



Full length article

Type-II AlAs/GeH van der Waals heterostructure: A promising platform for efficient solar-driven water splitting

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ABSTRACT

The rapid development of two-dimensional (2D) materials has opened new opportunities for designing high-performance systems for optoelectronic and photocatalytic applications. In this work, we utilize a first-principles approach to conduct a systematic analysis of the AlAs/GeH van der Waals heterostructure, focusing on its structural, electronic, and photocatalytic behaviors, as well as its optical and transport properties. Our findings demonstrate that the proposed heterostructure possesses both energetic and dynamic stability. Furthermore, the weak nature of the interlayer coupling ensures that the fundamental properties of the individual monolayers remain largely intact. The identification of a type-II band alignment in the AlAs/GeH heterostructure suggests that the heterostructure can efficiently separate photogenerated charge carriers across different spatial regions. Furthermore, the heterostructure exhibits a reduced band gap compared to the individual layers, leading to significantly enhanced optical absorption in both visible and ultraviolet regions. Carrier mobility calculations based on deformation potential theory show high electron mobility and a pronounced asymmetry between electron and hole transport, which is beneficial for suppressing charge recombination. Furthermore, the AlAs/GeH heterostructure can potentially operate via a Z-scheme mechanism, preserving strong redox capabilities. These findings highlight the AlAs/GeH heterostructure as a versatile platform for future light-driven electronic and catalytic technologies.

1. Introduction

Over the past decade, research on two-dimensional (2D) materials [1] has expanded rapidly, largely driven by the distinct physical properties that emerge at reduced dimensionality. These materials have been considered have been widely explored for advanced nanoelectronic [2], optoelectronic [3] and energy conversion systems [4]. The isolation of graphene [5] marked an important milestone, motivating the exploration of other layered compounds with similar structural characteristics. Since then, various classes of 2D materials, such as transition metal dichalcogenides (TMDs) [6], phosphorene [7], MXenes [8] and MA₂Z₄ family [9,10] have been investigated, each offering different electronic structures and functional possibilities. Despite this progress, several challenges still limit the practical application of 2D

materials. For example, graphene, although possessing exceptionally high carrier mobility, has a zero band gap, which restricts its use in applications requiring effective switching behavior [11]. Moreover, many 2D semiconductors exhibit limited photocatalytic performance, primarily due to inappropriate band edge positions relative to water redox potentials and the rapid recombination of photogenerated electron-hole pairs [12,13].

To address these limitations, several strategies have been proposed to tailor the physical properties of 2D materials. Methods such as strain engineering [14], chemical functionalization [15], and defect modulation [16] have been widely investigated, as they enable tuning of the electronic structure. However, these approaches may compromise structural stability or remain challenging to control with high precision

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in experimental implementations. An alternative and increasingly effective strategy is the assembly of van der Waals (vdW) heterostructures by integrating distinct 2D materials in a layered architecture [17–22]. This approach allows the integration of complementary properties from individual constituents while largely preserving their intrinsic characteristics, thereby providing greater flexibility in designing materials with enhanced performance. Specifically, vdW heterojunctions featuring type-II band offsets have emerged as a prominent area of study because they inherently facilitate the spatial decoupling of photogenerated carriers [23–26]. In those heterostructures, the conduction band minimum (CBM) and valence band maximum (VBM) are localized in different layers, which drives photogenerated electrons and holes to spatially separate regions. This separation suppresses electron–hole recombination and prolongs carrier lifetimes, thereby enhancing the efficiency of photoinduced processes. As a result, type-II heterostructures are considered especially promising for photocatalytic applications, including water splitting, where efficient charge separation and migration are essential for driving redox reactions under light irradiation.

Among the various 2D material candidates, group III–V [27–29] and hydrogenated group-IV [30,31] materials have become promising candidates for electronic and energy-related applications because of their highly tunable electronic responses and favorable carrier mobility. In particular, monolayer AlAs has been reported to exhibit semiconducting behavior and good structural stability, making it a promising candidate for electronic and optoelectronic applications [32]. Moreover, the electronic and optical properties of monolayer AlAs can be further engineered by forming heterostructures with other 2D semiconductors, such as ZnSe [33], InS [34], Ge [35], Ga₂SeTe [36] and Sb [37]. Interestingly, the interfacial band alignment in these AlAs-based heterostructures belongs to the type-II category, enabling electrons and holes to accumulate in separate layers and thus prolonging the lifetime of photoexcited carriers. For instance, Ma et al. [34] predicted that the AlAs/InS heterostructure possesses a type-II band alignment and operates via a Z-scheme photocatalytic mechanism, enabling efficient hydrogen production from water splitting. Similarly, Guo et al. [36] reported that the Ga₂SeTe/AlAs heterostructure exhibits type-II band alignment and an estimated solar-to-hydrogen (STH) conversion efficiency reaching 36.06%, making it a promising candidate for photocatalytic water splitting.

On the other hand, germanane (GeH), a fully hydrogenated derivative of germanium, has recently attracted considerable attention due to its direct band gap and high carrier mobility [38,39]. The physical properties of monolayer GeH are highly sensitive to external perturbations, such as strain [40], chemical functionalization [41,42], defects [43] and stacking with other 2D materials [44–47]. Furthermore, pristine GeH is predicted to be a nonmagnetic semiconductor, whereas appropriate chemical functionalization can induce magnetic ordering depending on the type and arrangement of the functional groups [42]. In particular, the formation of heterostructures with other 2D materials has been predicted to significantly enhance its electronic and optical properties, especially by improving charge separation efficiency, thereby making it suitable for photocatalytic applications. For instance, Li et al. [46] reported that a GeH-based heterostructure exhibits type-II band alignment and enhanced optical absorption, indicating its potential for efficient photocatalytic water splitting. Similarly, Kheshti et al. [44] demonstrated that GeH/GeCH₃ and GeH/InSe heterostructures can exhibit Z-scheme photocatalytic behavior, leading to improved charge separation and enhanced efficiency in water splitting. Taken together, these findings suggest that GeH is a promising candidate for photocatalytic applications, particularly when incorporated into van der Waals heterostructures.

