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Investigation of Electronic Properties of AlGaSe/GaSe Heterostructure: A Density Functional Study

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Abstract

The scientific community has shown significant interest in the field of two-dimensional (2D) materials. Due to the phenomenon of quantum confinement in a specific direction, 2D materials exhibit fascinating properties that are not present in their bulk form. With the emergence of semiconducting 2D materials, there is a wide array of electronic properties to explore, opening up exciting possibilities for developing next-generation electronics. An emerging class of materials includes the III-VI monochalcogenides, with indium selenide (InSe) and gallium selenide (GaSe) being two prominent members. Unlike transition metal dichalcogenides, researchers have been drawn to investigate the underlying physical phenomena and technological applications of materials with high intrinsic mobility and a direct bandgap at small thicknesses. In this work, we explore the structural and electronic characteristics of AlGaSe/GaSe heterostructure by density functional theory. The GaSe forms a relatively weak bond with the AlGaSe monolayer, exhibiting an adsorption energy of 9.089 meV/atom. The heterobilayer has been determined to be energetically advantageous, with an interlayer distance of 3.379 Å, suggesting an interaction of the van der Waals (vdW) type. Several deposition procedures are employed to verify the optimal layering arrangement. The AlGaSe/GaSe heterostructure exhibits the property of an indirect band gap semiconductor, with a bandgap value of 1.774 eV. The van der Waals heterostructure's potential for the development of innovative two-dimensional nanoelectronic devices is demonstrated by the results of our investigations.

Keywords: Heterostructure, first-principles calculations, two-dimensional materials, GaSe

AlGaSe/GaSe Heteroyapısının Elektronik Özelliklerinin İncelenmesi: Yoğunluk Fonksiyonel Çalışması

Öz

Bilim camiası iki boyutlu (2D) malzemeler alanına büyük ilgi göstermiştir. Belirli bir yönde kuantum kısıtlaması nedeniyle, 2D malzemeler yığın formlarında bulunmayan büyüleyici özellikler sergiler. Yarı iletken 2D malzemelerin ortaya çıkmasıyla birlikte, keşfedilecek çok çeşitli elektronik özellikler ortaya çıkmakta ve bu da yeni nesil elektronik cihazların geliştirilmesi için heyecan verici olanaklar sunmaktadır. Bu bağlamda ortaya çıkan bir malzeme sınıfıda III-VI monokalsojenidleri (InSe; indiyum selenid ve GaSe; galyum selenid) olmuştur. Geçiş metal dikalkojenitlerin aksine, araştırmacılar III-VI monokalsojenidlerin yüksek içsel hareketliliğe ve küçük kalınlıklarda doğrudan bant aralığına sahip olmalarından dolayı teknolojik uygulamaları bu malzeme sınıfını araştırmaya yönelmiştir. Dolayısıyla bu çalışmada, AlGaSe/GaSe heteroyapısının yapısal ve elektronik özelliklerini yoğunluk fonksiyonel teorisi ile araştırıyoruz. GaSe, AlGaSe tek tabakası ile nispeten zayıf bir bağ oluşturmakta ve 9,089 meV/atom adsorpsiyon enerjisi sergilemektedir. AlGaSe/GaSe heteroyapısının van der Waals (vdW) tipi bir etkileşimi gösteren 3,379 Å'luk bir ara katman mesafesi ile enerjik olarak elverişli olduğu bulunmuştur. En kararlı istifleme konfigürasyonu farklı biriktirme dizileri ile doğrulanmıştır. AlGaSe/GaSe heteroyapısı, 1,774 eV band aralığı değeri ile dolaylı bir bant aralığı yarı iletken özelliği sergilemektedir. Bulgularımız, vdW AlGaSe/GaSe heteroyapısını kullanarak yeni iki boyutlu nanoelektronik cihazlar oluşturmak için heyecan verici olasılıkları ortaya koymaktadır.

