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Effects of an external electric field on the electronic properties and optical excitations of germanane and silicane monolayers

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Abstract. Using density functional theory in conjunction with many-body perturbation theory, we theoretically investigated the electronic structures of monolayers germanane and silicane in an applied out-of-plane uniform electric field. Our results show that although the band structures of both monolayers are affected by the electric field, the band gap width cannot be reduced to zero even for high field-strengths. Moreover, excitons are shown to be robust under electric fields, so that Stark shifts for the fundamental exciton peak is only of the order of a few meV for fields of $1 \text{ V}/\text{\AA}$. The electric field has also no significant effect on electron probability distribution, as the exciton dissociation into free electron-hole pairs is not observed even at high electric field strengths. Franz-Keldysh effect is also studied in monolayers germanane and silicane. We found that, due to the shielding effect, the external field is prevented to induce absorption in the spectral region below the gap and only above-gap oscillatory spectral features are allowed. One can benefit from such a characteristic where the absorption near the band edge is not altered by the presence of an electric field, especially since these materials have excitonic peaks in the visible range.

1. Introduction

Due to their rich and dense spectrum of unusual physical and chemical properties, atomically thin two-dimension materials (2D) are considered as the materials of the 21st century. Besides their fascinating properties, they provide a route to sharply reduce the characteristic lengths of electronic devices thus opening a large avenue for a wealth of low-power applications such as ultra-thin-channel field-effect transistors, optoelectronic devices, and solar cells. This family of materials includes a broad range of components such as graphene, transition metal dichalcogenides (TMDs) and hexagonal boron nitride (hBN) just to cite a few.[1, 2, 3]

Germanene[4, 5, 6, 7] and silicene [8, 9, 7] are the kind of 2D materials that share similar characteristics with graphene. This includes the geometry, the shape of the band structure, the high carrier mobility [10, 11], as well as the quantum spin Hall effect [12, 13]. These novel silicon and germanium 2D allotropes are promising for the next generation of the electronic devices due to their reduced dimensionality.

However, both monolayers suffer from the absence of a band gap, which strongly limits their applications in the electronic devices such as field-effect transistors (FETs), and optoelectronic devices. To remedy this limitation, silicene and germanene would need to acquire a semiconducting behavior, which is the key to the on-off switching operations performed by electronic components. Several strategies have been elaborated to open band gaps in these materials, such as doping, adsorption, and chemical functionalization. [14, 15, 16] Similar to the fully hydrogenated graphene (named graphane) [17], the so-called, germanane and silicane obtained by fully hydrogenation of germanene and silicene, exhibit semiconducting characters with band gap of about 1.4 eV and 2.2 eV respectively. [18, 19, 20, 21].

The natural next step is to try to build optoelectronic devices with germanane and silicane monolayers. The controllable band gap engineering of semiconductors is highly desirable for a wide range of energy and sensing applications. In this respect, it is interesting to know if the optical properties can be tuned in a controlled way. External electric field is a powerful tool for tailoring and tuning electronic and optical properties in nanosized materials due to the Stark effect.[22, 23, 24, 25, 26]

Several theoretical studies have shown the possibility of employing a similar strategy to reduce the band gap in germanane monolayer and bilayer, and silicane monolayer, even trigger a complete semiconductor-metal transition.[24, 25] These calculations have been performed on the level of Density Functional Theory (DFT) [27, 28], neglecting the effects of electron-electron self-energy effects. These effects, however, have been shown to be strongly large in reduced-dimensional semiconducting materials due to the quantum confinement effect as well as the reduced Coulomb screening.[29, 30] Furthermore, to our knowledge, there have been no studies on the effects of electric field on the optical spectra of germanane nor silicane so far.

In light of the foregoing, there are critical few questions that remain unanswered: *i*) How the electric field affects electron correlations in the band-structure? *ii*) how the

transverse electric field changes the nature of optical excitations, the spatial extension of excitons, and the spatial separation of the electron-hole pairs? *iii*) What is the effect of an electric field on the optical absorption spectra of germanane and silicane; is it as less pronounced as for boron nitride nanotubes (BNNTs) [22] or strong as for bulk parents[31, 32].

