation for H-ASiCNRs. From table 1 it is obvious that the family behaviour of DFT and GW band gaps follows the hierarchy $3p > 3p + 1 > 3p + 2$, in good agreement with earlier studies of DFT band gaps of H-ASiCNRs [17], and quite unlike H terminated graphene [46] and boron-nitride [49] nanoribbons which follow the hierarchy $3p + 1 > 3p > 3p + 2$.

3.3. Optical absorption spectra of H-ASiCNRs

Based on GW quasiparticle band structures, we calculated optical absorption spectra of H-ASiCNRs, with (GW-BSE)

Table 1. The values of GGA and quasiparticle band gaps and their difference for H-ASiCNRs are tabulated.

| $N_a$   | $E_{\text{GGA}}$ | $E_{\text{GW}}$ | $\Delta E$ | $E_\phi$ |
|---------|----------------|----------------|------------|--------|
| 6 (3p)  | 2.41           | 4.18           | 1.77       | 1.07   |
| 7 (3p + 1) | 2.38       | 4.17           | 1.79       | 1.76   |
| 8 (3p + 2) | 2.31       | 3.91           | 1.60       | 1.93   |

Note: The last column gives the highest exciton binding energy. All energy values are in eV.

![Figure 1. Geometric structures of (a) 2D SiC sheet, and (d) hydrogen passivated and (e) bare armchair SiCNRs. Both types of SiCNRs correspond to $N_a = 6$, and unit cells employed for the calculations are shown in the dashed boxes. Panels (b) and (c) show the calculated GW band structure and optical absorption spectra of the SiC sheet. Panels (f) and (g) display 2D charge density (in the units of $e$/Bohr$^3$) plots of 6-H-ASiCNR and 6-ASiCNR, respectively.](image)
Figure 2. For 6-H-ASiCNR: (a) DFT-GGA band structure (pink arrows show the charge densities corresponding to VBM and CBM). (b) GW band structures (red arrows denote interband transitions). $\delta \pi$ character of bands is also pointed out. (c) Atom projected density of states (black dashed line denotes the Fermi level).

Figure 3. (a) Quasiparticle self-energy corrections to the GGA Kohn–Sham energies. Corrections to the nearly free electron states are enclosed by ellipses (red dashed), and (b) variation of the GGA band gap and quasiparticle gaps with ribbon width for H-ASiCNRs.
and without (GW-RPA) electron–hole interaction, and results are presented in figure 4. BSE calculations were performed by including five valence and five conduction bands. The polarization direction of the radiation is assumed to be along the length of the ribbons, as significant quenching occurs in 1D systems for perpendicular directions. The blue colored curves denote the absorption due to interband transitions at the GW-RPA level. The red colored curve denotes the absorption obtained by solving the Bethe–Salpeter equation, including both the electron–electron and electron–hole interactions.

As compared to the independent particle absorption spectra, BSE-based spectra exhibit changes both in the positions of the peaks, as well as the line shapes, with excitonic states having binding energies in the range 1.07–1.93 eV. We adopt the following notation to label interband transitions: $E_{nm}$ denotes the interband transitions from the $n$th valence band to the $m$th conduction band, with the band indices counted from the Fermi level. The underlying band-to-band transitions are also marked with arrows in the band structure plot in figure 2(b). The first peak ($E_{11}$) of ribbon arises due to transitions between the highest valence band and the lowest conduction band at the zone center, while other prominent peak arises due to transitions between the second valence and conduction bands. Weak peaks in between include contributions from cross transitions between these bands. For the case of $N_w = 6, 7$, $E_{22}$ peak is the most intense one, while for $N_w = 8$ case, $E_{11}$ peak acquires significant oscillator strength and becomes the most intense peak. The binding energies of the excitons corresponding to the $E_{11}$ peak are 1.07 eV, 1.76 eV, and 1.93 eV, and for $N_w = 6, 7$, and 8, respectively. In comparison, our computed value of exciton binding energy of the SiC sheet is 1.5 eV, while that of bulk 2H-SiC is reported to be 0.1 eV [21]. Thus, exciton binding energy for and without (GW-RPA) electron–hole interaction, and results are presented in figure 4. BSE calculations were performed by including five valence and five conduction bands. The polarization direction of the radiation is assumed to be along the length of the ribbons, as significant quenching occurs in 1D systems for perpendicular directions. The blue colored curves denote the absorption due to interband transitions at the GW-RPA level. The red colored curve denotes the absorption obtained by solving the Bethe–Salpeter equation, including both the electron–electron and electron–hole interactions.