Anahtar Kelimeler: Heteroyapı, birinci prensipler hesaplamaları, iki boyutlu malzemeler, GaSe

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1. Introduction

For many years, scientists believed that 2D materials were impossible to exist due to their thermodynamic instability. Nevertheless, the domain of 2D materials has been acknowledged since the 1940s, as reported in Refs. (Wallace, 1947; El - Mahalawy and Evans, 1977). Novoselov et al. (2004) successfully extracted and examined graphene, which is a sheet of carbon that is just one atom thick, at the University of Manchester. Their groundbreaking discovery resulted in them being awarded the prestigious Nobel Prize in Physics in 2010. This remarkable achievement also inspired scientists to explore and utilize other two-dimensional materials in a wide range of applications. Over the past few years, there has been a significant emphasis on finding new 2D materials with properties similar to graphene (Bhimanapati et al., 2015; Sangwan et al., 2018; Wang et al., 2018). For 2D materials to be suitable for use in electronics and optoelectronics, such as transistors, photodetectors, photovoltaics, sensors, and light-emitting diodes, they must possess a restricted bandgap, exceptional transport properties, and mechanical flexibility. Transition metal dichalcogenides (TMDCs) such as MoS_2, $MoSe_2$, WS_2, and WSe_2 are highly valued in the field of two-dimensional materials because of their notable bandgaps (1-2 eV), stability under typical settings, and ability to minimize short-channel effects (Wang et al., 2012; Ahmed et al., 2017). Comparing Si to TMDCs, it has been shown that TMDCs display a more gradual fall in carrier mobility as the thickness lowers, especially at the sub-5 nm scale (Cao et al., 2015). Moreover, their elongated form maintains significant mobility, indicating the possibility of investigating flexible electronics. Nevertheless, the growing interest in 2D semiconductors is not limited just to TMDCs but has also expanded to include other unconventional materials (Miró et al., 2014; Naguib et al., 2014; Liu et al., 2018). Despite the wide range of electrical characteristics shown by semiconducting TMDCs, their inherent mobility is much lower than that of Si, measuring just a few hundreds of $cm^2\ V^{-1}\ s^{-1}$ (Fiori et al., 2014). Additionally, the absence of a direct bandgap in multilayers has limited their use in optoelectronics only to monolayers. The family of III-VI monochalcogenides has gained considerable attention in recent years owing to its intriguing features and the fundamental physics involved in low-dimensional applications in electronics and optoelectronics. III-VI monochalcogenides are stratified substances with the chemical formula MX. The metallic component (M) in these materials is derived from group 13 elements, namely Ga and In, whereas the chalcogen component (X) may be either S, Se, or Te. The III-VI monochalcogenides provide many benefits compared to 2D materials. These characteristics include of a direct bandgap, increased intrinsic mobilities and charge densities, enhanced photoresponsivities, and exceptional nonlinear optical properties (Luo et al., 2015; Mudd et al., 2015; Bhuiyan et al., 2019). Monolayers of InSe and GaSe possess exceptional electrical characteristics and lack inversion symmetry, making them ideal for studying second-order optical nonlinearities, single-photon emission, and terahertz applications (Jie et al., 2015; Tonndorf et al., 2017; Zhou et al., 2018). Hence, it is clear that these III-VI monochalcogenides have the potential to significantly influence the trajectory of technology in the near future.

According to a study by Tamalampudi et al. (Tamalampudi et al., 2014), it has been shown that photodetectors made from few-layered InSe have the ability to detect a wide range of light wavelengths, from the visible to near-infrared region (450-785 nm). These photodetectors have high photoresponsivities, surpassing those of other 2D materials. Furthermore, few-layered GaX and InX have shown great potential for use in optoelectronics, field-effect transistors (FETs), and solar energy conversion (Hu et al., 2013; Jin et al., 2016). In addition, heterostructures based on InX and GaX (X = S, Se, Te) were proposed in previous studies (Wei et al., 2015; Jin et al., 2016). The tunable electronic properties, excellent photoresponse, and impressive photovoltaic performances indicate that group-III