The present paper addresses those issues by means of first-principles calculations based on many-body perturbation theory. Our results indicate that the electronic band structure of germanane and silicane exhibit similar behavior, where both are found to be very robust to respond to the application of an external electric field. We show how the latter impact the absorption onset, keeping the excitonic binding energy almost unaffected. The paper is organized as follows. Descriptions of the computational methods are given in Section 2. In Section 3, we report and discuss our results, and finally we summarize our main conclusions.

2. Method

All the calculations are carried out using Quantum espresso [33] and YAMBO[34] codes. We calculate the ground-state properties using DFT with norm-conserving pseudopotentials and plane wave basis sets.[33]

The most stable chair conformation has been simulated using a two dimensional triangular lattice with a basis of two SiH (GeH) units where the ionic potential has been modeled using the Optimized Norm-Conserving Vanderbilt (ONCV) scalar relativistic pseudopotentials.[35]

We adopted the generalized gradient approximation with Perdew- Burke-Ernzerhof (PBE) exchange correlation functional. [36] The calculations were done in the supercell arrangement using a 80 Rydberg plane-wave cutoff for the electronic wave function expansion and a $9 \times 9 \times 1$ k Monkhorst-Pack[37] mesh for Brillouin zone (BZ) integration.

To prevent the unphysical interlayer interaction between the periodic images, a large vacuum of 20 Å is used in the out-of plane direction. The convergence criterion of self-consistent calculations for ionic relaxations is 10^{-10} eV between two consecutive steps. All atomic positions and unit cells are optimized until the atomic force convergence of 10^{-2} eV/Å were reached. The above criteria ensure the absolute value of stress is less than 0.01 kbar.

DFT underestimates the band gap of semiconductors due to the poor treatment of the electron-electron effects by the local and semi-local exchange correlation functional. To overcome this limitation and thus capture the physics of electronic correlations, we performed GW calculations. This method corrects the Kohn–Sham eigenvalues, thereby re-normalizing the band gaps to values close to their experimental counterparts.

The quasiparticle energies (single-particle excitation energies) were computed within the G_0W_0 by solving the Dyson equation [38, 39] using the following equation:

$$E_{nk}^{QP} = \epsilon_{nk} + Z_{nk} \langle \phi_{nk}^{KS} | \Sigma(\epsilon_{nk}) - V_{xc} | \phi_{nk}^{KS} \rangle, \quad (1)$$

where ϵ_{nk} , ϕ_{nk}^{KS} and V_{xc} describe the Kohn-Sham eigenvalues, orbitals, and exchange-correlation potential. The normalization factor Z is defined as: $Z_{nk}^{-1} = [1 - \frac{d\Sigma_{nk}}{d\omega}]^{-1}$.

We used DFT eigenvalues and eigenfunctions to construct G_0 and the dynamical screening effects in the self-energy are evaluated using the generalized plasmon-pole model.[40] The sampling of the BZ is performed with a $30 \times 30 \times 1$ uniform k -point mesh. We included 100 empty states for both self energy and dynamical dielectric screening. We used a cutoff energy of 4 Ha to evaluate the dielectric function included in the self energy operator.

In the calculation of the absorption spectra, two schemes were considered: the random-phase approximation (RPA) and the Bethe–Salpeter equation (BSE) formalism. In the RPA scheme, the coulomb interaction between the photo-excited electron (in the conduction band) and the hole that it leaves behind in the valence band (excitonic effects) is neglected. This shortcoming of the RPA can cause significant errors when considering systems that exhibit strong excitonic effects, such as for germanane and silicane. To capture the physics of excitonic effects one should resort to an appropriate formalism by solving the equation of motion of the two particles Green’s function, known as the Bethe–Salpeter equation (BSE). This method gives a reliable and accurate description of the optical excitations thus giving results very close to the experimental data.