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### Table 2. Values of GGA and GW band gaps and their difference for bare ASiCNRs are tabulated.

| N   | $E_{GOA}$ | $E_{GW}$ | $\Delta E$ | $E_b$ |
|-----|-----------|-----------|------------|-------|
| 6 (3$p$) | 1.74      | 3.72      | 1.98       | 0.62  |
| 7 (3$p$ + 1) | 1.51      | 3.48      | 1.97       | 1.26  |
| 8 (3$p$ + 2) | 1.62      | 3.56      | 1.94       | 2.48  |

**Note:** The last column gives the highest exciton binding energy for the given width. All energies are in eV units.

ASiCNRs is comparable to that of the monolayer, but significantly larger than that of the 3D bulk SiC. This large difference between the exciton binding energies of ASiCNRs and bulk SiC can be attributed to their reduced dimensionality, because in reduced dimensions, electron–hole interactions get stronger as quantum confinement increases the overlap between electron and hole wave functions, leading to the formation of small radius excitons [49]. When we compare the exciton binding energies of nanoribbons of different widths, we find a strong width dependence, implying that the strength of electron–hole interactions is also strongly width dependent. This suggests that one can tune the optoelectronic properties of H-ASiCNRs which are direct band gap materials by manipulating their width, a property highly useful from the point of view of device applications.

3.4. Quasiparticle energies of bare armchair SiC nanoribbons

In this section, we present and discuss the quasiparticle band structure of bare ASiCNRs. Figure 1(e) displays the relaxed geometric structure of bare 6-ASiCNR, from which it is obvious that it undergoes significant edge reconstruction because of the dangling bonds, and the Si–C bond length at the edge is reduced from 1.78 Å to 1.69 Å. The effect of edge reconstruction is also obvious in total charge density plot of the ground states of bare 6-ASiCNRs (figure 1(g)), when compared with that of 6-H-ASiCNR (figure 1(f)). Furthermore, we find that, at all levels of theory, for the same width the band gaps of bare ASiCNRs are smaller as compared to those of H-ASiCNRs. At the DFT-GGA level, they are smaller by ≈0.7 eV , a result in agreement with the results of previous theoretical studies [18], while at the GW level, the difference reduces to ≈0.3–0.4 eV. For bare ASiCNRs we also studied the family behavior by considering widths of $N_w = 6$ (3$p$), 7 (3$p$ + 1), 8 (3$p$ + 2); the results of our calculations are presented in the table 2. Figure 5 displays the calculated GGA and GW band structures for $N_w = 6$. From the figure and the table it is obvious that, as in the case of hydrogen-passivated ribbons, quasiparticle corrections due to the GW approach broaden the band gaps of bare ASiCNRs also by about 2 eV. However, unlike the hydrogen-passivated ribbons, the bare ASiCNRs exhibit an indirect band gap because the top of the valence band and the bottom of the conduction band are located at points $\Gamma$ and $Z$ of the Brillouin zone, respectively, whereas in H-ASiCNRs both were located at the $\Gamma$ point. As shown in figure 5, as compared to H-ASiCNRs, for the case of bare ASiCNRs we can observe that two new, relatively flatter bands, appear near both
the CBM and the VBM. As far as the CBM region is concerned, it is now entirely composed of these two new bands, while for the valence band case, the new bands are slightly away from the VBM. This restructuring of the band structure caused by hydrogen removal leads not only to a reduced band gap, but also transforms bare ASiCNRs into indirect band gap materials, as compared to H-ASiCNRs. Charge density analysis reveals that these additional valence and conduction bands are due to the dangling edge bonds and because the electrons involved do not participate in the bond formation, they have relatively less interaction with each other, leading to flatter bands. Partial charge density plots for VBM and CBM of bare ASiCNRs are presented in figure 5(a). A comparison with the corresponding plots of H-ASiCNRs reveals that: (a) VBM of bare ribbons are similar to the case of hydrogen saturated ones in that they derive their charge density contributions from the same set of carbon atoms, and (b) CBMs of bare ribbons are entirely different from those of the saturated ones in that their charged density is almost entirely due to the edge silicon atoms. From the PDOS plots of bare ASiCNRs presented in figure 5(c), one can deduce that the main contribution to the states near VBM is from interior C atoms, while the contribution to the states near CBM is mainly due to the edge Si atoms.