monochalcogenide materials have significant potentials for high-performance electronic and optoelectronic applications. Regarding this matter, we conduct a comprehensive theoretical analysis of the structural and electronic properties of AlGaSe/GaSe heterostructures by employing density functional theory. With a total energy calculation, the thermal stability of AlGaSe/GaSe and the high quality of its heterostructure have been successfully achieved. This is attributed to the low lattice mismatches between GaSe and AlGaSe, resembling the work of a materials scientist. Through geometry optimization calculations, the most energetically stable configuration is achieved. In this configuration, the Ga atoms of the GaSe monolayer are positioned directly above the Se atoms of the AlGaSe monolayer. Additionally, the Se atoms of GaSe are situated directly on top of the Al atoms of the AlGaSe monolayer, resulting in a well-structured AlGaSe/GaSe heterostructure. The distance between the layers is measured to be 3.379 Å, and the adsorption energy is determined to be 9.089 meV/atom, indicating a van der Waals type interaction between the layers. Our research revealed that the AlGaSe/GaSe heterostructure exhibits an indirect band gap, measuring at 1.774 eV. The discussion on the nature of the indirect band gap is supported by calculations of the projected density of states.

2. Method

The computations were performed using the plane wave self-consistent field (PWSCF) software built in Quantum ESPRESSO (Giannozzi et al., 2009). An approach known as DFT/GGA was used to account for long-range dispersive interactions in the AlGaSe/GaSe heterostructure. The long-range dispersive interactions namely van der Waals interactions were included via the empirical correction (Grimme, 2006; Grimme, Hansen et al., 2016). It is well known that Local density (LDA) and generalized gradient approximation (GGA) density functionals generally underestimate band gaps for semiconductors. Hybrid functionals such as HSE06 that include some exact Hartree−Fock exchange are known to be better. However, it is unfeasible for many large and/or complex systems due to their high computational cost and large memory requirements. Therefore, we used GGA functionals in all calculations. The analysis of electron-ion interactions was carried out using ultrasoft pseudopotentials (Vanderbilt, 1990). The cutoff energy for the plane waves was set at 150 Ryd. A 18×18×1 Γ-centred Monkhorst-Pack k-points mesh was utilized for integrations across the 2D Brillouin zone (Monkhorst et al., 1976). To ensure the accuracy and reliability of our DFT calculations, we carefully selected the cutoff energy and k-point mesh parameters. These parameters were determined based on convergence tests specific to our system. We found that all total energies converged within 0.01 eV with respect to the number of k-points and cutoff. The repeated slab approach was used to imitate individual 2D crystals by using a vacuum layer with a thickness of 30 Å in the perpendicular direction. In order to achieve structural optimization, the locations of all the atoms were let to relax until certain conditions were satisfied. The criteria included energy convergence accuracy, maximum residual force on atoms, and maximum displacement. The thresholds for these criteria were set at less than 1×10^{-6} eV/atom, 0,03 eV $Å^{-1}$, and 5×10^{-4} Å, respectively. In the self-consistent calculations, the electron state was populated using the Methfessel-Paxton scheme (Methfessel and Paxton, 1989) with a smearing width of 0,05 eV.

3. Results and Discussion

Firstly, we begin the process of optimising the lattice constants of monolayer GaSe and AlGaSe. The lattice constants are measured to be 3.793 Å and 3.798 Å, respectively. The Ga-Se bond length is 2.503 Å, whereas the Al-Ga bond length measures 2.537 Å. The computed lattice constants and bond lengths exhibit a significant concurrence with the values that have been previously documented in the Ref. (Zhuang et al., 2013). Figure 1 depicts the optimized configurations of monolayer GaSe, monolayer AlGaSe, and the AlGaSe/GaSe heterostructure. The lattice

mismatch between the monolayers is less than 0,13% based on their lattice constants. This makes a little strain on the monolayers that the electronic properties of two dimensional (2D) materials can be extensively tuned through strain engineering. By strain engineering, the crystal structure of GaSe and AlGaSe monolayer may be affected by the strain, since the strain distorted electron cloud and changed the Se-Ga-Se bond angle, thus strongly affecting the band structure and the effective mass. In general, the band gap of 2D materials can also be varied with strain. Based on the lattice constants of the monolayers, the lattice mismatch between them is less than 0,13 %. Thus, utilizing 1×1 unit cells of monolayer GaSe and AlGaSe is sufficient for constructing the heterostructure and is experimentally feasible. The AlGaSe/GaSe structure is created by adjusting the lattice constants of monolayer AlGaSe, causing a slight contraction of materials by 0,13 %. This mismatch has relatively little effect on the total energy and the electrical properties of the structure in the following calculation. Based on our analysis, it appears that the lattice constants used for the AlGaSe/GaSe heterostructure have a minimal impact on its electronic properties.

