Tuning the Electronic and Optical Properties of the ZrS$_2$/PtS$_2$ van der Waals Heterostructure by an External Electric Field and Vertical Strain

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ABSTRACT: Two-dimensional (2D) material-based heterostructures gain increasing interest due to their extraordinary properties and excellent potential for the optoelectronic devices. This study deals with modulation of electronic and optical properties of the ZrS$_2$/PtS$_2$ van der Waals heterostructure under vertical strain and an external electric field based on first principles calculation. Different stacking of ZrS$_2$ and PtS$_2$ layers are considered for the heterostructure formation and the most stable structure with lowest binding energy is selected for further calculations. The stable ZrS$_2$/PtS$_2$ heterostructure shows an indirect band gap of 0.74 eV, which is smaller than that of both ZrS$_2$ and PtS$_2$ monolayers. With the applied external electric field, the band gap value of the ZrS$_2$/PtS$_2$ heterostructure increases with the negative electric field and decreases with the positive electric field. It is observed that the indirect-to-direct band gap transition occurs when the highest negative value of the electric field is applied. In the case of vertical strain applied to the heterostructure, with an increase in compressive strain, the band gap decreases and vice versa for tensile strain. Optical absorption spectra show significant absorption in the visible light region to the ultraviolet light region. This study shows that the electronic and optical properties of ZrS$_2$/PtS$_2$ heterostructures can be modulated by using vertical strains and an external electric field.

1. INTRODUCTION

Two-dimensional (2D) materials have drawn significant attention due to their unique electrical, optical, mechanical, and thermal properties such as transition metal dichalcogenides (TMDs), e.g., MoS$_2$, MoSe$_2$, WS$_2$, WSe$_2$, and ZrS$_2$ show fascinating properties.\textsuperscript{1−3} Based on their extraordinary properties, 2D materials are widely used in applications such as catalyst, solar cells, lithium-ion batteries, and superconductivity. ZrS$_2$ is thermodynamically stable and shows high sensitivity and environmental suitability\textsuperscript{4−13} and due to its higher carrier mobility and current density is used in the nanoelectronic devices and vastly used in photodetectors and solar cell applications.\textsuperscript{14} The PtS$_2$ monolayer has higher carrier mobility than phosphorene which shows its application in optoelectronics.

Nowadays, van der Waals heterostructures based on 2D materials are extensively studied theoretically and experimentally. These heterostructures are obtained by vertically stacking two or more different monolayers and show extraordinary properties as compared to monolayers, thereby providing opportunities to be used in nanoelectronic and optoelectronic device applications. Some examples of heterostructures based on different 2D materials are graphene/TMDs, CdO/GaS, and so on.\textsuperscript{16,17} Three types of band alignments can be observed in van der Waals heterostructures such as straddling type-I, staggered type-II, and broken-gap type-III. Due to these band alignments, these heterostructures have different applications such as light-emitting diodes, quantum well lasers, photovoltaics, photocatalysts, and field-effect transistors (FETs).

For example, the CdO/GaS vdw heterostructure is a direct band gap semiconductor and due to type-II band alignment, it shows excellent photocatalytic performance in the whole visible region under biaxial strain.\textsuperscript{16} A type-II heterostructure InSe/β-Sb shows the efficient carrier separation for optoelectronics applications.\textsuperscript{18} The silicene/Sc$_2$CF$_2$ heterostructure...
looks promising for high-performance FETs with high carrier mobilities in nanoelectronics.\textsuperscript{19}

Ge/GaGeTe is an excellent heterostructure with electric field-induced archetype data storage device having high carrier mobility and tunable band gaps. Its band structure can be flexibly modulated surprisingly, when strain or bias voltage is applied. Being a new type in electronic devices, it has potential advantage for high-speed effective FETs and promising application in nanoelectronics.\textsuperscript{20}

2D ZrS\textsubscript{2} and PtS\textsubscript{2} have similar lattice parameters and hexagonal crystal structures which make it possible to form stable heterostructures in a laboratory. It is a well-established strategy to tune the electronic and optical properties of the 2D materials by applying strain and an external electric field such as in the case of graphene/g-GeC,\textsuperscript{21} AlN/InSe,\textsuperscript{22} SnSe/GeSe,\textsuperscript{23} and g-ZnO/2H-TiS\textsubscript{2} due to their unique layered structures. These studies show that the electronic properties of both ZrS\textsubscript{2} and PtS\textsubscript{2} can be tuned by creating vdW heterostructures and applying an external electric field and vertical strain.