In figure 6(a), we show the self-energy corrections for ASiCNRs as a function of energies. The corrections to the GGA eigenvalues of bare ribbons are qualitatively similar to those for H-ASiCNRs, with the corrections to the $\pi$ states being larger as compared to those for the $\sigma$ states, and exhibit a linear variation with respect to the energy. The states enclosed in a red circle, which deviate from the main region, represent corrections to the conduction band states localized on the edge atoms. In figure 6(b) we present the variation of the band gap as a function of the ribbon width, and it is clear that bare ASiCNRs follow the same trends as H-ASiCNRs in that the band gap exhibits oscillatory behavior. For the largest width considered ($N_y = 12$), the GW band gap of H-ASiCNR is 0.64 eV larger than that of the SiC sheet, while for bare ribbon the same difference is 0.46 eV. With increasing width, band gaps of hydrogen-passivated nanoribbons are expected to approach the band gap of the SiC monolayer, while in the case of bare ones it is unlikely because of the presence of flat bands (figure 5(a)).

3.5. Optical absorption spectra of bare ASiCNRs

In figure 7 we present the optical absorption spectrum of bare ASiCNRs for $N_y = 6–8$. For the calculations of the BSE spectra, five valence and five conduction bands were included. As for the case of H-ASiCNRs, once the electron–hole interaction effects are incorporated, the resulting BSE spectrum of bare ribbons looks completely different as compared to the band-to-band absorption spectrum computed at the GW-RPA level. Similar to the case of H-ASiCNRs, the excitons in bare ribbons are also strongly bound, with the binding energies in bare ribbons, for the same ribbon widths, being larger than in the hydrogen-passivated ones (see tables 1 and 2). We can also find strongly bound excitons in bare ASiCNRs with binding energies in the range 0.62–2.45 eV. The reasons behind these large binding energies are the same as in case of H-ASiCNRs, i.e. stronger electron–hole interactions due to quantum confinement, and reduced screening in lower dimensions.

One qualitative difference in the optical properties of bare ribbons as compared to the hydrogen-passivated ones is that bare ribbons do not absorb at the band gap because they exhibit an indirect band gap, as discussed in the previous section. Therefore, the prominent peaks displayed in figure 7 do not have an $E_{11}$ contribution. In all the ribbons considered, the first peak corresponds to an $E_{13}$ transition, while the strongest peak is due to $E_{13}$ transition. Because of the indirect nature of excitons, bare ASiCNRs cannot be used in devices such as LEDs, however, they may be useful in transport oriented applications. As far as the location of first absorption peak is concerned, both hydrogen-passivated and bare nanoribbons follow the pattern $E(3p + 2) > E(3p + 1) > E(3p)$. Because of the presence of an indirect band gap in bare ASiCNRs, these materials will have poor photoluminescence efficiency, and thus will not be useful in light-generation applications.