To account for electron-electron effects in the calculation of excitonic spectra, we solved the BSE on top of the G_0W_0 quasiparticle spectrum [39, 38]:

$$(E_{ck} - E_{vk})A_{vck}^S + \sum_{k',v',c'} \langle vck | K_{eh} | v'c'k' \rangle A_{v'c'k'}^S = \Omega^s A_{vck}^S \quad (2)$$

where E_{ck} and E_{vk} describe the quasi-particles energies of valence and conduction bands. Ω^s and A_{vck}^S are amplitudes and excitation energies of excitonic states, respectively. K_{eh} is the interaction kernel that contains the repulsive unscreened exchange interaction (V) and attractive screened coulomb interaction (W) between electron-hole states. The BSE calculations were performed using a denser $90 \times 90 \times 1$ k -point grid. Five conduction band and four valence band were used to construct the kernel interaction in BSE and a Lorentzian broadening of 0.15 eV is adopted to visualize absorption spectra. In both GW and BSE calculations, the coulomb interaction was truncated at 18 Å to avoid unphysical interaction between the adjacent layers [41] as implemented in YAMBO code.[34]

An electric field along the out-of-plane direction is accounted for by using a model capacitor (sawtooth potential). This model mimics gated germanane and silicane sheets. The limit boundary conditions in the out-of plane direction are imposed on the electrostatic potential, which gives rise to an artificial electric field across the surface of the sheets. A dipole correction is added to the bare ionic potential to cancel this spurious effect.[42] We mention that the electric field is introduced in the ground state at the optimized geometry with unstrained symmetry. Then, the GW and BSE calculations are carried out on top of that, using the Kohn-Sham eigenvalues and eigenfunction obtained under the effect of the electric field.

3. RESULTS AND DISCUSSION

3.1. Structural properties

Before investigating the effect of an external electric field on the electronic structures of germanane and silicane it is worth to check the consistency of our results obtained for free structures with previous findings.

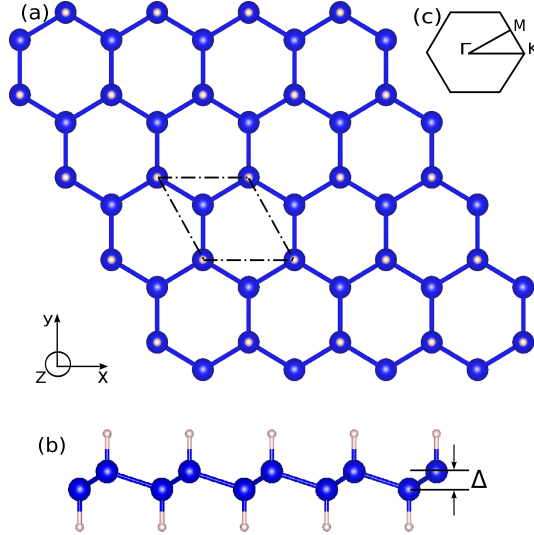


Figure 1. (a) Top and (b) side views atomic structure of germanane and silicane. The Ge (Si) and H atoms are represented by large blue and small white spheres respectively. (c) First Brillouin zone.

Figure 1 displays the optimized structures of germanane and silicane for the most energetically favorable like-chair configuration with c_{3v} symmetry.[18, 43] We note that both pristine germanene and silicene exhibit buckled structures. Such a buckling becomes more pronounced upon the decoration with H atoms. These structures illustrate their great similarities with the puckered geometry of graphane but with the slight difference of buckling heights Δ . As it can be seen, the puckered structures of germanene and silicene (not shown here) undergo reconstructions after the decoration with H atoms. The Si (Ge) atoms move upward and downward leading to a buckling of about 0.71 Å (0.73 Å), being comparable with that of graphane (0.45 Å).[44] It is worth to notice that this structural parameter is higher in germanane than in silicane due to the large ionic radii of germanium atom. This structural change can be guessed as a transition from an sp^2 - sp^3 bonding towards sp^3 bonding.