Motivated by the above considerations, we perform a comprehensive first-principles investigation to elucidate the structural, electronic, optical, and transport properties, as well as the photocatalytic performance, of the AlAs/GeH heterostructure. The AlAs/GeH heterostructure

exhibits favorable band alignment for efficient charge separation, enhanced optical absorption in the visible region, and promising carrier transport characteristics. These findings not only provide new insights into the design of GeH-based heterostructures but also highlight the potential of the AlAs/GeH system for applications in photocatalysis and optoelectronics.

2. Computational methods

First-principles calculations were carried out within the framework of density functional theory (DFT) using the Quantum Espresso [48]. We accounted for ion–valence electron interactions via the projector augmented wave (PAW) technique [49]. For the exchange–correlation potential, the generalized gradient approximation (GGA) in the form of the PBE functional was implemented [50]. To properly account for the weak interlayer interactions in the AlAs/GeH heterostructure, dispersion corrections were included through the DFT-D2 scheme [51]. The plane-wave basis set was expanded with a kinetic energy cutoff of 500 eV. Brillouin zone integrations were performed using a $15 \times 15 \times 1$ Monkhorst–Pack k-point grid. A vacuum layer exceeding 30 Å was introduced along the perpendicular direction to avoid artificial interactions between periodic images. Structural optimization was conducted until the total energy variation was below 10^{-6} eV, and the Hellmann–Feynman forces on each atom were reduced to less than 0.01 eV/Å. The energetic stability of the heterostructure was evaluated through its binding energy. To achieve a more reliable description of the electronic structure, particularly the band gap, selected calculations were further refined using the Heyd–Scuseria–Ernzerhof (HSE) functional [52].

3. Results and discussion

We start by examining the geometric and electronic features of the pristine AlAs and GeH monolayers. Both systems crystallize in a hexagonal lattice with a characteristic buckled configuration, as shown in Fig. 1. The degree of buckling differs between the two materials, with AlAs exhibiting a height of 0.46 Å, while a more pronounced distortion of 0.74 Å is observed for GeH. The optimized lattice parameters are found to be 4.04 Å for AlAs and 4.03 Å for GeH, indicating a close lattice match between the two monolayers. The calculated band structures indicate distinct electronic characteristics for the two systems. AlAs is identified as an indirect-gap semiconductor, with the VBM located at the K point and the CBM at the Γ point. In contrast, GeH exhibits a direct band gap, with both the VBM and CBM situated at the Γ point. The band gap values obtained from the PBE functional are 1.78 eV for AlAs and 1.15 eV for GeH, while the use of the HSE functional increases these values to 2.67 and 1.90 eV, respectively. It is worth noting that the difference between the PBE and HSE results mainly originates from the upward shift of the CBM, while the position of the VBM remains nearly unchanged. However, both methods consistently describe the same band dispersion and preserve the fundamental electronic characteristics of the materials, including the nature of the band gap and the locations of the band extrema.

We further construct the AlAs/GeH van der Waals heterostructure by considering several possible stacking configurations, as illustrated in Fig. 2. Six distinct stacking arrangements are examined, namely AB@1, AB@2, AC@1, AC@2, AA@1, and AA@2. After full structural relaxation, the interlayer distance d between the AlAs and GeH layers is determined to be 2.87, 2.59, 2.17, 2.10, 2.86, and 2.25 Å for the AB@1, AB@2, AC@1, AC@2, AA@1, and AA@2 configurations, respectively, as listed in Table 1. Among these, the AC@2 configuration exhibits the shortest interlayer distance, whereas the largest separation is found for the AB@1 stacking. Interestingly, the obtained interlayer distances are comparable to those reported for other GeH-based [44,46] and SiH-based heterostructures [53–55]. Furthermore, these values are significantly larger than the H–As covalent bond length (1.52 Å), revealing