In 2D materials, strain arise due to externally applied stress, pseudomorphic growth, and 2D material layers clamped to the substrate.\textsuperscript{25}

Recent experimental and theoretical work has explained that with application of external strains, such as biaxial strain and uniaxial strain, the optical, electronic, mechanical, and chemical properties of 2D materials can be manipulated. For band structure manipulation, the application of large strains is allowed for the incredible strength of TMDCs, as compared to their conventional semiconducting counterparts. For example, a semiconductor to metal phase transition and a direct to indirect band gap transition are expected to occur in a semiconductor to metal phase transition and a direct to indirect band gap transition.\textsuperscript{20}

However, there is no study available to tune the electronic and optical properties of the ZrS\textsubscript{2}/PtS\textsubscript{2} heterostructure by applying an external electric field and vertical strain. In the present study, first principles calculations are performed to investigate the electronic and optical properties of the ZrS\textsubscript{2}/PtS\textsubscript{2} vdWH heterostructures using vertical strain and the external electric field, and from the results, a significant change in properties of the heterostructure is observed. Our study shows that the ZrS\textsubscript{2}/PtS\textsubscript{2} heterostructure is a suitable material for nanoelectronic and optoelectronic devices.

2. COMPUTATIONAL METHODS

All calculations are performed using density functional theory (DFT)-based code quantum espresso. The generalized gradient approximation (GGA) of Perdew–Burke–Ernzerhof (PBE) is used to describe the exchange–correlation functional. van der Waals interactions between different heterostructures are considered by using the semiempirical correction DFT-D3 scheme proposed by Grimme. A cutoff energy of 60 Ry is set for a plane wave expansion, and a grid of 10 × 10 × 1 k-points is sampled using the Monkhorst-Pack method in the Brillouin zone (BZ) for both monolayers and the heterostructure. Structural relaxation was obtained with the convergence criteria of 10^{-6} Ry and 10^{-3} Ry/Bohr for energy and force, respectively. A vacuum distance of 20 Å perpendicular to the layers is added to remove interactions between adjacent slabs.

3. RESULTS AND DISCUSSION

3.1. Structural Properties. First, optimized lattice parameters of monolayers and heterostructures were obtained then stable configuration of the heterostructure was selected for further calculation. The optimized lattice constants of the PtS\textsubscript{2} and ZrS\textsubscript{2} monolayer are 3.56 and 3.63 Å, respectively, which are in excellent agreement with the lattice parameter obtained by previous researchers 3.58 Å of the PtS\textsubscript{2} monolayer\textsuperscript{27} and 3.67 Å of the ZrS\textsubscript{2} monolayer.\textsuperscript{28}

We used 2 × 2 monolayers of PtS\textsubscript{2} and ZrS\textsubscript{2} to construct the ZrS\textsubscript{2}/PtS\textsubscript{2} vdWHs and the lattice mismatch is 1.7%. Three possible stacking patterns of the ZrS\textsubscript{2}/PtS\textsubscript{2} vdWHs were considered to find the suitable stable configuration. The top and the side views of the three configurations are shown in Figure 1 named AB, A′B, and A′B′ where A represents the ZrS\textsubscript{2} monolayer, B represents the PtS\textsubscript{2} monolayer, and A′ and B′ represent the 180° rotation of the monolayers from each other.
The most stable structure was obtained by calculating the binding energy of different interlayer spacings for all three stacking patterns. Binding energy can be solved by the following equation:

\[
E_b = E_{(PtS_2/ZrS_2)}^{vdWHs} - E_{PtS_2} - E_{ZrS_2}
\]

where \(E_{(PtS_2/ZrS_2)}^{vdWHs}\), \(E_{PtS_2}\), and \(E_{ZrS_2}\) are the total energies of the ZrS\(_2\)/PtS\(_2\) heterostructure, the PtS\(_2\) monolayer, and the ZrS\(_2\) monolayer, respectively. The variation of binding energy with the interlayer distance is shown in Figure 2. The equilibrium interlayer distance for the AB structure is 2.83 Å corresponding to lowest binding energy, and for the A′B and AB′ layers, it is almost the same, i.e., 3.1 Å. The binding energy with a negative value shows that the obtained heterostructure is a stable structure.

**3.2. Electronic Properties.** We studied the electronic properties by carrying out partial density of states (PDOS) and electronic band structure analysis of the ZrS\(_2\)/PtS\(_2\) heterostructure. The PDOS analysis of the ZrS\(_2\)/PtS\(_2\) heterostructure shows that VBM originates from maximum contribution of d-orbitals of Pt and p-orbitals of S, while CBM has equal contribution from the d-orbitals of Zr and p-orbitals of S as shown in Figure 3.

To study the band structure of the ZrS\(_2\)/PtS\(_2\) heterostructure, first band structures of ZrS\(_2\) and PtS\(_2\) monolayers are calculated and shown in Figure 4. ZrS\(_2\) shows an indirect band gap of 0.98 eV, at \(\Gamma\) and between \(\Gamma\) and M point of the BZ as shown in Figure 4a which is similar in result with previous DFT study based on GGA approximation. PtS\(_2\) represents an indirect band gap of 1.70 eV as shown in Figure 4b. Figure 4c represents the band structure of the ZrS\(_2\)/PtS\(_2\) heterostructure which shows that the band gap is indirect in nature of 0.74 eV and this band gap value is lower than that of both ZrS\(_2\) and PtS\(_2\) monolayers. For the ZrS\(_2\)/PtS\(_2\) heterostructure, the CBM is positioned between the \(\Gamma\) point, while VBM is positioned between \(\Gamma\) and M points. As it can be observed that the VBM is contributed from PtS\(_2\) and CBM is contributed from ZrS\(_2\), so it can be concluded that the VBM and CBM of the heterostructure are a feature of two different layers. It shows that the ZrS\(_2\)/PtS\(_2\) heterostructure forms a type-II band alignment.\(^{29,30}\) This type of band alignment offers an opportunity to separate electron–hole pair spontaneously which is useful for solar energy conversion and photocatalytic applications.

Figure 5 represents the electrostatic potential of the ZrS\(_2\)/PtS\(_2\) heterostructure along the Z-direction at equilibrium. It can be seen that the ZrS\(_2\) monolayer has a more negative potential than the PtS\(_2\) monolayer which results in a potential difference of about 0.4 eV between the heterostructure layers. Due to this potential difference in the layers a strong built-in electric field is developed between the layers. This built-in electric field decreases the recombination rate of the photogenerated electron–hole pair which shows its potential application in optoelectronic devices. To further explore the understanding of the charge separation and charge transfer in the ZrS\(_2\)/PtS\(_2\) heterostructure, we obtained the charge density difference between the layers using this equation

\[
\Delta \rho = \rho_{ZrS_2/PtS_2} - \rho_{ZrS_2} - \rho_{PtS_2}
\]
where \( \rho_{\text{ZrS}_2/\text{PtS}_2} \), \( \rho_{\text{ZrS}_2} \), and \( \rho_{\text{PtS}_2} \) represent the charge density of the \( \text{ZrS}_2/\text{PtS}_2 \) heterostructure and charge density of the \( \text{ZrS}_2 \) monolayer and the \( \text{PtS}_2 \) monolayer, respectively. Figure 5b shows the charge density difference plot where electron’s depletion and accumulation are represented by the blue area and red area, respectively, and it can be observed that charge redistribution occurs between the heterostructure layers. It is observed that charge depletion occurs in the \( \text{PtS}_2 \) layer and accumulated to the \( \text{ZrS}_2 \) layer which results in the built-in electric field in the monolayers.