The calculated lattice constants, bond lengths and bond angles are summarized in Table 3.1, These values are in good agreement with previous theoretical works.[45, 18]

3.2. Effects of an external electric field on the band structures

To illustrate the effect of an electric field, we have calculated the projected density of states (PDOS) of germanane and silicane with and without the presence of the field

	a (Å)	d_{X-X} (Å)	d_{X-H} (Å)	Δ (Å)	\angle HXX (degrees)
Germanane	4.07	2.46	1.55	0.73	82.19
Silicane	3.88	2.35	1.50	0.71	82.19

Table 1. Structural parameters of germanane and silicane: lattice constants a , bond lengths d_{X-X} and d_{X-H} ($X = \text{Ge}$ and Si), buckling height Δ , and bond angles \angle HXX.

and the results are displayed in Fig. 3. In the absence of the electric field, the main features of the PDOS curves are quite similar for both materials (see Fig. 3(a) and 3(e)). The valence band maximum (VBM) is dominated by $p_x + p_y$ states of Ge (Si) while the conduction band minimum (CBM) arises from s and p anti-bonding states of Ge (Si) with negligible contribution of H s anti-bonding states.

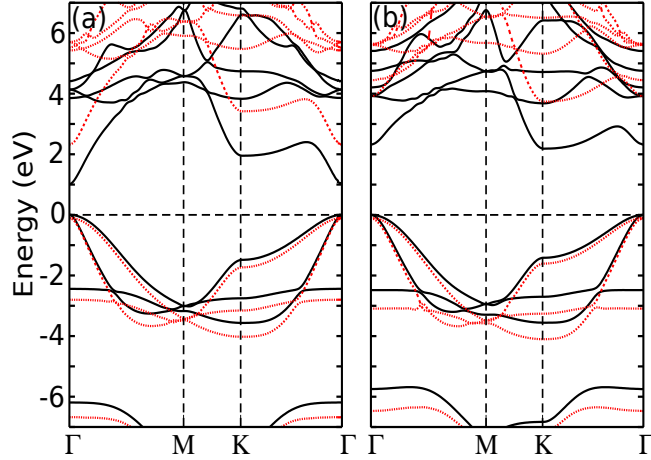


Figure 2. PBE (black full line) and G_0W_0 (red dashed line) band structures of (a) germanane and (b) silicane.

The VBM is followed at lower energies by a sharp peak around -2.5 eV below the Fermi level which is made up of a heavily mixture of p_z states of Ge(Si) atoms and H s with a small contribution from the Ge(Si) s and $p_x + p_y$ states. The CBM is followed at higher energy by a peak at around 4.3 eV above the Fermi level essentially formed by hybridization of H s and Ge(Si) p anti-bonding states of Ge (Si). One can conclude that the valence band is formed by the orbitals of Ge (Si) atoms while H atoms give rise to states far way from the band edges in the energy gap. It is worth mentioning the good agreement of our results with the recent theoretical data.[46, 47]

The calculated PBE and G_0W_0 band structures without including the field are depicted in Fig 2. (a) and (b). We clearly see that the sp^3 hybridization of Ge and Si orbitals causes the opening of a band gap in germanene and silicene. At the DFT level of theory, their corresponding band structure dispersions look quite similar due to the same symmetry. Germanane is predicted to have a direct band gap of 1.01 eV at the Γ -point, with doubly degenerated valence bands predominantly of $p_x + p_y$ character. Silicane has

an indirect band gap of 2.19 eV at K-point and a direct gap of 2.32 eV at Γ -point. Its valence band is also twofold degenerate with p_x+p_y character. It is noteworthy that a very small difference between the direct and the indirect gap of silicane indicates that the material may be of importance for optoelectronic applications as it is still a good emitter of light.