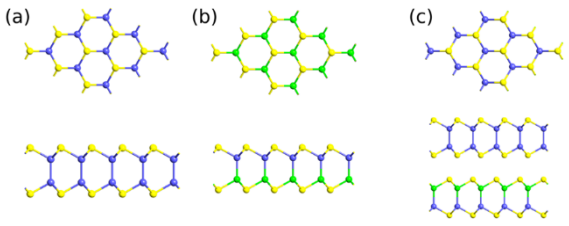

Figure 1. The relaxed atomic structure of (a) GaSe monolayer, (b) AlGaSe monolayer, and (c) AlGaSe/GaSe heterostructure. The yellow, blue, and green balls are Se, Ga, and Al atoms, respectively.

In order to determine a thermodynamically stable arrangement for the AlGaSe/GaSe heterostructure, we are investigating several stacking arrangements. (i) In one arrangement, the aluminum (Al) atoms of a single layer of aluminum gallium selenide (AlGaSe) are located above the selenium (Se) atoms of gallium selenide (GaSe), while the gallium (Ga) atoms of the GaSe layer are positioned on top of the selenium atoms of AlGaSe. (ii) In an alternative configuration, the Se atoms of a single layer of GaSe are positioned on top of the Se atoms of AlGaSe, while the Ga atoms of the GaSe layer are put above the Al atoms of AlGaSe. (iii) In an alternate situation, the Ga atoms of a single layer of GaSe are positioned on top of the Al atoms of AlGaSe, whereas the Se atoms of the GaSe single layer are located in the core of the AlGaSe hexagon. (iv) An alternative scenario is that the selenium (Se) atoms of a single layer of gallium selenide (GaSe) are positioned on top of the selenium atoms of aluminum gallium selenide (AlGaSe), and the gallium (Ga) atoms of the GaSe layer are precisely aligned with the centre of the AlGaSe hexagon. (v) Likewise, the selenium (Se) atoms in a single layer of gallium selenide (GaSe) may be arranged on top of the aluminum (Al) atoms in aluminum gallium selenide (AlGaSe), with the gallium (Ga) atoms in the GaSe layer precisely aligned above the hexagonal structure of AlGaSe. (vi) Finally, the Ga atoms of a single layer of GaSe are positioned on top of the Se atoms of AlGaSe, whereas the Al atoms of the single layer of AlGaSe are centred over the GaSe hexagon.

Following the geometry optimization calculations, the configuration with the most negative binding energy is determined to be the most stable in all considered configurations. As a result, the more negative binding energy compared to other configurations is an indication that the interfaces between AlGaSe and GaSe are energetically stable and easy to realize in experiments.

Calculating the binding energy (E_b) per unit cell is essential in determining the thermal stability of AlGaSe/GaSe. The formula used for this calculation is as follows:

$$E_b = E_{\mathrm{AlGaSe/GaSe}} - E_{\mathrm{GaSe}} - E_{\mathrm{AlGaSe}} \quad (1)$$

where the total energy of the heterostructure is denoted as $E_{\mathrm{AlGaSe/GaSe}}$, while E_{GaSe} represents the total energy of the free-standing GaSe and E_{AlGaSe} represents the total energy of the AlGaSe monolayer. The calculated value for E_b in the

heterostructure is 9.089 meV/atom. It is evident that the formation of the heterostructure releases energy. In addition, the binding energy is more negative compared to bilayer graphene and is similar to the typical van der Waals binding energy of around 20 meV. Based on our calculations, the interlayer distance for the AlGaSe/GaSe heterostructure is approximately 3.379 Å.