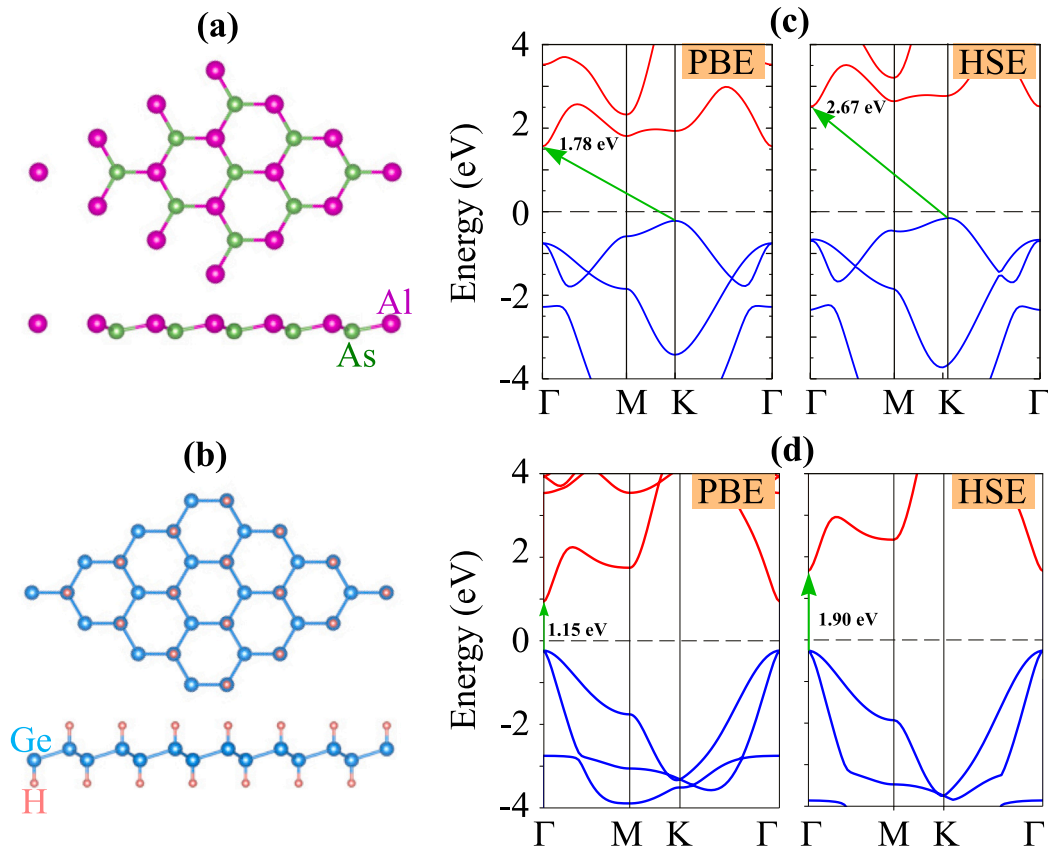


Fig. 1. Geometric optimizations of (a) AlAs and (b) GeH monolayers. Band structures of (c) AlAs and (d) GeH monolayers obtained from PBE and HSE functional.

that the interface is dominated by long-range vdW coupling instead of covalent bond formation.

Furthermore, the thermodynamic stability of the AlAs/GeH heterostructure is further evaluated through the binding energy (E_{BE}), defined as follows:

$$E_{BE} = E_{AlAs/GeH} - E_{AlAs} - E_{GeH} \quad (1)$$

where $E_{AlAs/GeH}$, E_{AlAs} and E_{GeH} correspond to the total energies of the combined system, the isolated AlAs layer, and the GeH monolayer, respectively. The resulting binding energies are calculated to be -0.032 , -0.106 , -0.112 , -0.115 , -0.033 , and -0.107 eV for the AB@1, AB@2, AC@1, AC@2, AA@1, and AA@2 configurations, respectively, as summarized in Table 1. Among the investigated arrangements, the AC@2 configuration is found to be the most stable due to its lowest E_b . The observation that all stacking modes yield negative binding energy values serves as evidence that the formation of the AlAs/GeH heterostructure is an energetically spontaneous process. Moreover, it is worth noting that beyond band alignment engineering, interlayer sliding in vdW heterostructures can provide an effective route for tuning electronic and valley-dependent properties by modulating the interlayer coupling and symmetry [56]. Such findings suggest additional opportunities for tailoring the functionalities of lattice-matched heterostructures.

To elucidate the role of interfacial stacking on the electronic properties, we compare the projected band structures and density-of-states profiles of the six AlAs/GeH heterostructures, as summarized in Fig. 3. Due to the weak vdW interaction between the two layers, the electronic characteristics of the individual constituents are largely retained upon heterostructure formation. In particular, the GeH layer preserves its direct band gap nature, while the AlAs layer maintains its intrinsic indirect semiconducting character. Even though the primary electronic features of each layer remain mostly intact, the resulting AlAs/GeH system exhibits a band gap that is notably narrower than those of

Table 1

Calculated structural and electronic parameters of the AlAs/GeH heterostructure for different stacking configurations, including the equilibrium interlayer distance (d), binding energy (E_b), band gap (E_g), and band alignment.

Patterns	d (Å)	E_{BE} (eV)	E_g (eV)	Alignment
AB@1	2.87	-0.032	0.96	Type-II
AB@2	2.59	-0.106	1.01	Type-II
AC@1	2.17	-0.112	1.00	Type-II
AC@2	2.10	-0.115	0.95	Type-II
AA@1	2.86	-0.033	0.96	Type-II
AA@2	2.25	-0.107	1.04	Type-II

its constituent monolayers. For the different stacking arrangements, the band gap values are calculated to be 0.96, 1.01, 1.00, 0.95, 0.96, and 1.04 eV for AB@1, AB@2, AC@1, AC@2, AA@1, and AA@2, respectively. This band gap narrowing is expected to have a significant impact on the optical response of the heterostructure. In particular, a smaller band gap enables optical transitions to occur at lower photon energies, thereby extending the absorption edge toward the visible region. As a result, the AlAs/GeH heterostructure is likely to exhibit enhanced light-harvesting capability under solar irradiation, which is advantageous for optoelectronic and photocatalytic applications. The calculated projected band structures and DOS show that the VBM at Γ point originate from GeH layer, while the CBM at Γ points are provided by AlAs layer. This staggered arrangement of energy levels leads to the spatial separation of photogenerated carriers, confirming that the AlAs/GeH vdW heterostructure forms a type-II heterojunction. This separation effectively suppresses the recombination of electron-hole pairs and prolongs their lifetime.

To verify the structural robustness of the AlAs/GeH system, we performed phonon spectrum analysis and AIMD modeling to examine its dynamical and thermal properties, as shown in Fig. 4. The

