Strain and electric field-modulated indirect-to-direct band transition of monolayer GaInS$_2$

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Abstract
The strain- and electric field-dependent electronic and optical properties of monolayer GaInS$_2$ have been calculated using density functional theory (DFT) and time-dependent DFT (TD-DFT). GaInS$_2$ monolayer shows an indirect band gap of 1.79 eV where valence band maxima (VBM) and conduction band maxima (CBM) rest between the K and Γ point and at the Γ point, respectively, while at 4% compressive strain, the material changes from indirect to direct band gap of 2.22 eV having the VBM and CBM at the Γ point. With a further increase in compressive strain, the CBM shifts, from the Γ to the M point, which leads to an indirect band gap again. The electric field also affects the band structure of monolayer GaInS$_2$ and shifts the transition from direct to indirect band gap at a positive electric field of 4 V/nm, which acts normal to the surface. The strain-dependent optical properties are also calculated, which suggests that the absorption coefficient increases with compressive strain. Our work demonstrates a wide range of band gap variation and optical properties improvement upon application of biaxial strain and electric field on the monolayer of GaInS$_2$.

Keywords Two-dimensional materials · Monolayer · Band transition · Strain engineering · Electric field effects · Electronic properties · Optical properties

1 Introduction
The discovery of graphene [1, 2], a two-dimensional (2D) material, has made researchers curious about further research on new low-dimensional materials due to their magnificent physical, electronic, and optical properties. Owing to their excellent electronic, optical, mechanical, and thermoelectric properties, 2D materials can be used as nanoelectronic and optical devices [3–7]. Enormous research has been done on developing the properties, for that 2D materials such as arsenic sulfide [8, 9], silicene [10, 11], and black phosphorus are being studied. Along with these materials, other novel 2D materials like transition metal dichalcogenides (TMDC) [12, 13], metal diiodides [14, 15], metal chalcogenides [16, 17], and bilayer heterostructures [18, 19] are now at the peak of interest for the researchers. Low-dimensional TMDCs were used for various applications such as transistors, gas sensors, photodetectors, solar cells, and light-emitting diode [20–25]. Metal diiodides monolayers with hexagonal honeycomb structures can be used as thermoelectric devices due to their ultra-low lattice thermal conductivity [26, 27]. Metal monochalcogenides are being studied for their recent application in nanoelectronic devices. However, band modulation is required for various device applications, which can be done by applying strain or external electric field on 2D materials. By strain engineering, enhancement of materials’ properties has been reported [28].

Two-dimensional group III monochalcogenides are being studied because of their exceptional optoelectronic properties, and these properties can be modified by applying strain and external electric fields. Gallium and indium chalcogenides are the well-known 2D materials with indirect band gap and are layered hexagonal structures [29]. Among them, gallium chalcogenides are being focused on due to their possibilities to be utilized in experiments. Experimental synthesis of the monolayers has been done to study their properties [30, 31]. With gallium chalcogenides, indium chalcogenides are also studied widely. Along with these materials, different
types of designed materials are required for the development of nanoscale devices. Because of that, different types of material structures have been designed, Janus structure is one of them. It is well known that optical and electronic properties depend on the structure and symmetry of the materials. Janus structure gives different and improved results because of its symmetry breaking to meet the requirement of applications [32]. Bui et al. designed Janus Ga2SSe, Ga2STe, and Ga2SeTe monolayers and showed their optical and electronic properties [33]. In this study, they showed that Ga2SSe has an indirect band gap, while Ga2STe and Ga2SeTe have a direct band gap. The optical absorption peaks are observed in the UV region.

In this work, we have designed a Janus GaInS2 monolayer by replacing one Ga atom with an In atom from the Ga2S2 monolayer structure. After atomic relaxation, its electronic and optical properties have been studied. Unstrained structure exhibits an indirect band gap of 1.79 eV. Application of biaxial compressive strain causes indirect-to-direct band gap for the material. The external electric field also causes indirect-to-direct band gap transition for the material. Our work showed that upon applying biaxial strain the band gap varies in a wide range from 2.22 to 0.26 eV, while Chen et al. showed in their work that with application of 8% uniaxial strain on monolayer InSe, the band gap varies from 1.87 to 1.06 eV [34]. Similarly, at 9.23 V/nm electric field, InSe changes its property from semiconducting to metallic [35]. So, GaInS2 monolayer showed a wide range of band gap variation. It shows a high absorption coefficient starting at the visible range and has a peak at the UV region. This work indicates that the material can be used in optoelectronic devices as a photovoltaic absorber layer, UV photodetector, and many more applications.