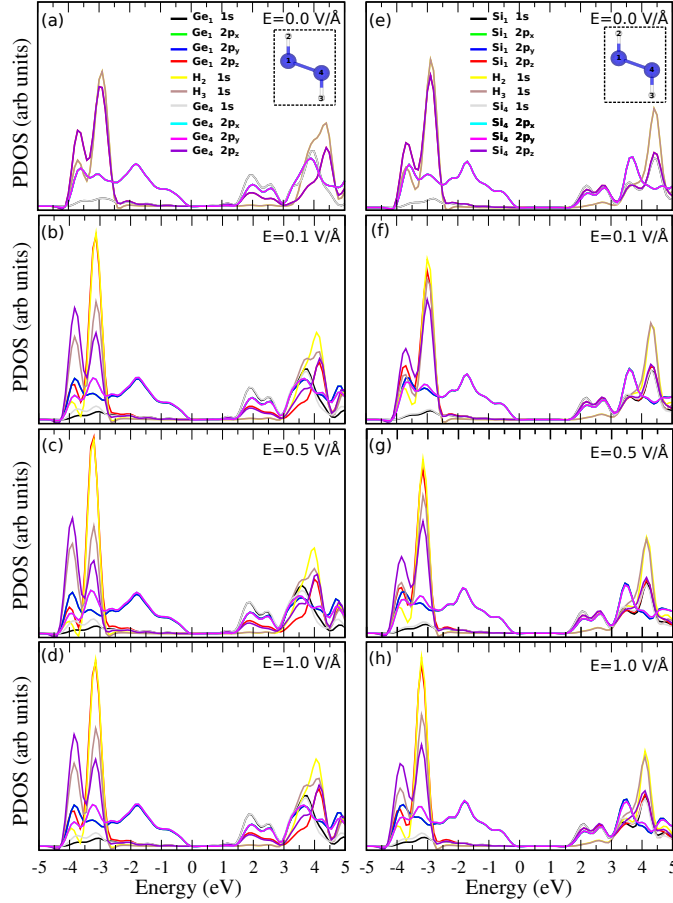


Figure 3. Projected electronic density of states at different values of the electric field for (a-d) germanane and (e-h) silicane.

The inclusion of the electron-electron self-energy effects strongly modifies (more than 80%) the band structures. The direct bandgap of germanane increases from 1.01 to 2.32 eV while the indirect band gap of silicane increases from 2.42 to 4.01 eV. This feature is in close agreement with previous theoretical studies.[45, 47, 48] The large quasiparticle corrections to the PBE band gap originates from the increase of the electron-electron interaction and the weakening of the screening response within two-dimensional materials. Such a low screening gives rise to bound excitons with large binding energies.

As mentioned above, the external electric field is a powerful tool for tuning and controlling the electronic properties of 2D materials. The band structure variations with perpendicular electric field come from the well-known Stark effect which causes the shifting of the valence band and conduction bands.

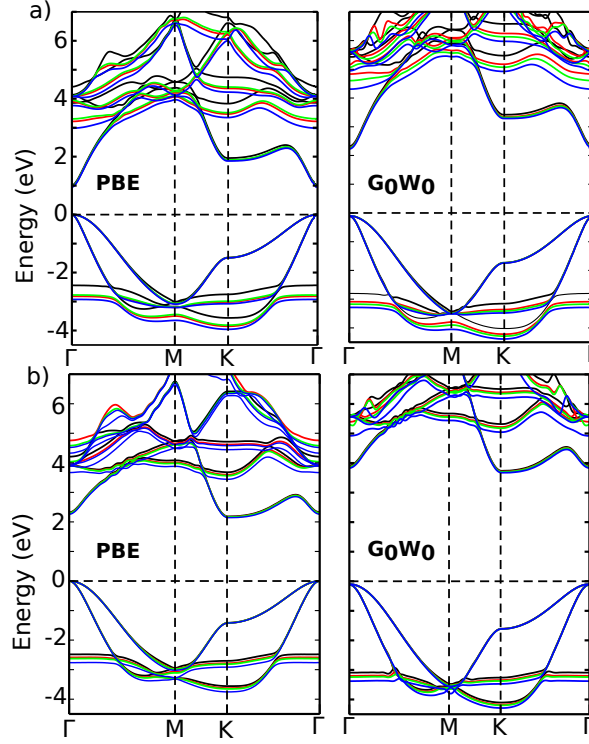


Figure 4. PBE and G_0W_0 band structures under external field for (a) germanane and (b) silicane respectively, $E = 0.0$ V/Å (black), $E = 0.1$ V/Å (red), $E = 0.5$ V/Å (green) and $E = 1.0$ V/Å (blue).

In Fig 4, we depict the band structures of both monolayers calculated at different value of the field. As it can be seen, the band structures of germanane and silicane have qualitatively similar responses to the external field. Both valence and conduction bands are pushed down towards lower energies. The effect is more pronounced for lower valence bands and higher conduction bands starting from the second valence band (VBM -1) and the second conduction band (CBM $+1$) where energies downshift are in the range of 0.3 to 1.0 eV. The conduction band minimum is shown to be less sensitive while the valence band maximum remains almost unchanged.

