

Monolayer Transition Metal Dichalcogenide Channel-Based Tunnel Transistor

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Abstract—We investigate the gate controlled direct band-to-band tunneling (BTBT) current in monolayer transition-metal dichalcogenide (MX_2) channel-based tunnel field effect transistor (TFET). Five MX_2 materials (MoS_2 , MoSe_2 , MoTe_2 , WS_2 , WSe_2) in their 2-D sheet forms are considered for this purpose. We first study the real and imaginary band structure of those MX_2 materials by density-functional theory (DFT), which is then used to evaluate the gate-controlled current under the Wentzel-Kramers-Brillouin (WKB) approximation. It is shown that all five MX_2 support direct BTBT in their monolayer sheet forms and offer an average ON current and subthreshold slope of $150 \mu\text{A}/\mu\text{m}$ (at $V_d = 0.1\text{V}$) and $4 \text{ mV}/\text{dec}$, respectively. Furthermore, we also demonstrate the strain effect on the complex band structures and the performances of MX_2 based TFETs. It is observed that a certain tensile strain becomes favorable for the improvement of ON-current performances.

Index Terms—Tunnel field effect transistor, 2-D crystal, atomistic simulation, complex band structure, band-to-band tunneling.

I. INTRODUCTION

THE TUNNEL field effect transistors (TFETs) with gate controlled band-to-band tunneling (BTBT) have emerged as a thrust area of research for low-standby power (LSTP) application due to its sub-60 mV/dec subthreshold swings (SS) and very high $I_{\text{ON}}/I_{\text{OFF}}$ ratio [1], [2]. However, poor SS and low ON-current have been seen in all conventional Silicon TFETs due to the large indirect energy band gap ($\sim 1.12 \text{ eV}$). As a result, there has been an extensive investigation on the alternative materials for TFET applications [1]–[3] which do not require phonon assistance in the tunneling process. In order to replace Si, atomically thin layered materials have found great significance as alternate MOSFET channel materials due to their planar structure, excellent electrostatic integrity and mechanical flexibility. Recently, layered transition-metal dichalcogenide materials (MX_2) (Fig. 1), especially MoS_2 , have received much attention for their application in nano-scale electronic devices as an alternative to Graphene [4]–[6].

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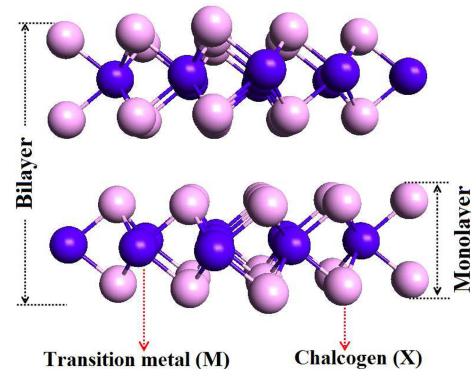


Fig. 1. Side view of the layer structure of 2D-hexagonal MX_2 crystals. Monolayer consists of a sandwich of three hexagonally packed atomic layers, X-M-X, where within two X layers, the M atoms in the intermediate layer are bonded with the X atoms through ionic-covalent interactions in a trigonal prismatic arrangement.

The bulk MX_2 crystals, which are composed of stacked layers, have indirect band gaps whereas these band gaps become direct in monolayer MX_2 form at the K point along the Γ -M-K- Γ path of the Brillouin zone [7]–[16] and thus may become a potential material for TFET applications.

In this paper, we first explore the BTBT in five monolayer MX_2 sheets (MoS_2 , MoSe_2 , MoTe_2 , WS_2 , and WSe_2) by considering the complex dispersion relationship within the band gap region. These complex band structure calculations have been evaluated by using Atomistix ToolKit (ATK) which uses DFT-LDA method [17]. Finally, computing the least action integral from the complex band structure and considering the analytical Poisson solution we compute the drain current of a symmetric double gate (DG) TFET and compare the performances of different MX_2 materials. Further, the impact of isotropic biaxial (ϵ^{bi}) and uniaxial (ϵ^{uni}) strains on the complex band structures and the performances of MX_2 based TFETs have also been investigated.