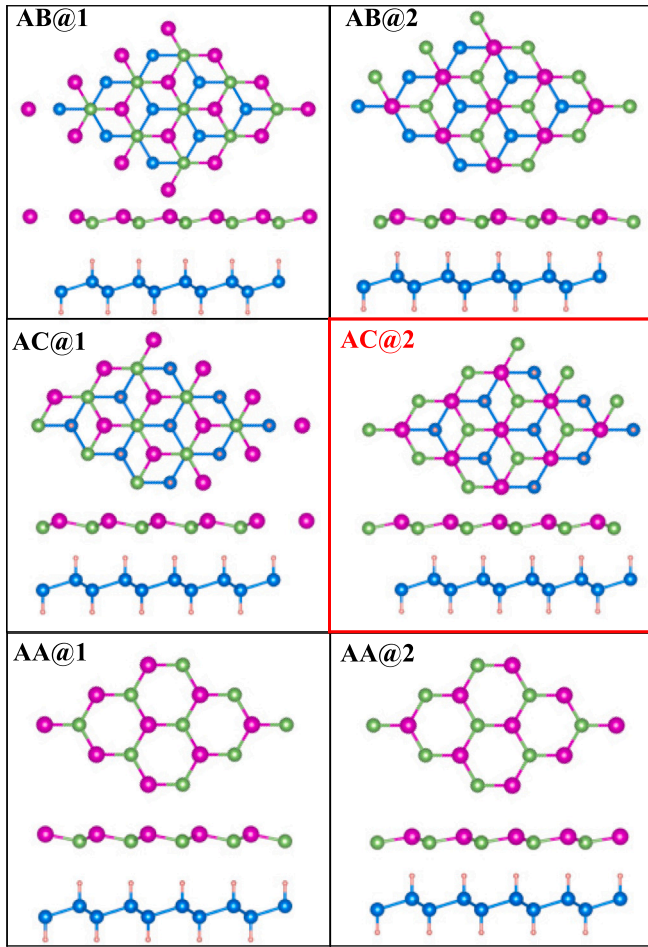


Fig. 2. Optimized geometric structures of the AlAs/GeH heterostructure for different stacking configurations.

phonon dispersion shown in Fig. 4(a) contains no imaginary modes across the entire Brillouin zone, confirming its dynamical stability. Thermal stability is further evaluated via AIMD simulations performed at 300 K, as depicted in Fig. 4(b). The fluctuations in temperature and total energy are negligible throughout the trajectory, as they oscillate narrowly around their equilibrium points. Additionally, no noticeable structural reconstruction or bond dissociation is observed throughout the simulation, thereby confirming the thermal robustness of the AlAs/GeH heterostructure. Taken together, these results confirm that the AlAs/GeH heterostructure is both dynamically and thermally stable, supporting its feasibility for practical applications.

To further explore the mechanical properties of the AlAs/GeH heterostructure, the in-plane elastic constants and elastic anisotropy are analyzed, as presented in Fig. 5. For a 2D hexagonal system, the independent elastic constants include C_{11} , C_{12} and C_{66} , where C_{66} can be expressed as $C_{66} = (C_{11} - C_{12})/2$. A comparison of the elastic constants for the AlAs/GeH system and its individual components is provided in Fig. 5(a). The in-plane stiffness, represented by C_{11} , reaches 98 N/m for the heterostructure, which is considerably higher than the corresponding values of 50 N/m and 52 N/m for the GeH and AlAs monolayers, respectively. A similar trend is observed for C_{12} , which increases from 11 N/m (GeH) and 18 N/m (AlAs) to 29 N/m in the heterostructure. These results indicate a clear enhancement of the mechanical rigidity upon heterostructure formation. The mechanical integrity of the AlAs/GeH heterostructure is evidenced by the calculated elastic constants, which fulfill the essential 2D stability requirements, i.e. $C_{11} > 0$ and $C_{11} - C_{12} > 0$.

To further characterize the elastic response, the orientation-dependent Young's modulus is evaluated using the relation:

$$Y(\theta) = \frac{C_{11}C_{22} - C_{12}^2}{C_{11}\sin^4\theta + C_{22}\cos^4\theta + \left(\frac{C_{11}C_{22} - C_{12}^2}{C_{66}} - 2C_{12}\right)\sin^2\theta\cos^2\theta} \quad (2)$$

For a hexagonal system, where $C_{11} = C_{22}$, the above expression can be simplified accordingly. The in-plane elastic response of the AlAs/GeH system is found to be isotropic, as evidenced by the perfectly circular contour of the Young's modulus angular dependence presented in Fig. 5(b). Furthermore, the Young's modulus of the AlAs/GeH heterostructure is calculated to be 89 N/m, which is significantly higher than those of the AlAs (46 N/m) and GeH (47 N/m) monolayers. This enhancement reflects the improved mechanical stiffness arising from interlayer interactions, suggesting that the heterostructure can better withstand external mechanical deformation compared to its individual constituents.

For a more profound understanding of the charge transfer mechanisms and interfacial physics, the electrostatic potential and charge density difference for the AlAs/GeH heterostructure are evaluated and displayed in Fig. 6. We define the difference in charge density using the following relation:

$$\Delta\rho(\mathbf{r}) = \rho_{\text{AlAs/GeH}}(\mathbf{r}) - \rho_{\text{AlAs}}(\mathbf{r}) - \rho_{\text{GeH}}(\mathbf{r}), \quad (3)$$

where $\rho_{\text{AlAs/GeH}}(\mathbf{r})$, $\rho_{\text{AlAs}}(\mathbf{r})$ and $\rho_{\text{GeH}}(\mathbf{r})$ represent the charge densities of the AlAs/GeH heterostructure, isolated AlAs, and GeH monolayers, respectively, with all components taken at the same atomic positions as in the heterostructure. Positive and negative values of $\rho(\mathbf{r})$ denote electron accumulation and depletion, respectively. Fig. 6(a) reveals a significant redistribution of charge density at the AlAs/GeH interface, characterized by the coexistence of accumulation and depletion regions on opposite sides of the junction. This interfacial charge transfer generates an intrinsic electric field, which can facilitate the separation of photogenerated carriers and suppress their recombination. Specifically, charge depletion is mainly localized on the AlAs layer (green region), while charge accumulation occurs on the GeH layer (orange region), indicating that electrons are transferred from AlAs to GeH upon contact. Furthermore, this behavior is consistent with the difference in work function between the two constituents, where AlAs (4.84 eV) has a lower work function than GeH (5.59 eV), as illustrated in Fig. 6(b). As a result, electrons tend to flow from AlAs to GeH until equilibrium is established. As a consequence of the electron transfer between the constituent layers, an internal electrostatic field of 0.75 eV is generated at the interface, extending from the electron-deficient GeH side to the electron-enriched AlAs side.