To further explore these features, we examine the PDOS for three different finite values of the field displayed in Fig. 3. The PDOS curves show that the electric field has a negligible impact on the valence and conduction band edges. The application of the electric field, however, induces significant changes in the Ge-H (Si-H) bonding states on one side of the monolayer (the high potential side) leading to the lifting of the degeneracy of p_z orbitals of Ge (Si) atoms (see Fig 3). The bonding states on the other side (low potential side) remain almost unaffected. The cause of this trend is the negatively charged H atoms that screen largely the electric field, and therefore its weak influence on other atoms.

In Fig. 5, we show the evolution of the band gap width of germanane and silicane as a function of applied external field estimated at both DFT and GW levels. Because of the inversion symmetry of the layers, we have carried out the calculations by increasing

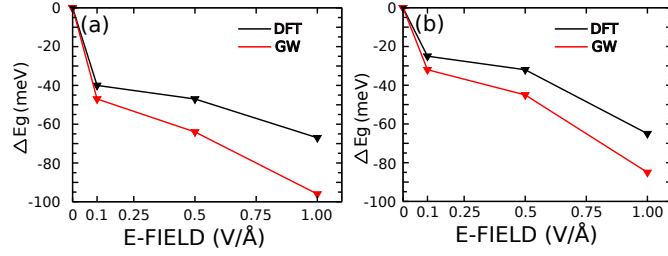


Figure 5. Variation of the band gap ΔE_g in the DFT and GW levels under electric field for (a) germanane and (b) silicane. $\Delta E_g = E_g(E) - E_g(0)$.

the strength of the field from 0 up to a higher value of 1.0 V/Å. At first glance, the band gap in all cases decreases with increasing field strength. The response of germanane band structure to the field is more sensitive than that of the silicane. The cause for this trend may be the heavy mass of germanium atoms, and therefore their electrons behave differently in the presence of an electric field than those of silicon which is a light atom due to relativistic effect.

Overall, Fig. 5 shows that the band gaps of both monolayers do not significantly reduce even at high field values (up to 1 V/Å), indicating their robust electronic properties. The inclusion of electron-electron self-energy effects does change this trend; it only increases the threshold value of field for gap closure. Moreover, for a field strength of 1.0 V/Å, the difference between $\Delta E_g(\text{GW})$ and $\Delta E_g(\text{DFT})$ is about 29 meV and 20 meV for germanane and silicane, respectively, which values are much smaller compared to their respective band gaps. Thus, one can speculate that the band gaps of both germanane and silicane monolayers are difficult to be reduced to zero by applying an external electronic field. We conclude that the electronic properties of germanane and silicane monolayers can not be efficiently tuned from semiconducting to metallic under practical external electric field.

3.3. Effects of an external electric field on the optical absorption spectra

In Fig. 6, we depicted the absorption spectra of both monolayers computed at GW+BSE and GW+RPA. The optical absorption spectra of germanane and silicane including electron-hole interaction reveal a more pronounced red-shift of the spectral profile with respect to the RPA spectrum (which ignores excitonic effects). Our calculation shows a redistribution of the oscillator strength and a global shift of the spectrum towards lower energies, with the rise of excitonic resonances well below the onset of single-particle transition continuum.

In the absorption spectrum of silicane, the major peak around 4 eV (labeled with B in Fig. 6) originates from electronic transitions between VBM and CBM+1 at the Γ -point. Both VBM and VBM+1 states are twofold degenerate with predominantly $p_x + p_y$ character (see Fig. 3(e) and Fig. 4). This bound exciton is double degenerate with a binding energy E_b of 100 meV.