Figure 2 (a) and (b) display the electronic structure and projected density of states for monolayer GaSe, respectively. The band gaps of monolayer GaSe are calculated to be 2.153 eV. These values are in good agreement with previous studies. It is worth noting that the band gap value for monolayer GaSe was found to be smaller than the experimental value of 3.30 eV reported in Ref. (Jung et al., 2015). This finding highlights the accuracy of the computational method employed in this study. This is a common issue where density functional theory tends to underestimate band gap values.

The explanation for this can be found in detail in Ref. (Crowley et al., 2016). Figure 2 (b) presents PDOS for GaSe monolayer. The valance band maximum is contributed by Ga-p and Se-p orbits, and the conduction band minimum (CBM) is mainly contributed by Se-p orbitals. In addition, the AlGaSe/GaSe heterostructure has not been studied experimentally. Therefore, this research will provide valuable guidance for future experiments.

The electronic structure and projected density of states for monolayer AlGaSe are shown in Figure 3 (a) and (b). The AlGaSe monolayer has an indirect band gap of 2.334 eV, with the VBM found between **Γ** and **K** points and the conduction

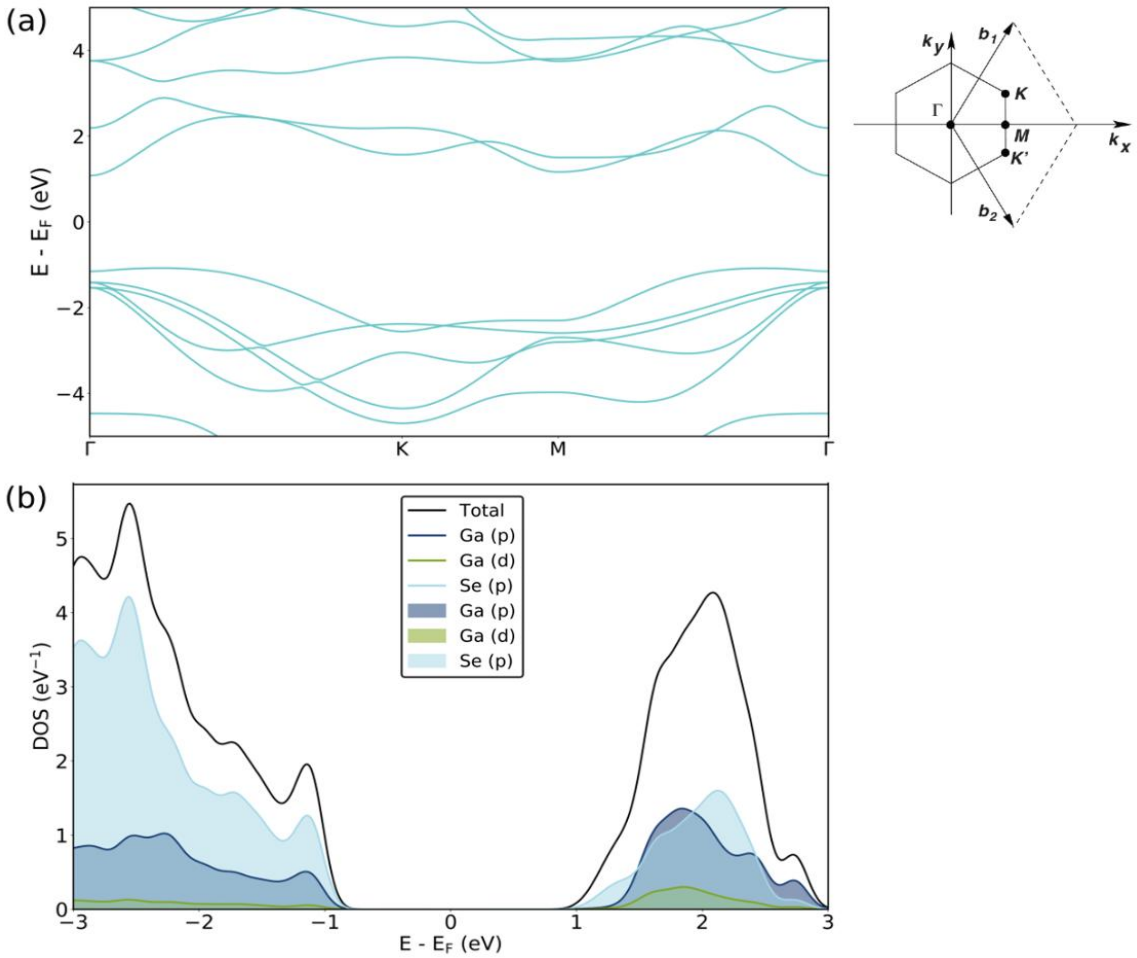