II. APPROACH, RESULTS AND DISCUSSIONS

A. Study of Complex Band Structure

The band structure calculations of geometrically optimized MX_2 have been evaluated by using the ATK simulation package [17]. Our band structure computations are based on the self consistent density-functional theory (DFT). The exchange correlation energies are treated within local density approximation (LDA) combining with Perdew and Zunger correlation functional and double zeta polarized basis set.

TABLE I
ELECTRONIC, DIELECTRIC AND PHYSICAL PROPERTIES OF MX₂

MX ₂	E _g (eV)		ξ _I (V nm ⁻¹)	ε _s (ε ₀)		c/2 (nm)	λ (nm)
	Cal. ⁱ	Exp.		ε _s	ε _s [⊥]		
MoS ₂	1.81	1.89 ⁱⁱ	1.02	8.29	3.92 ⁱⁱⁱ	0.62	0.38
MoSe ₂	1.58	1.55 ^{iv}	0.85	9.05	6.07	0.65	0.45
MoTe ₂	1.12	1.15 ^v	0.81	33.70	16.10	0.70	0.72
WS ₂	1.90	2.05 ^{vi}	1.25	7.95	5.14	0.62	0.42
WSe ₂	1.60	1.49 ^{vii}	0.96	7.25	5.16	0.65	0.43

E_g is the energy band gap of monolayer MX₂. i = comparable with [7]–[9]. ii, iv–vii: [10]–[14].

ξ_I is the “least action integral” and has been calculated according to Eq. (1).

ε_s is the static dielectric constant of bulk, Re[ε(ω = 0)], where “||” and “⊥” represents the lateral and perpendicular directions of the material, respectively. iii = comparable with [6].

c/2 (c: bulk lattice constant) is the monolayer thickness, obtained from ab-initio structure optimization, which is close to the experimental value [4], [10], [15]–[16].

λ is natural length scale and has been calculated from Eq. (3) by considering 2 nm thick HfO₂ (ε_{ox} = 25ε₀) as a gate dielectric.

The tolerance parameter was 10⁻⁵ with maximum steps of 200, and a Pulay mixer algorithm [18] was used as the iteration control parameter. In addition, the k-point sampling of 27×27×1 grid was used with a mesh cut-off energy of 10 Hartree. In case of monolayer MX₂ sheets we used a supercell with a 15Å vacuum region along the c axis (keeping the lattice parameters a and b same as bulk) so that it effectively behaves as an isolated 2D layer. Band gap values obtained from DFT are also in good agreement with existing experimental results as shown in Table I.

The static dielectric constant, Re[ε(ω = 0)], [Table I] is computed by using DFT-LDA and double zeta double polarized basis set along with the k-point sampling of 15×15×15 grid with a mesh cut-off energy of 75 Hartree. The Kubo-Greenwood formula has been used to calculate the susceptibility tensor (χ(ω)) [19], [20] which is related to the dielectric constant as ε(ω) = (1 + χ(ω))ε₀, where ε₀ is the vacuum permittivity. In Table I, the bulk values of the dielectric constants are presented since the monolayer values are nearly same as those of the bulk. For example, the ε_s[⊥] of bulk MoS₂ is 3.92ε₀ whereas it is 3.86ε₀ for a monolayer sheet. So, for our device applications we approximated the monolayer dielectric values with the bulk values.

Recently, the complex band theory was successfully applied in the modeling of tunneling devices [21], [23], [24] for a deeper understanding of band-to-band tunneling (BTBT) phenomenon. Physically, during this BTBT process, when a carrier tunnels through a band gap region, it transits in an evanescent mode and its wave vector becomes imaginary within this forbidden gap. In case of direct band gap semiconductors, when the complex band that starts from the top of valence band ‘wraps’ itself to the bottom of the conduction band, constituting one continuous band then only the direct BTBT can take place. However, if the band that starts from the valence band edge ‘crosses’ with the band starting from the conduction band edge then the tunneling process requires phonon to ensure the momentum conservation [23] which reduces the transmission rate quite significantly [23], [25]. It