To evaluate the potential of the AlAs/GeH heterostructure for optoelectronic and photocatalytic applications, it is essential to examine its optical absorption characteristics, as efficient light harvesting plays a decisive role in determining the overall device performance. In particular, strong absorption in the visible region is highly desirable for maximizing solar energy utilization. The optical properties of the AlAs/GeH heterostructure are therefore investigated through the absorption coefficient and compared with those of the individual monolayers. The absorption coefficient $\alpha(\omega)$ is expressed through real ($\epsilon_1(\omega)$) and imaginary ($\epsilon_2(\omega)$) part as [43]:

$$\alpha(\omega) = \frac{\sqrt{2}\omega}{c} \left[(\epsilon_1^2(\omega) + \epsilon_2^2(\omega))^{1/2} - \epsilon_1(\omega) \right]^{1/2} \quad (4)$$

The optical absorption of the heterostructure, along with those of the individual AlAs and GeH monolayers, are presented in Fig. 7. A significant enhancement in the absorption intensity is observed upon the formation of the heterostructure, covering both the visible and ultraviolet regions. This enhancement can be attributed to the reduced band gap and the increased density of electronic states near the band edges, which facilitate optical transitions. Specially, in the

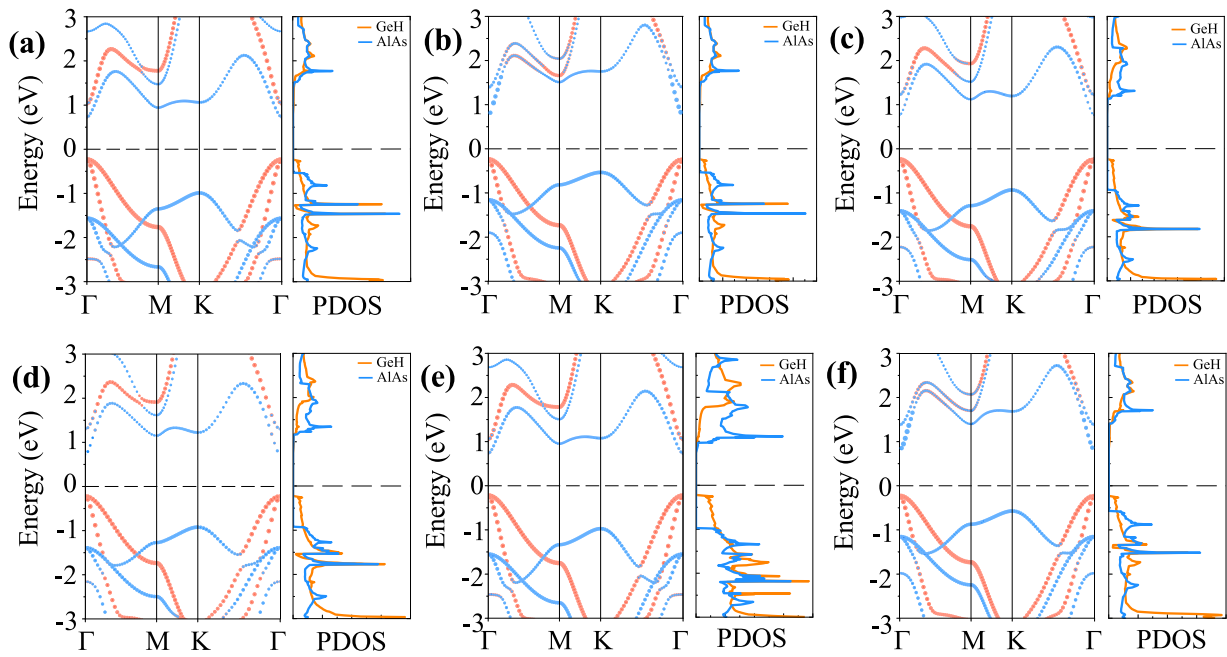


Fig. 3. Projected band structures and density of states of the AlAs/GeH heterostructure for the (a) AB@1, (b) AB@2, (c) AC@1, (d) AC@2, (e) AA@1, and (f) AA@2 stacking modes. Orange and blue colors denote the electronic states originating from the GeH and AlAs layers, respectively. The Fermi energy is taken as the reference level (0 eV) and is marked by the dashed line.

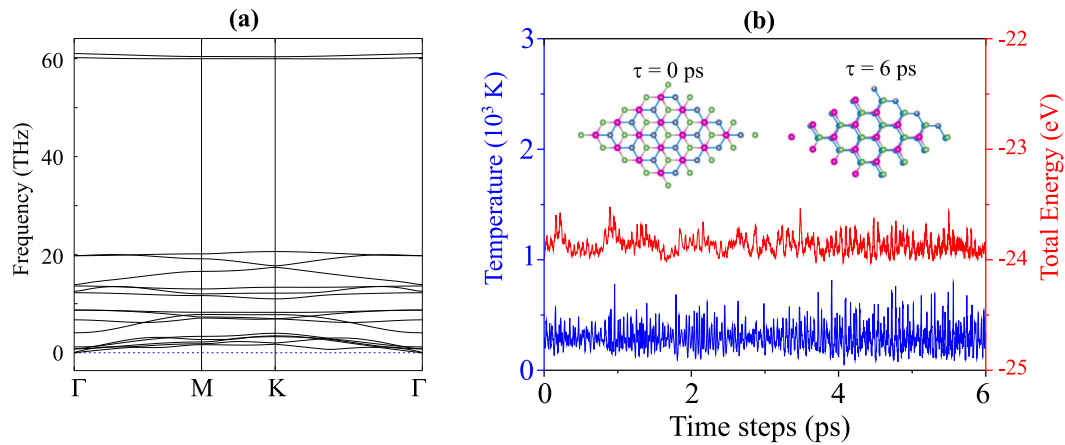


Fig. 4. (a) Phonon spectrum and (b) AIMD simulations of the temperature and total energy of the AlAs/GeH heterostructure as a function of simulated time steps.