Figure 2. (a) Electronic structure and (b) projected density of states for monolayer GaSe and its Brillouin zone. Fermi level is set to zero.

band minimum (CBM) found at the Γ point of its Brillouin zone. From the projected density of states (PDOS) in Figure 3 (b), it can be seen that both the VBM is mainly contributed by Se p orbitals and the CBM is mainly contributed by the hybridized Se p and Al p orbitals. When the AlGaSe monolayer is deposited on the GaSe monolayer, it maintains its indirect band gap nature with a gap value of 1.774 eV as shown in Figure 4 (a), which is lower compared to both monolayer GaSe and AlGaSe. Additionally, we observe the position of the CBM remains the same at Γ point when the heterostructure is formed. Recently, it has been shown that ZnO/GaSe and ZnO/Ga_2SSe heterostructures lead to the reduction of the band gaps of monolayer GaSe and monolayer GaSe Janus monolayer (Zhang et al., 2023). Also, the indirect band behavior of monolayer GaSe is changed when forming heterostructures (Zhang et al., 2023). Figure 4 (b) displays the overall density of states (TDOS) and the projected density of states (PDOS) for the AlGaSe/GaSe heterostructure. The purpose of these computations is to further our comprehension of the electrical configuration and interactions between monolayer GaSe and AlGaSe at the atomic level. The electronic states of AlGaSe/GaSe near the Fermi level primarily