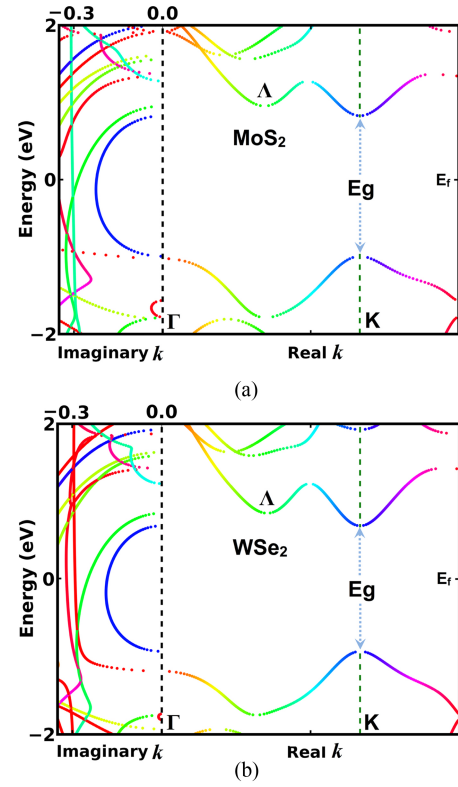


Fig. 2. Complex and real bands of monolayer MX₂ sheets. Here, we have shown the band structures of MoS₂ and WSe₂ only, as remains have same nature. The color-coding of the k-values applies to both real and imaginary parts of the band structure to make it easier to realize where the complex bands are attached to the real ones. E_g and E_f are band gap and the Fermi level respectively.

should also be noted that the inter-band tunneling probability (T_{BTBT}) depends on the minimum area that is enclosed by the complex band which connects the valence band edge to conduction band edge [21]–[24], [26]. Fig. 2 shows the complex bands within the band gap region of monolayer MX₂ monolayers. For clarity, only a few bands are shown here. It appears that, for all monolayer MX₂ monolayers, the complex band is characterized by a continuous band that connects the highest valence subband to the lowest conduction subband allowing for direct tunneling.

Now, using the Wentzel-Kramers-Brillouin (WKB) approximation the direct tunneling probability for the BTBT process can be approximated as [21], [27]

$$T_{BTBT} = \exp \left\{ -\frac{2}{q\xi} \int_0^{E_g} k(E) dE \right\} \equiv \exp \left\{ -\frac{\xi_I}{\xi} \right\} \quad (1)$$

where q is the electronic charge, ξ the electric field; $E = 0$ the valence band edge, $E = E_g$ the conduction band edge, $k(E)$ the magnitude of the imaginary wave vector with “least action for tunneling” within the forbidden gap, and $\xi_I = \frac{2}{q} \left(\int_0^{E_g} k(E) dE \right)$ is basically the “least action integral” which is an intrinsic property of the material.

As a result, in any applied electric field, controlled by a third terminal (the gate) in TFET applications, T_{BTBT} can be figured out instantly when ξ_I is enumerated. Since monolayer MoTe₂

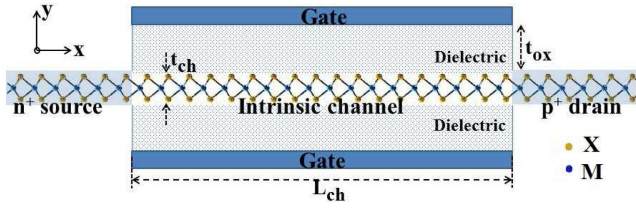


Fig. 3. Schematic cross section of a monolayer MX₂ based double gate TFET with n⁺ source, p⁺ drain and intrinsic channel.

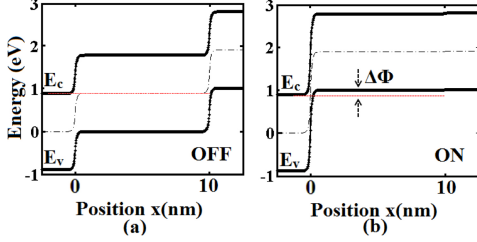


Fig. 4. Energy band diagrams for a symmetric n⁺-i-p⁺ DG TFET having monolayer MoS₂ sheet as a channel material in (a) the OFF-state and (b) the ON-state respectively.

sheet has lowest direct band gap than others, it provides the lowest ξ_I value [Table I]. It is recently noticed that the presence of spin orbit coupling can split the valence band maximum at the K-point [28]. However, the curvatures of the conduction band minima and valence band maxima remain same. It is also observed that the band gap remains nearly same for with or without spin orbit coupling. Therefore, the inclusion of spin-orbit coupling does not affect the tunnelling effective mass as well as the band gap which are responsible to find ξ_I to calculate the band to band tunnelling probability.