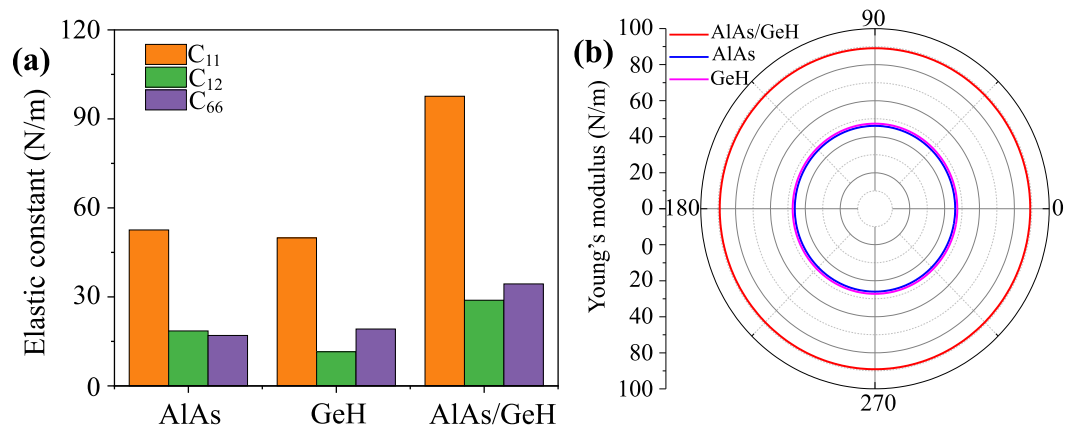


Fig. 5. (a) Calculated in-plane elastic constants and (b) polar representation of the orientation-dependent Young's modulus for the AlAs/GeH heterostructure.

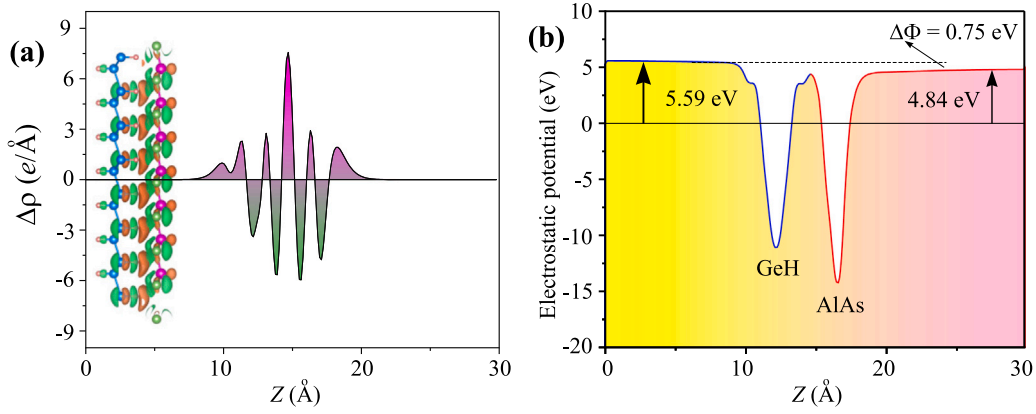


Fig. 6. (a) Spatial distribution of the plane-averaged charge-density difference and (b) electrostatic potential variation along the out-of-plane direction of the AlAs/GeH heterostructure. The orange and green regions represent charge accumulation and depletion, respectively.

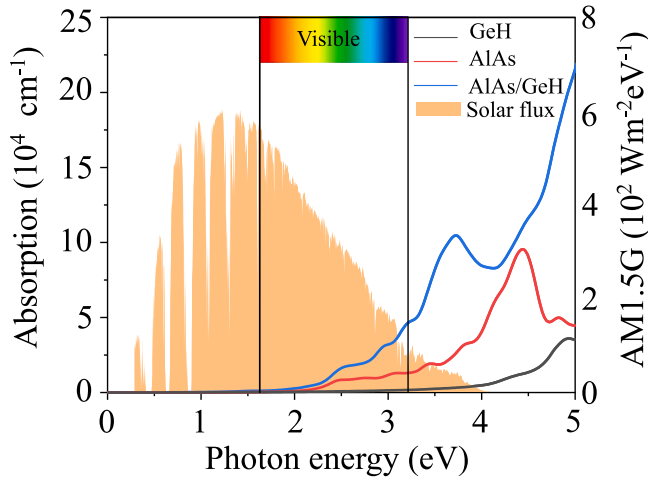


Fig. 7. Optical absorption coefficient of the AlAs/GeH heterostructure and its constituent AlAs and GeH monolayers.

visible range, the AlAs/GeH heterostructure exhibits a maximum absorption coefficient of $4.56 \times 10^4 \text{ cm}^{-1}$ at the photon energy of 3.2 eV. This value is substantially higher than those of the GeH monolayer ($1.7 \times 10^3 \text{ cm}^{-1}$) and AlAs ($1.3 \times 10^4 \text{ cm}^{-1}$), indicating a pronounced improvement in visible-light absorption. A similar trend is observed in the ultraviolet region. The heterostructure reaches a peak absorption coefficient of $2.15 \times 10^5 \text{ cm}^{-1}$ at 5 eV, which is approximately five times higher than that of AlAs ($4.5 \times 10^4 \text{ cm}^{-1}$) and about six times greater than that of GeH ($3.54 \times 10^4 \text{ cm}^{-1}$) by 6 times. These results clearly demonstrate that the formation of the AlAs/GeH heterostructure significantly enhances light absorption over a wide energy range, particularly in the visible region, which is crucial for efficient solar energy utilization.