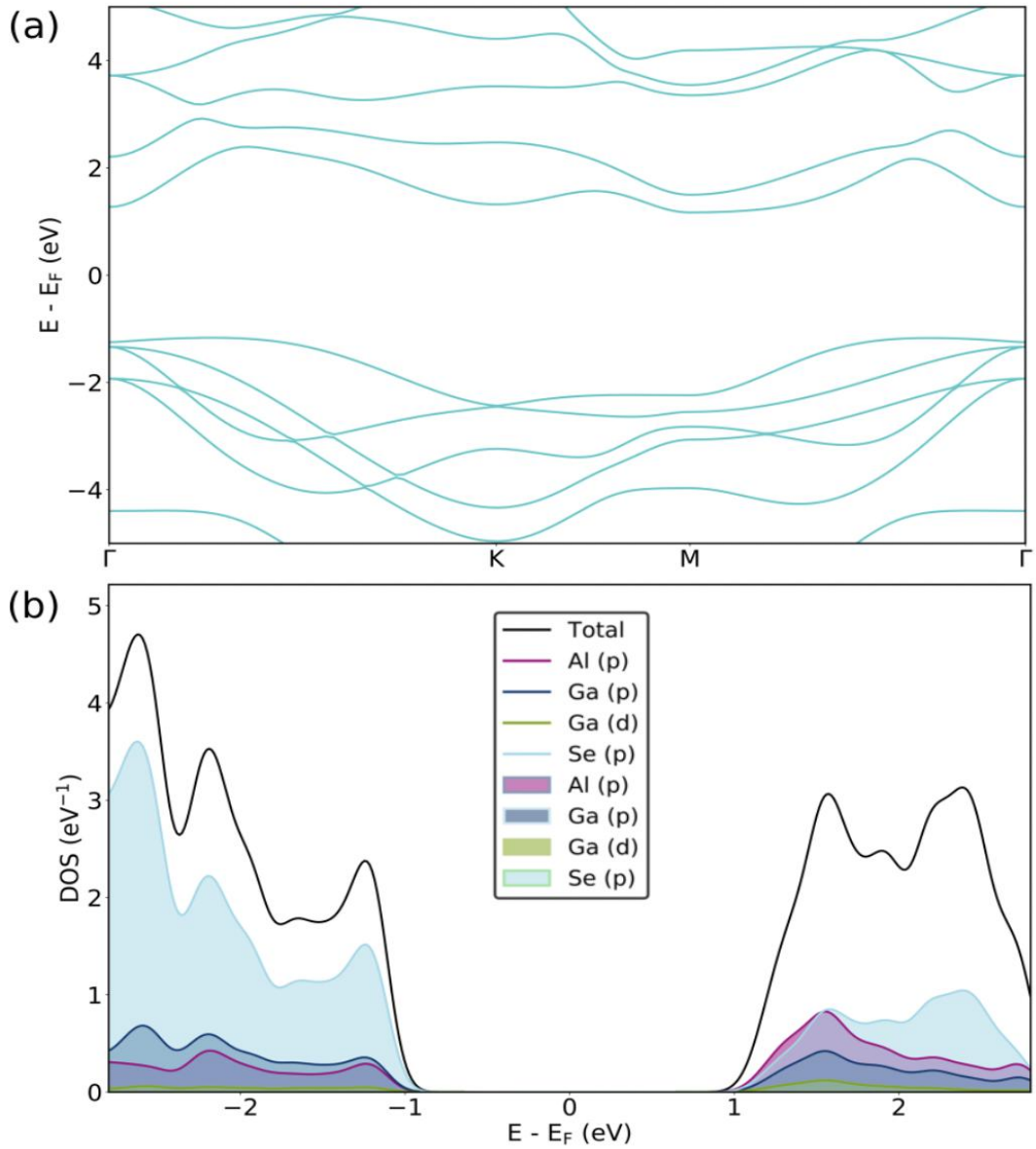

Figure 3. (a) Electronic structure and (b) projected density of states for AlGaSe. Fermi level is set to zero.

consist of Al p, Se p, Ga p and Ga d orbitals. The CBM of the AlGaSe/GaSe heterostructure is mainly influenced by the p orbitals of Se and Ga atoms. There is a small contribution from d orbital of Ga atoms. On the other hand, the VBM of the AlGaSe/GaSe heterostructure is primarily determined by the p orbitals of Se atoms. In the unoccupied region, the GaSe monolayer doesn't play a key role, but the p orbitals of the Ga have an impact on the VBM. There is an interesting observation of the overlap of electronic states between the p orbitals of Se and Ga in the region around $E_f - 2.5$ eV.