2 Computational details

First principle calculations of monolayer GaInS2 were performed using DFT. Structural optimization and electronic properties were calculated using ultrasoft pseudopotential [36] with nonlinear core correction and Perdew–Burke–Ernzerhof (PBE) functional [37] as implemented in Quantum ESPRESSO (QE) package [38]. The calculations were performed with 15×15×1 k-mesh sampling for monolayer with Methfessel–Paxton first-order spreading. Atoms were relaxed until force convergence minimum of 10−3 Ry/bohr has been attained. 45 Ry cutoff energy of plane wave was considered to perform the calculations. A vacuum space of 20 Å has been taken along the Z-direction to prevent the periodic interaction between layers. As PBE underestimates the band gap of material, hybrid (HSE06) functional has been used to calculate band structure of the monolayer. The biaxial strain was applied on the unit cell and can be calculated using the equation $\epsilon = \frac{a-a_0}{a_0} \times 100\%$, where $a$ and $a_0$ are lattice constants with and without strain. The positive and negative values of the applied strain are known as tensile and compressive strain, respectively. The optical properties were calculated by using the time-dependent density functional perturbation theory (TD-DFPT) with SIESTA package [39]. Imaginary and real parts of dielectric function were optimized from momentum space formulation and Kramers–Kronig transformation [40], respectively. From dielectric function, other optical properties like absorption coefficient ($\alpha$), refractive index ($\eta$), and extinction coefficient ($K$) can be obtained from the following equations:

$$\eta = \frac{\left[\left(\varepsilon_1^2 + \varepsilon_2^2\right)^{1/2} + \varepsilon_1\right]}{2}^{1/2}$$

$$K = \frac{\left[\left(\varepsilon_1^2 + \varepsilon_2^2\right)^{1/2} - \varepsilon_1\right]}{2}^{1/2}$$

$$\alpha = \frac{2K\omega}{C}$$

where $\varepsilon_1, \varepsilon_2, \omega, C$ are the real and imaginary functions of dielectric, frequency of incident light, and speed of light, respectively.

3 Results and discussion

3.1 Structural details and stability study

GaInS2 monolayer has a hexagonal structure with four atomic layers stacked in the order of S-In-Ga-S. The geometric design is the same as Ga2S2, which is a layered structure having broken inversion and mirror symmetry. The GaInS2 structure is modeled from the structure Ga2S2 by replacing one Ga atom with an In atom. This Janus structure belongs to P3m1 (C3v) with space group number 156. The side view and top view of a 4×4×1 supercell are shown in Fig. 1a, b, respectively. It shows that the Ga atom and S atom are exactly vertically above the In and S atom, respectively. The lattice constant of the hexagonal unit cell was optimized by relaxing the structure and gives a value $a=b=3.78$ Å, which matched well as reported previously [41]. The distance between Ga-In, Ga-S, In-S, and S–S atoms is 2.66 Å, 2.41 Å, 2.52 Å, and 4.95 Å, respectively. The atoms make the following angles between them: $\angle$ Ga-In-S, $\angle$ In-Ga-S, $\angle$ In-S–S, and $\angle$ Ga-S–S, and their corresponding values are 119.98°, 115.29°, 60.01°, and 64.7°, respectively.
Dynamical stability of the structure has been studied from the phonon dispersion curve of monolayer GaInS$_2$ as shown in Fig. 1c. There are twelve frequency modes available, out of which three are acoustic modes and nine are optical modes for four atoms in a unit cell. No negative frequency in the dispersion curve indicates the dynamical stability of monolayer structure. The phonon dispersion curve was taken along the high symmetric path $\Gamma$-K-M-$\Gamma$. The phonon density of states (PDOS) is also plotted with the figure. The figure shows that the Ga atom has more contribution for acoustic modes, whereas for optical modes the contributions of In and S atoms are the dominating factor. Thermal stability of the structure has been studied with the help of molecular dynamics (MD) with micro-canonical ensemble NVE for 4500 fs time at 300 K temperature as shown in Fig. 1d. The figure shows that the temperature oscillates near 300 K, suggesting the thermal stability of the structure.