B. Calculation of TFET Drain Current

Now, we investigate the performance of the symmetric DG TFET with these materials as channel materials (Fig. 3) with a thickness of t_{ch} ($= n \times \frac{\epsilon}{2}$; n is the number of layers) and an oxide thickness of t_{ox} . The source region is heavily n⁺ doped and drain is heavily p⁺ doped, while the channel of length L_{ch} is intrinsic. We also consider that, in an electrostatically well-designed device, the Fermi level is at the conduction band edge (E_c) at the n⁺ source and at the valence band edge (E_v) at the p⁺ drain whereas it is at the mid-gap of the intrinsic channel at thermal equilibrium. To demonstrate the surface potential profile (Ψ_s) in this DG TFET, here we use an analytical model which shows that the electrostatic of such TFET can be described by a modified 1-D Poisson equation [29]

$$\frac{d^2\Psi_s}{dx^2} - \frac{\Psi_s - V_g + V_{bi}}{\lambda^2} = 0 \quad (2)$$

where x is the direction along the channel, V_g and V_{bi} ($\approx \frac{E_g}{2q}$) are the gate and built-in potentials respectively, and λ is the natural length scale of the potential variation and is given by

$$\lambda = \sqrt{\frac{\epsilon_{ch}}{2\epsilon_{ox}} \left(1 + \frac{\epsilon_{ox} t_{ch}}{4\epsilon_{ch} t_{ox}} \right) t_{ch} t_{ox}} \quad (3)$$

Here, ϵ_{ch} ($= \epsilon_s^\pm$) and ϵ_{ox} are the channel and oxide dielectric constants respectively. Applying the following boundary conditions (i) zero electric field at $x = \pm\infty$ and (ii) continuous

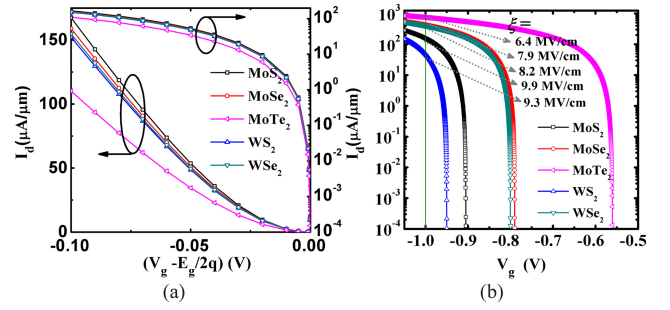


Fig. 5. Direct tunneling current variation with (a) $(V_g - \frac{E_g}{2q})$ and (b) V_g in a symmetric n⁺-i-p⁺ DG TFET having monolayer MX₂ sheets as channel materials at $V_d = 0.1$ V and $T = 300$ K.

electric field and potential at the source-channel and drain-channel junction, and (iii) $L_{ch} \gg \lambda$, (2) can be solved analytically and leading to a solution of the form $\Psi_s \propto \exp(-\frac{x}{\lambda})$. The electric field calculated from the surface potential profile can then be expressed as $\xi \propto \frac{1}{\lambda} (\frac{E_g}{2q} - V_g) e^{-\frac{x}{\lambda}}$. Now, from (3) it is also seen that λ is a function of t_{ch} and this solution reflects that the source-channel junction will become very thin in case of an atomically thin planar structure (see Table I). Being a function of t_{ox} and ϵ_{ox} , it can also be seen that λ decreases as t_{ox} decreases and the gate dielectric constant increases. If we compute the λ of MoS₂ by considering 2 nm thick HfO₂ ($\epsilon_{ox} = 25\epsilon_0$) as a gate dielectric then it gives only 0.38 nm whereas 5 nm thick ultrathin-body Si or InAs provides a λ of 2.35 or 2.48 nm. Thus these MX₂ provides 6–7 times smaller value of λ than the conventional ultrathin materials. In case of low band gap materials (e.g. III–V materials) the ξ_I is significantly low, however as the tunneling probability is controlled by the product $\lambda \times \xi_I$ thus higher λ reduces the tunneling probability. So the use of high- κ oxide and atomically thin planer channel materials will improve the device performance significantly [30]. In this context, it should be noted that the change in Ψ_s at the middle of the channel should not depend on drain voltage for proper BTBT process in TFET operation. This can be achieved if $L_{ch} \gg \lambda$ and the scaling of the device is in the quantum capacitance limit (QCL) that can also be achieved in monlayer 2-D MX₂ sheets due to their low DOS value [6], [9], [31].