To further evaluate the transport performance of the AlAs/GeH heterostructure, the carrier mobility is investigated, as it plays a crucial role in determining the efficiency of charge transport in nanoelectronic, optoelectronic, and photocatalytic devices. High carrier mobility facilitates rapid migration of photogenerated electrons and holes, thereby reducing recombination probability and improving device performance. In this work, the carrier mobility is estimated based on the deformation potential (DP) theory as below:

$$\mu = \frac{e\hbar^3 C_{2D}}{k_B T m^* m_d E_1^2} \quad (5)$$

Table 2

Calculated carrier mobility and related parameters in the AlAs, GeH monolayer and their AlAs/GeH heterostructure.

Material	Direction	Carrier type	$m^* (m_e)$	C_{2D} (N/m)	E_1 (eV)	μ_{2D} ($\text{cm}^2 \text{ V}^{-1} \text{ s}^{-1}$)
AlAs	x direction	e^-	0.16	77.73	9.96	651.30
		h^+	0.76	77.73	0.66	7235.15
	y direction	e^-	0.16	77.73	9.96	651.27
		h^+	0.61	77.73	0.66	9013.86
GeH	x direction	e^-	0.08	66.67	10.36	1932.74
		h^+	0.51	66.67	3.11	558.47
	y direction	e^-	0.09	66.67	10.36	1778.95
		h^+	0.50	66.67	3.11	578.46
AlAs/GeH	x direction	e^-	0.09	143.67	11.67	2629.25
		h^+	0.52	143.67	4.15	670.07
	y direction	e^-	0.10	143.67	11.67	2368.51
		h^+	0.50	143.67	4.15	707.11

In this equation, e is the elementary charge, while k_B and $\hbar$ denote the Boltzmann and reduced Planck constants, respectively. Unless otherwise stated, T is taken as 300 K. m^* is the effective mass of the carrier along the transport direction, and m_d is the average effective mass defined as:

$$m_d = \sqrt{m_x^* m_y^*} \quad (6)$$

Here, $m_{x,y}^*$ represents the effective masses along the x, y directions.

The deformation potential constant E_1 , which characterizes the sensitivity of the band edge to strain, is defined as:

$$E_1 = \frac{\partial E_{\text{edge}}}{\partial \epsilon} \quad (7)$$

where E_{edge} corresponds to the energy of the CBM for electrons or the VBM for holes.

Fig. 8 illustrates the strain-induced changes in the total energy and band edge levels, while the carrier mobility parameters for the AlAs/GeH system, alongside the results for standalone AlAs and GeH monolayers, are compiled in Table 2. The results show that the heterostructure exhibits relatively high electron mobility, reaching 2629.25 and 2368.51 $\text{cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ along the x and y directions, respectively. One can observe that the electron mobility of the AlAs/GeH heterostructure is greater than that of the constituent monolayers. The enhanced electron mobility in the AlAs/GeH heterostructure can be understood from the deformation potential theory. It is obvious that the carrier mobility is positively proportional to the in-plane stiffness C_{2D} and inversely proportional to both the effective mass and the square of the deformation potential constant E_1 . Compared with the pristine GeH monolayer, the heterostructure retains a small electron effective mass (0.09 m_e versus 0.08 m_e) while exhibiting a

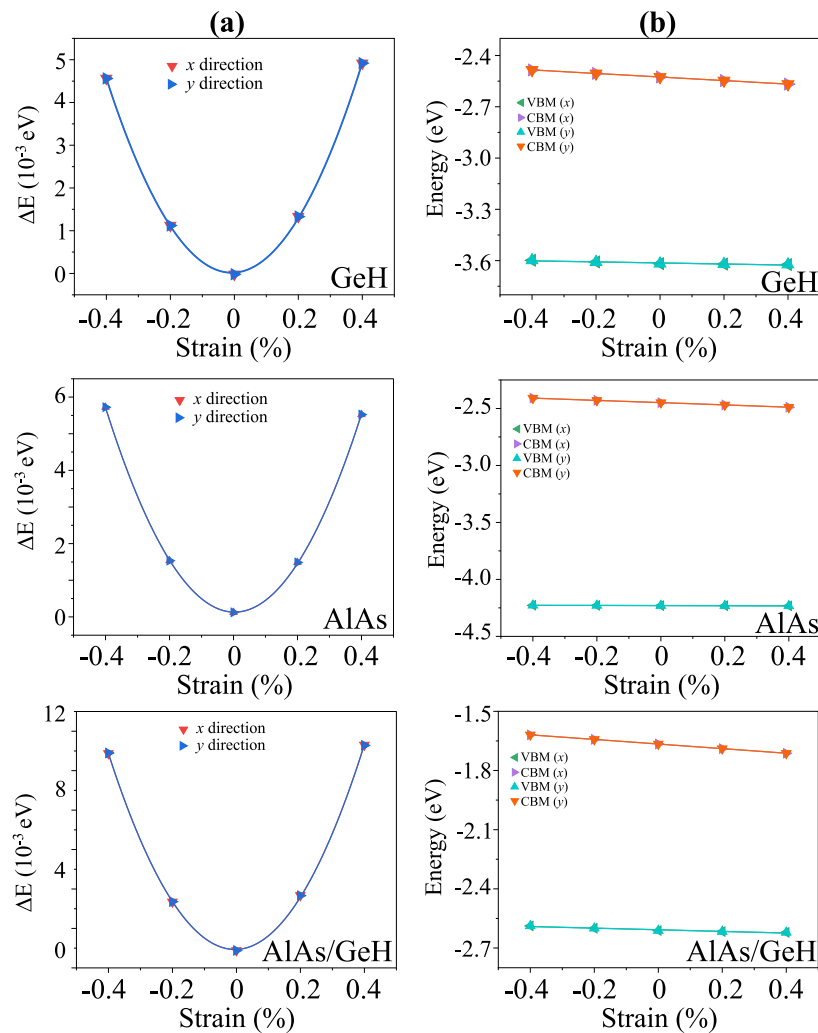


Fig. 8. Small strain-induced in (a) total energy and (b) band edge positions of the GeH, AlAs and the AlAs/GeH heterostructure.