At lower energies well below the onset of the single-particle transition continuum,

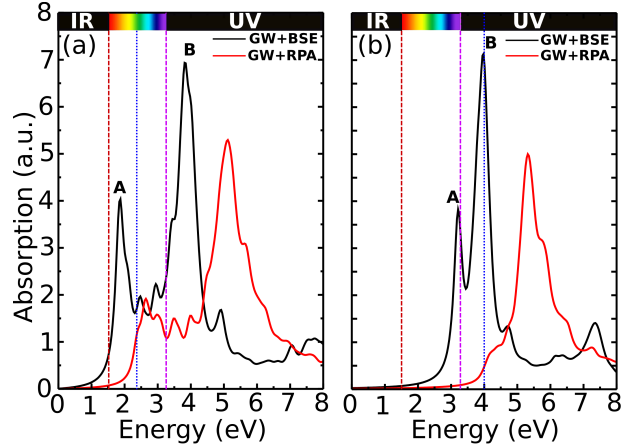


Figure 6. Optical absorption spectra of (a) germanane and (b) silicane computed on the top of GW approximation with (GW+BSE) and without (GW+RPA) including electron-hole interaction. The blue dashed line indicate the GW gap and A indicates the first bounded exciton.

the optically active (bright) bound exciton at 3.21 eV marked with A in Fig. 6 has a E_b of 0.8 eV. This exciton which is degenerated with a dark exciton with much smaller oscillator strength is related to the vertical transitions from the top two valence bands to the bottom of the conduction band close to the Γ -point. The dark exciton arises from transitions from the highest valence band to the first out-of-plane band. It is important to point out that the oscillator strengths of the exciton A and the dark exciton reverse when the light propagating direction changes. This behavior is due to the symmetry of the states that contribute to the formation of the bound excitons[49].

As for germanane, the optical absorption spectrum also shows a major peak B around 4 eV. This excitation is originated from a large number of transitions from VBM band to the third conduction band (CBM+2). CBM+2 states are twofold degenerate with predominantly p_x+p_y character (see Fig. 3 (a) and Fig. 4). The first bright exciton A, which is degenerate with a dark exciton, locates at 1.87 eV with a E_b of 0.56 eV. In both monolayers, the strong excitonic binding energy reflects the weak dielectric screening. It is noteworthy that our findings agree well with results reported in the previous works[47, 48].

The bottom of the conduction band of both germanane (silicane) has predominantly p character (see Fig. 3). This feature gives rise to first-class excitons in these materials due to the strong intra-atomic contributions that increase the dipole matrix elements. This kind of excitons cannot emerge (dipole forbidden) in graphane, due to the H s character of the bottom of its conduction band, hence giving rise to second-class excitons. [48].

Let us now move to the next part of this work that consists to study the evolution of the optical spectra of germanane and silicane with the external electric field. The BSE optical absorption spectra of germanane and silicane are shown in the top and bottom of Fig. 7, respectively. The structures are subjected to external out-of-plane

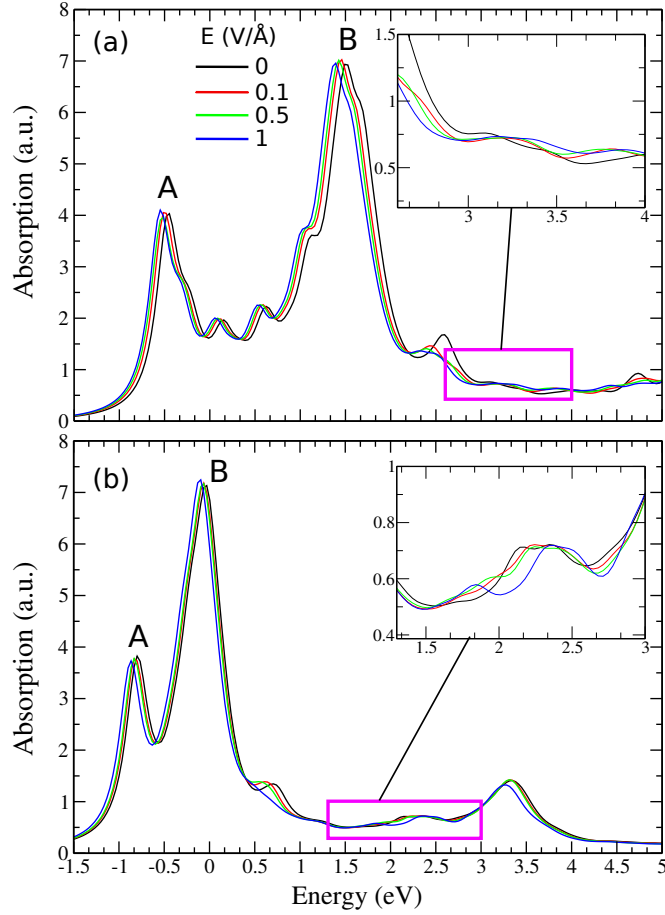


Figure 7. BSE optical spectra of germanane (a) and silicane (b) under external electric field. The onset of the single-particle transition continuum is shifted to zero. The inset is a zoom of the field-induced above-gap (Franz-Keldysh) oscillations.