3.2 Electronic properties

The electronic band structures of the relaxed system have been calculated using PBE functional as shown in Fig. 2a. Band structure of monolayer has been studied along the high symmetric k-path K-$\Gamma$-M-K of hexagonal Brillouin zone. The GaInS$_2$ monolayer shows an indirect band gap of 1.79 eV. The conduction band minima (CBM) rests at $\Gamma$ point, while the valence band maxima (VBM) rests between K and $\Gamma$ point, and Fermi level rests between VBM and CBM. The valence band has two nearly degenerate states, rest between K-$\Gamma$ and $\Gamma$-M point, which is because two S atoms contributed to the valence band. The band structure considering spin orbit coupling (SOC) has been studied as shown in Fig. 2b. Due to the consideration of SOC, the band gap changes slightly to 1.65 eV. The band has not split at high symmetric $\Gamma$ point but slightly split at K and M point. The band split by 8.8 meV at VBM which rests between K and $\Gamma$ point. To get realistic idea of electronic properties, HSE06 functional has been used to study the band structure. The band structure has been calculated along the path $\Gamma$-M-K-$\Gamma$ as shown in Fig. 2c. The CBM and VBM rest at $\Gamma$ point and between K and $\Gamma$ point with a band gap of 2.70 eV.

To know the contribution of atoms in the VBM and CBM, total DOS and partial DOS have been studied. Figure 2d indicates that VBM is contributed mainly by the p orbital of the S atoms. CBM is contributed by P orbitals of Ga and In atoms. Further insight revealed that the VBM is contributed
primarily by $P_x$ orbital and some of $P_y$ and $P_z$ orbitals of S atom and minor contribution of $P_x$ orbitals of Ga and In atoms. The CBM is contributed by $P_y$, $P_z$ orbital of Ga and In atoms and $P_x$ orbital of S atom. Two-dimensional charge density of the monolayer has been plotted to know about charge distribution. The different color shows the amount of charge accumulation as shown in the scale bar. It can be easily concluded that the maximum charge is accumulated on S atoms and less amount of charge is on Ga and In atoms. The more accumulation of charge on S atom can be understood by its electronegativity property. Sulfur is more electronegative than Ga and In atoms and that causes more charge accumulation on it.

3.3 Effect of biaxial strain:

The effect of biaxial strain on the band structure of GaInS$_2$ monolayer was studied. We have applied up to 10% tensile and compressive strain with an increment of 2% to the studied band structure. The band structure and projected density of states (PDOS) with 4% and 10% tensile strain and compressive strain ($-4\%$ and $-10\%$) are shown in Fig. 3a, b, c, d. At 4% tensile strain, the band remained indirect, as shown by the red arrow. The band gap was found to be decreasing to 0.98 eV. At 10% strain as shown in Fig. 3b, the band gap decreases to 0.26 eV. The band gap values calculated with HSE06 functional are 2.11 eV, 1.65 eV, and 1.46 eV at 4%, 8%, and 10% tensile strain, respectively. Compressive strain results in indirect-to-direct-type semiconducting properties and little increase in the band gap. At $-4\%$ strain, monolayer changes its semiconducting state from indirect to direct type. The VBM and CBM rest at $\Gamma$ point, and the band gap for the monolayer at that particular strain is 2.22 eV. The position of VBM remains at $\Gamma$ point for further increase in compressive strain, but CBM shifted from high symmetric $\Gamma$ to M point at $-6\%$ strain, and again CBM shifted from M to K point at $-8\%$ strain. The band gap at $-6\%$, $-8\%$, and $-10\%$ strain is 2.08 eV, 1.73 eV, and 1.28 eV, respectively, using PBE, while the band gap values are 3.31 eV, 3.22 eV, and 3.00 eV at $-6\%$, $-8\%$, and $-10\%$ strain, respectively, using HSE06.

3.4 Effect of the electric field:

A finite electric field is applied to the monolayer along the perpendicular direction of the surface (Z-direction) using the modern theory of polarization as implemented in QE. The effect of finite electric field on electronic band structure has been studied. Upon application of a finite electric field, the structural change is negligible. An external electric field is applied up to 4 V/nm and $-4\$ V/nm with an increment of 2 V/nm, which can be considered as a perturbation on a
stable system or application of gate voltage on field effect transistor (FET) device. The field-dependent modification of band structures is shown in Fig. 4a, b, c, d. For the 2 V/nm applied field, the band type remains the same, although the band gap reduced to 1.54 eV. With 4 V/nm, the material becomes a direct band gap semiconductor with a gap of 1.03 eV. The negative electric field does not affect the band structure much, and the band gap also does not change.
significantly. At the $-2$ eV/nm field, the band gap decreases slightly to 1.77 eV, while at -4 V/nm, the gap increases to 1.82 eV. Band structure remains indirect for both negative electric fields.