Considering HfO₂ as a dielectric ($\epsilon_{ox} = 25\epsilon_0$, $t_{ox} = 2$ nm) and monolayer MoS₂ sheet as a channel ($L_{ch} = 10$ nm), the computed band diagrams for a symmetric n⁺-i-p⁺ DG TFET are shown in Fig. 4(a) for the OFF-state at $V_g = 0$ and in Fig. 4(b) for the ON-state at $V_g = -1.0$ V with a supply voltage (V_d) of 0.1 V. It can be seen from Fig. 4(b) that under this condition, the reverse-bias V_g opens an energy window, $\Delta\Phi$, through which the effective tunneling current flows and this $\Delta\Phi$ can be derived as $(qV_g - \frac{E_g}{2})$. It should also be noted that this $\Delta\Phi$ is derived here for relatively small V_g , so that the effective electric field do not change appreciably from its equilibrium value. Under these circumstances, the BTBT tunneling current can be then written in the form [22]

$$I_{BTBT} = \frac{g_s g_v q}{h} \int_0^{\Delta\Phi} T_{BTBT} \{ f_i(E) - f_f(E) \} dE \quad (4)$$

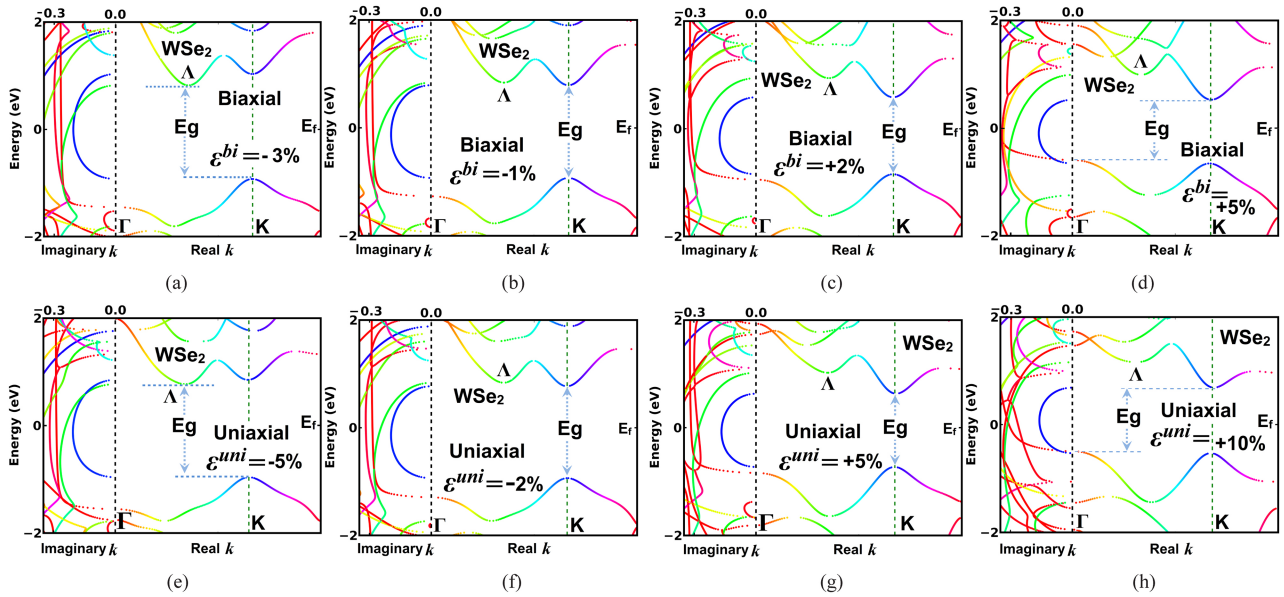


Fig. 6. Effect of various biaxial ((a)–(d)) and uniaxial ((e)–(h)) strains on the complex and real bands of monolayer WSe₂ sheet. ‘+’ and ‘-’ represent the tensile and compressive strain respectively. The color-coding of the k -values indicates where the complex bands are attached to the real ones.