3.6. Energetic stability

Energetic stability of hydrogen-terminated ASiCNRs is well known from previous theoretical studies [17]. In order to

Figure 5. (a) DFT-GGA and (b) GW band structures of bare 6-ASiCNR. Red color arrows denote the interband transitions, pink color arrows show the VBM and CBM, black color arrows denote the additional valence and conduction bands. $\delta \pi$ character of bands is also pointed out. (c) Partial density of states for 6-ASiCNR, Fermi level shown with black dashed lines.
check the stability of bare ASiCNRs, we performed calculations of their formation energies, and compared them with those of H-ASiCNRs. The following formula was employed for computing the edge formation energy per unit length of edge of a given nanoribbon,

\[ E_f = \frac{E_c - N_h E_{H_2} - 0.5N_h E_{H_2}}{2L}, \]

where \( E_c \) is the total energy/cell of the nanoribbon under consideration, \( E_{2D} \) is the total energy/cell of an infinite 2D SiC sheet, \( E_{H_2} \) is the total energy of a hydrogen molecule, \( N_d \) is the total number of SiC units in the unit cell, \( N_h \) is the total number of H atoms in the unit cell (\( N_h = 0 \) for bare nanoribbons), while \( L \) is the length of the edge (in Å unit). It is easy to see that a lower value of \( E_f \) will imply higher stability of the considered nanoribbon.

Formation energy as a function of nanoribbon width for both bare and H-saturated nanoribbons studied here is presented in figure 8. The fact that both types of nanoribbon exhibit little change in the value of edge formation energy with increasing width implies a weak width dependence. H-ASiCNRs studied here have a much lower average formation energy of 0.07 eV Å\(^{-1}\) as compared to 0.76 eV Å\(^{-1}\) of the bare ones, clearly demonstrating that H-ASiCNRs will be much more stable compared to the bare ones. Therefore, based upon the formation energy data, we conclude that the synthesis of H-ASiCNRs in laboratory will be much more favorable compared to the bare ones.

4. Conclusions

To summarize, we performed large-scale first-principles calculations on armchair-type SiC nanoribbons of widths in the range 4 ≤ \( N_a \) ≤ 12, in order to study their electronic structure and optical properties. Both hydrogen-passivated and bare edge configurations were considered, sophisticated many-body methods such as the GW approximation for the band structure and BSE for the optical absorption were adopted, and the convergence of the calculations was carefully checked. Therefore, the results presented here are fairly accurate, and constitute to the best of our knowledge the first set of GW and BSE calculations for SiCNRs. From our calculations we conclude that hydrogen-passivated ribbons are direct band

Figure 6. For bare ASiCNRs: (a) quasiparticle self-energy corrections to the GGA Kohn–Sham energies. Corrections to the states corresponding to flat bands in conduction (valence) band regions are enclosed inside the red-dashed circle (ellipse). (b) Variation of the GGA and quasiparticle band gaps as a function of the ribbon width.

Figure 7. Optical absorption spectrum of bare 6-ASiCNRs, with (GW-BSE), and without (GW-RPA) electron–hole interactions. Lorentzian broadening of 0.03 eV has been used.

Figure 8. Formation energies of bare ASiCNRs and H-ASiCNRs as a function of width.
gap semiconductors, and bare edge-ribbons undergo significant edge reconstruction, and become indirect band gap semiconductors. As expected, self-energy corrections widened the band gaps, and excitonic effects modified optical absorption spectra dramatically for both the H-saturated and the bare ribbons. Our results predict that quasiparticle band gaps of hydrogen-passivated and bare ASiCNRs are ≈2 eV larger than their DFT-GGA band gaps, due to the inclusion of many-body effects within the GW approximation. These large quasiparticle corrections to the band gaps suggest enhanced Coulomb correlation effects in reduced dimensions. Our BSE-based calculations of the excitonic effects predict large excitonic binding energies in the range 0.62–2.45 eV in optical absorption spectra of both types of ASiCNRs, which is yet another consequence of reduced dimensions. Key results of our calculations can be tested in future experiments once these nanoribbons are synthesized in laboratories. Theoretically speaking, it will also be of interest to explore other ribbon geometries of SiC, and also ribbons with unequal proportions of Si and C.

Acknowledgments

All authors gratefully acknowledge computational support from Monash Sun Grid cluster and the National Computing Infrastructure, Australia. NA gratefully thanks P Chan and S Ayyub for helping in allocating the required CPUs to carry out the calculations.

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