### 3.3. Electric Field Effects on the Band Structure of the \( \text{ZrS}_2/\text{PtS}_2 \) Heterostructure

Electronic and optical properties can be tuned by applying the external electric field to the heterostructure. An external electric field is applied normal to the heterostructures.

Figure 4. Band structure of (a) \( \text{ZrS}_2 \), (b) \( \text{PtS}_2 \), and (c) \( \text{ZrS}_2/\text{PtS}_2 \) vdW heterostructures.

Figure 5. (a) Electrostatic potential of the \( \text{ZrS}_2/\text{PtS}_2 \) heterostructure along the Z-direction and (b) charge density difference of the \( \text{ZrS}_2/\text{PtS}_2 \) heterostructure, red and blue colors correspond to the accumulation and depletion of electronic densities.
the ZrS$_2$/PtS$_2$ heterostructure, its positive direction is taken from ZrS$_2$ to PtS$_2$ and the negative direction from PtS$_2$ to ZrS$_2$ along the z-axis. The applied electric field ranges from $-0.6$ to $0.6$ V/Å, and the interval is $0.2$ V/Å. Band structures of the ZrS$_2$/PtS$_2$ heterostructure under different electric fields is shown in Figure 6.

The band gap value of the ZrS$_2$/PtS$_2$ heterostructure increases with the electric field intensity from 0 to $-0.6$ V/Å and decreases with electric field intensity from 0 to $+0.6$ V/Å. With the external electric field applied, the indirect-to-direct band gap transition occurs in the electric field $-0.6$ V/Å, as shown in Figure 6b. Our results show that applying the vertical external electric field not only changes the band gap but also changes the band gap type from indirect to direct. From the band structure graphs it can be observed that the CBM at the $\Gamma$ point and the VBM at the $\Gamma$–M path of the ZrS$_2$ monolayer moved upward and the CBM and the VBM of the PtS$_2$ monolayer at the $\Gamma$ point moved downward with the application of a negative field. This shows that increasing the strength of the negative electric field decreases the band gap of the heterostructure.

3.4. Vertical Strain Effects on the Band Structure of the ZrS$_2$/PtS$_2$ Heterostructure. The band structures of the ZrS$_2$/PtS$_2$ heterostructure under vertical strain are shown in Figure 7. The interlayer distance is varied under vertical strain, i.e., the tensile (positive) strain means the increasing interlayer

Figure 6. Band structures of the ZrS$_2$/PtS$_2$ heterostructure under different electric fields.

Figure 7. Band structures of the ZrS$_2$/PtS$_2$ heterostructure under different vertical strains.
distance or vice versa. The strain in the range between $-6$ and $6\%$ is applied by changing the lattice parameter with $d = d_o = d_{\text{str}}$, where $d$ and $d_o$ represent the strained and unstrained vertical distance of the $\text{ZrS}_2/\text{PtS}_2$ heterostructure. The tensile strain shifts the VBM to lower energy and the CBM to higher energy and thus the band gap of the $\text{ZrS}_2/\text{PtS}_2$ heterostructure increases with increasing tensile strain as shown in Figure 7. Therefore, the band alignment of the $\text{ZrS}_2/\text{PtS}_2$ heterostructure can also modulate by applying a vertical strain. It is observed that the change of the band gap is approximately linear with varying the strain. In case of compressive strain applied to the $\text{ZrS}_2/\text{PtS}_2$ heterostructure the band gap decreases with increasing compressive strain due to the strong interlayer coupling.