in which h is the Planck’s constant; $g_s (= 2)$ and $g_v (= 2)$ are the spin and valley degeneracies [7]; $f_i(E)$ and $f_f(E)$ are the Fermi functions of the initial and final states from and to which the tunneling occurs, respectively. Using (1) and (4), taking $\Delta\Phi$ and ξ across the source-channel junction ($x=0$) from the band diagram calculations for different channel materials, the drain-current (I_d) at room temperature can be then calculated as a function of the V_g . It can be seen from Fig. 4(b) that, to open an energy window for tunneling, a reverse-bias $V_g = \frac{E_g}{2q}$ should require and that will be different for different channel materials. So, to compare the On-current performances, in Fig. 5 we have presented the variation of the direct BTBT current per micron width as a function of $(V_g - \frac{E_g}{2q})$ for monolayer MX₂ sheets at a supply voltage $V_d = 0.1$ V. It appears from Fig. 5 that, in all cases the drive tunneling currents show the same kind of variations, however, MoS₂ has the best performance compared to others. Although it has relatively higher ξ_l value, a comparatively lower ε_{ch} and t_{ch} provides much lower λ (see Table I) and consequently it delivers better ON-performance. On the other hand, MoTe₂ has much lower band gap so the effective tunneling will start in very low V_g for this material. Thus, if we see the variation as a function of V_g only, then MoTe₂ sheet (lowest band gap) will provide highest performance for a particular V_g (Fig. 5(b)) which is consistent with the results in [32]. While in comparison to the conventional Si TFET which shows only $0.4 \mu\text{A}/\mu\text{m}$ for the comparable $V_d = 0.1$ and $V_g - V_{th} = 0.1$ V (V_{th} ; the threshold voltage) [33], MX₂ sheets provide much higher ON-currents. In case of Graphene nanoribbon (GNR), as investigated earlier by Q. Zhang et al. [34], it can be seen that the ON state current is $800 \mu\text{A}/\mu\text{m}$ for 5nm wide monolayer GNR ($E_g \sim 0.25$ eV). However, owing to much higher band gap, MX₂-TFET offers negligible OFF-current in comparison to GNR. Therefore, the atomically thin transition metal dichalcogenides have an advantage over

Graphene nanoribbons whose band gap decreases very rapidly with the increase of ribbon width and becomes very small above 5nm. An average subthreshold slope less than 4 mV/dec (extracted from the $I_d - V_g$ characteristics using the same method as in [30]), shows the immense potential of MX₂ based TFETs for realizing high performance LSTP devices.

C. Effect of Elastic Strain

Recently, strain dependent modulation of the transport properties of a channel material has successfully been employed in the CMOS technology to improve the carrier mobility and ON-current performances in the devices [35], [36]. Keeping that in mind, in the next part we have investigated the impact of strain on the performances of the MX₂ based TFETs. In our study, the strain is given by scaling the lattice constant of the MX₂ by an amount $\varepsilon = (a - a_0)/a_0$, where a_0 and a are the lattice constants of the unstrained and strained MX₂ sheet respectively.