electric fields applied parallel to the vector surface. For each monolayer, field strengths of 0, 0.1, 0.5 and 1.0 V/Å are considered, and represented by the black, red, green, and blue lines, respectively.

The binding energy of the bound exciton A increases with the field E due to the Stark effect and its value depends on the binding energy at zero field $\delta E_b = E_b(E) - E_b(0)$. For a field of 1.0 V/Å, we found Stark shifts of about 20 meV and 10 meV for germanane and silicane, respectively, reflecting the reduction of screening, predominantly by the valence electrons. The oscillator strength of its absorption peak shows small variations with increasing electric field, thus reflecting the weak effect of the electric field on the electron-hole pairs. The cause for this trend is the negatively charged H atoms on the high potential side that shields the electric field so that it interacts only weakly with Ge (Si) atoms from which this first-class exciton is originated. As a consequence, the magnitude of the wave function of the bound exciton A is little reduced. The mechanism driving the interaction between excitons and external field is not straightforward. Although the exciton is electrically neutral, it can be polarized by the electric field by pulling the electron and the hole farther apart, creating an electric

dipole field. The electric dipole field interacts with the electric field, and thus exerts a force on the exciton. It is important to notice that the bound exciton peak A can still be observed even for a larger electric field of 1.0 V/\AA , suggesting that the dissociation of this exciton into free electron-hole pairs requires extremely large fields. This in turn suggests that one should be able to observe an excitonic Stark effect in germanane and silicane experimentally.

Exciton Franz-Keldysh effect [50] is observed in the optical absorption of germanane and silicane. This effect has been previously investigated in bulk [51], and low-dimensional semiconductors. [52, 53] Its fingerprints is the appearance of the field-induced absorption below the band gap and characteristic oscillations in the absorption spectrum above it.[54] The Stark shift of excitonic states leads to a shift of absorption peaks towards lower energies in contrast to oscillations above the band gap, which exhibit shifts towards higher energies with increased electric field.[52]

Interestingly, from Fig. 7, we can see that there is no additional field-induced absorption below the gap. In the continuum above the gap, however, the oscillatory spectral features are clearly observed. Such a "truncated" Franz-Keldysh effect has not been reported elsewhere. It manifests itself only in induced characteristic oscillations in the absorption spectrum above the gap. This unique behaviour of Franz-Keldysh effect is a consequence of the shielding effect that prevent the electric field to induce additional absorption below the band gap. In other words, the absence of the absorption component is due to the negatively H atoms on the high-potential side that makes this spectral region not susceptible to the external electric field effect. As a result, the absorption is unaffected close to the band edge, making the dominant effect of the electric field is the Stark Shift. Therefore, one can benefit from such characteristic, especially as these materials have excitonic peaks in the visible range.

4. CONCLUSION

In summary, based on *ab-initio* calculations, we have shown that the electronic band structures of germanane and silicane are difficult to modulate by an external electric field. Moreover the band gap of both materials can not reach zero even at high field strengths. We have also investigated excitons and the absorption spectra of germanane and silicane in the presence of an applied out-of-plane electric field. Our calculations predict Stark shift for the fundamental exciton peak, which is of the order of 20 meV (10 meV) for germanane (silicane) for fields of 1 V/\AA . Furthermore, negligible loss of its absorption intensity with the field has been revealed indicating that very strong fields are required for this exciton to dissociate into free electron-hole pairs. Our findings suggest that exciton Stark effect can still be observed even at larger electric fields. Finally, we have found that the screening effect prevent the field to induce absorption below the gap and consequently, the Franz-Keldysh effect manifests itself only in field-induced above-gap oscillations.

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