### 3.5. Electric Field and Strain-Dependent Optical Properties

The optical properties of the $\text{ZrS}_2/\text{PtS}_2$ heterostructure are also investigated under an external electric field and strained conditions. The dielectric function describes the optical properties of the materials when incident electromagnetic waves passes through the materials. Frequency-dependent dielectric function is described as $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$ where $\epsilon_1(\omega)$ is the imaginary part and $\epsilon_1(\omega)$ is the real part of the dielectric function. The imaginary part is related to electronic band energy or summation of electronic states and the real part is obtained using the Kramers–Kronig relationship. The light absorption coefficient is obtained from the following formula:

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

where $\omega$ represents the frequency of incident light, and $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$ are real and imaginary parts of the dielectric constant, respectively.

The static dielectric constants (real part) of the $\text{ZrS}_2/\text{PtS}_2$ heterostructure as shown in Figure 8a,c increase with the positive electric field and tensile strain and decrease with the negative electric field and compressive strain.

Figure 8b,d shows the imaginary part of the dielectric function of the $\text{ZrS}_2/\text{PtS}_2$ heterostructure under different vertical strains and under electric field strength. The incident light is perpendicular to the surface of the $\text{ZrS}_2/\text{PtS}_2$ heterostructure. In case of the heterostructure without strain and electric field, the imaginary part shows that the interband transitions correspond to peaks at an energy level from 2 to 8 eV. These transition from the S-p state, Zr-d, and Pt-d states in

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Figure 8. Real and imaginary parts of dielectric functions of the $\text{ZrS}_2/\text{PtS}_2$ heterostructure under an external electric field (a,b) and vertical strain (c,d).
the valence band to Pt-d states and Zr-d states in the conduction band. The highest peak at 2.2 eV in the imaginary part graph represents the loss of photon energy at low energy. The application of strain on the \( \text{ZrS}_2/\text{PtS}_2 \) heterostructure optical properties causes the change in the optical gap. As tensile stain causes the shifting of the first optical gap toward lower energy or shows the red shift while in the case of compressive strain the first optical strain moves toward the higher energy region or shows a blue shift. The external electric field affects the optical gap to move toward lower energy in both the cases.

The optical absorption spectra for the \( \text{ZrS}_2/\text{PtS}_2 \) heterostructure under various external electric fields and vertical strains are shown in Figure 9. When the compression strain is applied, the absorption peaks shift to lower energy (red shift) which is consistent with the change of the band gap. A sufficient change in absorption spectra in the UV−visible region occurs. In the case of tensile strain, the absorption peaks shift to higher energy which shows a blue shift. The height of the absorption peaks decreases gradually with tensile strain and gradually increase with the compressive strain. Similarly, under an external electric field in the negative direction, the absorption spectra show the blue shift and with a positive external electric field increasing from 0.2 to 0.6 V/Å. The absorption spectra show a red shift. This shows that strain affects the absorption spectra of the \( \text{ZrS}_2/\text{PtS}_2 \) heterostructure so we can modulate the optical response with strain which can be used in the potential optoelectronic devices.

The high absorption coefficient in the ultraviolet region shows the potential application of the heterostructure for ultraviolet detection and protection. Therefore, strain can efficiently tune the optical properties of the \( \text{ZrS}_2/\text{PtS}_2 \) heterostructure, which provide the opportunities for new optoelectronic devices.

4. CONCLUSIONS

In conclusion, the electronic and optical properties of the \( \text{ZrS}_2/\text{PtS}_2 \) heterostructure under various external electric fields and vertical strains were studied using DFT calculation. The \( \text{ZrS}_2/\text{PtS}_2 \) heterostructure shows type-II band alignment with the VBM contributed from PtS2 and the CBM contributed from ZrS2. The value of the band gap increases 33% as the negative electric field increases from 0 to 0.6 V/Å and the value of the band gap decreases 44% as a positive electric field. Band gap modulation with vertical strain shows that compressive strain decreases 32% in the band gap whereas tensile strain increases the band gap 12% as compare to without strain, both the electric field and vertical strain does not change the band alignment type. The present work shows that the \( \text{ZrS}_2/\text{PtS}_2 \) heterostructures are more suitable for applications in tunneling devices based on the heterostructure.

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