substantial increase in the elastic modulus from 66.67 to 143.67 N/m. Although the deformation potential constant increases slightly from 10.36 to 11.67 eV, the pronounced enhancement in C_{2D} dominates the transport behavior, resulting in a higher electron mobility. In contrast, the hole mobility is considerably lower, with values of 670.07 and 707.11 $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$ along the x and y directions, respectively. This pronounced asymmetry between electron and hole mobilities is advantageous for suppressing the recombination of photogenerated charge carriers. Specifically, the higher mobility of electrons enables their rapid transport across the heterostructure, while the relatively slower holes tend to remain localized, thereby promoting effective charge separation.

The vacuum-aligned band edge positions for both the isolated monolayers and the AlAs/GeH system are provided in Fig. 9. For the AlAs monolayer, the VBM is located below the oxidation potential of water (OER), while the CBM lies above the reduction potential (HER). These results confirm that the AlAs monolayer fulfills the energetic criteria for overall water splitting, making it a viable candidate for simultaneous hydrogen and oxygen production. On the other hand, the GeH sheet exhibits a CBM above the HER, but its VBM fails to reach the necessary depth below the OER potential. This band alignment indicates that, although GeH possesses sufficient reducing power for hydrogen evolution, it lacks the necessary oxidizing capability to drive the oxygen evolution reaction. As a result, the GeH monolayer alone is not suitable for overall photocatalytic water splitting. In the AlAs/GeH heterostructure, the existence of a type-II band alignment ensures that

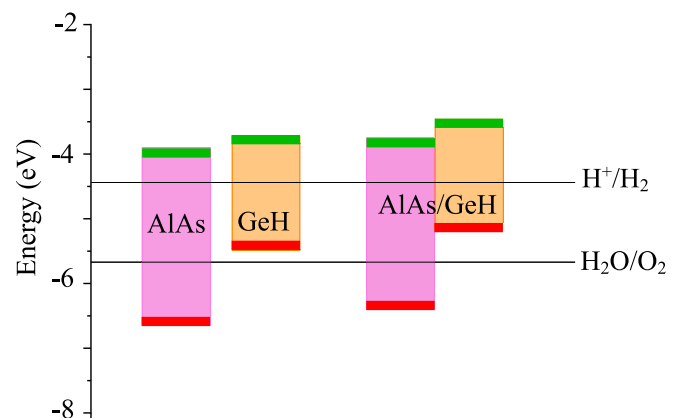


Fig. 9. Band edge positions calculated at HSE06 level for AlAs, GeH monolayers and the AlAs/GeH heterostructure referenced to the vacuum level.

photogenerated carriers are spatially decoupled across the interface, a feature that effectively mitigates the recombination of electrons and holes. However, in this configuration, the VBM of the heterostructure remains above the OER potential, indicating insufficient oxidizing power for the oxygen evolution reaction. As a result, the conventional type-II mechanism cannot support overall water splitting, despite its

advantage in charge separation. Nevertheless, it is worth noting that heterostructures with similar band alignments can still achieve overall water splitting through a direct Z-scheme mechanism. In such a mechanism, electrons in the CBM of AlAs layer recombine with holes in the VBM of the GeH layer, preserving the strong redox potentials of the remaining charge carriers. This allows the system to retain both strong reduction and oxidation capabilities simultaneously, thereby enabling overall water splitting. Therefore, the photocatalytic performance of the AlAs/GeH heterostructure should be further evaluated by considering the possibility of a Z-scheme charge transfer mechanism.

4. Conclusions

In summary, this study provides a comprehensive first-principles investigation into the structural, electronic, transport, and photocatalytic properties of the AlAs/GeH vdW heterostructure. Our results demonstrate that the AlAs/GeH heterostructure is energetically, dynamically, thermally, and mechanically stable. The electronic analysis reveals a staggered type-II band alignment, where the VBM and CBM are spatially localized on the GeH and AlAs layers, respectively. This feature is instrumental in facilitating the spatial separation of photo-generated carriers and suppressing charge recombination. Furthermore, the formation of the AlAs/GeH heterostructure leads to band gap narrowing, which significantly enhances optical absorption in both the visible and ultraviolet regions. The transport performance is characterized by exceptionally high electron mobility up to $2629.25 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ and a pronounced mobility asymmetry, further promoting efficient charge migration. Most importantly, while the individual GeH layer is limited, the AlAs/GeH heterostructure satisfies the thermodynamic requirements for overall water splitting. By operating through a direct Z-scheme mechanism, the AlAs/GeH heterostructure preserves strong redox potentials, enabling efficient solar-driven hydrogen and oxygen evolution. These findings highlight the AlAs/GeH vdW heterostructure as a highly promising candidate for next-generation optoelectronic devices and sustainable energy conversion technologies.

CRediT authorship contribution statement

Ho Kim Dan: Writing – original draft, Software, Resources, Methodology, Conceptualization. **Huynh Thi Phuong Thuy:** Software, Methodology, Data curation, Conceptualization. **Le Phuong Long:** Writing – original draft, Methodology, Investigation, Data curation. **Le Phuoc Dinh:** Software, Methodology, Investigation. **Nguyen D. Hien:** Writing – original draft, Supervision, Resources. **Khang D. Pham:** Writing – original draft, Supervision, Software, Resources, Data curation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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