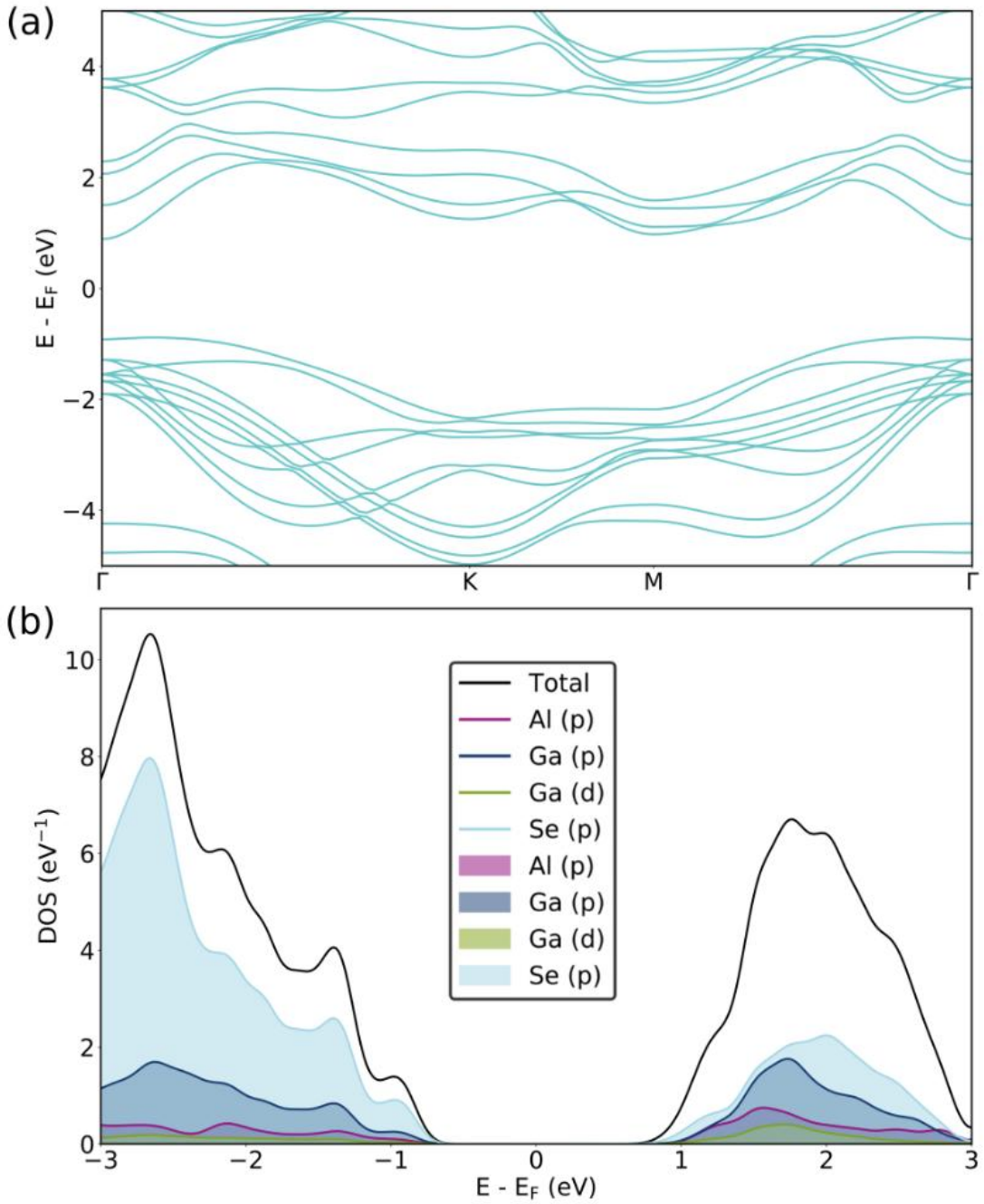

Figure 4. (a) Electronic structure and (b) projected density of states for GaSe/AlGaSe heterostructure. Fermi level is set to zero.

4. Conclusion

We have used density functional theory to examine the structural and electrical characteristics of AlGaSe/GaSe heterostructures. From the observed exothermic reaction, it seems that the development of AlGaSe can be accomplished by using the GaSe monolayer as a substrate. We achieved a high level of agreement with both actual and earlier computational data about the band gap of GaSe monolayers. The results of our study demonstrate that when a GaSe monolayer is combined with an AlGaSe monolayer, it leads to the formation of an indirect band gap with a value of 1.774 eV. A study was carried out to examine the influence of feeble interactions between the layers on the electrical structure. When AlGaSe is layered on top of a GaSe monolayer, the material maintains its indirect band gap, but the gap is reduced by 0.560 eV. Similar studies (Zhang et al., 2023) show that this is an effective approach to significantly modify the band structure through engineering stacking monolayer on GaSe and Janus structures. These discoveries provide useful insights for developing novel two-dimensional structures and their prospective applications in optoelectronics and field-effect transistor (FET) devices such as transistor channels, sensors, nano-generators, and high-frequency switches.

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Author contribution

C. Yelgel confirms sole responsibility for the following: study conception and design, data collection, analysis, theoretical calculations and interpretation of results, and manuscript preparation and writing.

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Conflict of interest

C. Yelgel declares that there is no conflict of interest.

Ethical statement

Ethics Committee approval is not required for this study.

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