The variation of VBM and CBM with applied strain and finite electric field along the transverse direction is shown in Fig. 5a, b. At the positive strain region, the band gap decreases linearly with applied strain. Along the negative region, nonlinear variation of band gap has occurred. The band gap increases linearly up to $-4\%$ compressive strain and then decreases linearly. We have divided the variation of VBM and CBM energy into four regions, namely A, B, C, and D. The VBM energy varies linearly with applied positive strain and at $-2\%$ strain, as shown in region A. As the negative strain increases, a jump in VBM energy has been observed, and again a linear variation with a different slope has occurred (region B). In CBM, linear variation of energy was observed from $-4\%$ to $10\%$ strain (region C). A nonlinear region (region D) was observed from $-6\%$ to $-10\%$ applied strain. In the whole A region, the VBM rests between $\Gamma$ and $K$, but at $-4\%$ strain, VBM shifts to $\Gamma$ point. This is why a certain jump in VBM energy has occurred. In the whole B region, VBM rests at $\Gamma$ point. Similarly, CBM rests at $\Gamma$ point throughout the C region, which causes linear variation there. At $-6\%$, CBM shifted to M point, and at $-8\%$ of strain again shifted to K point, resulting in a nonlinear region. To understand the linear trend of the states, PDOS has been studied as shown in Fig. 3a, b, c, d. Region A is dominated by the $P_x$ orbital of the S atom, while the $P_z$ orbital of the S atom dominates region B. Region C is dominated by, as expected, $P_y$ and $P_z$ orbital of Ga atom as CBM rests at the same $\Gamma$ point. In the region D, a change of high symmetric point from M to K has occurred and caused nonlinear characteristics. At $-6\%$ strain, CBM energy moves to the M point, and for $-8\%$ and $-10\%$ strain, it remains at K point.

External electric field-dependent variation of VBM and CBM has three different regions E–F. The slopes of linearly variant F and G are almost the same, which is responsible for not changing the band gap. At 4 V/nm electric field, VBM changes to $\Gamma$ point and causes a band gap reduction.

The variation of band gap with applied biaxial strain and electric field is shown in Fig. 5c, d, respectively. The change of band gap for PBE functional with and without SOC is almost similar, while for HSE06 functional the variation follows the same trend but the band gap value is greater than as for in the case of PBE. The band gap decreases for tensile strain for all cases, but for compressive strain the band gap first increases and then decreases. For an electric field, the band gap remains the same when a negative field has been applied, but it decreases when a positive field has been applied.
3.5 Optical properties

The optical properties of the GaInS$_2$ monolayer have been calculated along the transverse direction of the material. The real part of the dielectric function ($\epsilon_1$), the imaginary part of the dielectric function ($\epsilon_2$), and absorption coefficient ($\alpha$) varying with photon energy are shown in Fig. 6a, b, c. The zero-point value of $\epsilon_1$ for the unstrained structure is 3.16. With 4% tensile and compressive strain, the value does not change remarkably, but at 8% strain, the value increases to 3.39. The highest value peak arises at 3.49 eV with a value of 5.28 for the unstrained layer. The peak value increases slightly at − 4% strain but again decreases for − 8% applied strain. The lowest peak has been observed at 8% tensile strain with a value of 4.37 at 3.59 eV. Some negative value for $\epsilon_1$ has been observed with the highest value of − 0.81 for − 4% strain. All the $\epsilon_1$ values were found almost stable on a high photon energy range. The value of $\epsilon_2$ has started to increase at the visible energy region at 1.25 eV for all strained and relaxed layers. Only for 8% applied strain, it starts increasing at 0.3 eV. The peak value for the unstrained layer is 4.6 at 4.25 eV. The peak value is highest for 4% applied strain and decreases for compressive strain. The monolayer has been seen to be a very good absorber of light with high absorption coefficient. Although the strain does not have much effect on peak position, it changes the absorption value. The absorption starts in the visible region at 1.3 eV for unstrained monolayer, which starts decreasing for all strains except − 4% compressive strain. The absorption started at 0.65 eV for 8% strain. The first peak arises at 4.84 eV for the relaxed system, and the highest peak arises at 7.09 eV with a value of $8.54 \times 10^5$ cm$^{-1}$. The absorption decreases with tensile strain, but the first peak is getting prominent with tensile strain, while it started vanishing with applied compressive strain. The material shows absorption near visible and ultraviolet region.

4 Conclusions

We have studied the electronic and optical properties of the GaInS$_2$ monolayer. GaInS$_2$ monolayer has an indirect band gap which changes to direct band gap with applied 4% compressive strain. An external electric field with a value of 4 V/nm, applied normal to the plane, also changes the semiconducting property from indirect to direct band gap type. However, the band gap does not change effectively with the electric field. The Janus monolayer also possesses exciting optical properties with a high value of absorption coefficient and dielectric function.

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