Fig. 6 shows the effect of in-plane isotropic biaxial, ε^{bi} ($\varepsilon_{xx} = \varepsilon_{yy}$) and uniaxial ε^{uni} (ε_{xx}) strain on WSe₂ sheet. Previously, in the relaxed case we have seen that the band structure is direct in nature (Fig. 2), having both conduction band minima (E_c^{min}) and valence band maxima (E_v^{max}) at the K-point in the Brillouin zone; however, it appears from Fig. 6 that if we provide strain then the nature of WSe₂ band structure undergoes a direct to indirect band gap transition. If we provide a strain of $\varepsilon^{bi} \simeq +3.75\%$ (or $\varepsilon^{uni} \simeq +9\%$) then it is seen that the E_v^{max} at the Γ point moves up than the K point and makes the band gap as an indirect one. On the other hand, with the application of $\varepsilon^{bi} \simeq -1.5\%$ (or $\varepsilon^{uni} \simeq -3.5\%$), the E_c^{min} at the Λ moves down than the K point and band gap becomes indirect (see Fig. 6). It is worth noting that as the energy difference of the E_v^{max} (or E_c^{min}) between Γ (or Λ) and K point is different for the various MX₂, therefore the direct to indirect transition attains at various tensile or compressive

TABLE II
STRAINS TO ATTAIN DIRECT TO INDIRECT BAND GAP TRANSITION OF
VARIOUS MX_2

MX_2	ε^{bi} (%)		ε^{uni} (%)	
	Tensile	Compressive	Tensile	Compressive
MoS_2	+0.65	-1.25	+1.0	-1.0
MoSe_2	+3.6	-0.9	+8.0	-1.5
MoTe_2	+5.5	-1.0	+7.5	-2.0
WS_2	+0.5	-1.3	+1.05	-1.4
WSe_2	+3.75	-1.5	+9.0	-3.5

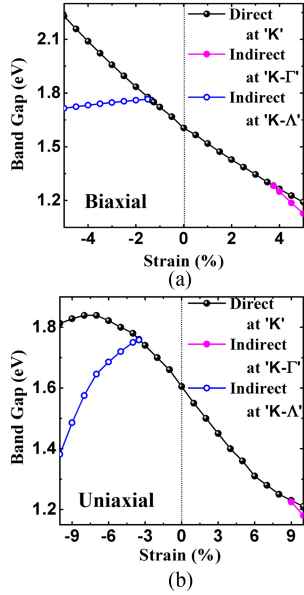


Fig. 7. The energy band gap variation of WSe_2 sheet under (a) isotropic biaxial and (b) uniaxial strains. The direct band gap is always measured at the K point of the Brillouin zone. The '+ve' and '-ve' side represent the tensile and compressive strain respectively.

strains for different MX_2 materials (see Table II). The nature of our computed band structure results are also in good agreement with the previous theoretical investigations [37], [38].

Moreover, it also appears from Fig. 7 that the band gap of WSe_2 (and other MX_2 also) changes significantly with the increase of both biaxial as well as uniaxial strain. With the increase of tensile strain, the direct band gap decreases for both ε^{bi} and ε^{uni} whereas it increases with the increase of compressive strain. However, this direct band gap again decreases slowly above $\varepsilon^{uni} = -7\%$. On the other hand, the indirect band gap decreases with the increase of both tensile and compressive strains after the direct to indirect transition. We can further see that the difference in indirect to direct band gap in the tensile zone is much less than the difference in the compressive zone.

Recently, it is also investigated that if the energy difference between the direct and indirect band gap is quite small then the transmission probability for direct band gap transitions dominates over the probability for indirect band gap transitions [26], [39]. Therefore, reducing the barrier height with the application of tensile strain will be an encouraging technique to increase the direct BTBT current in MX_2 based TFET applications.

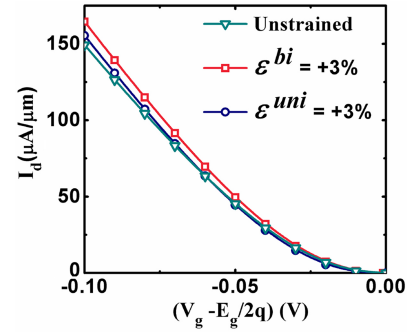


Fig. 8. Direct tunneling current variation with V_g in a symmetric DG TFET having monolayer WSe_2 sheet as channel materials at $V_d = 0.1$ V and $T = 300$ K for various strains.

In Fig. 8 we have shown the ON-current performances of WSe_2 sheet for various tensile strains by considering the same channel dielectric constant as the change in dielectric constant is negligibly small with strain (not shown here). It appears that the ON-current increases $\sim 13\%$ (or $\sim 9\%$) with the application of $\varepsilon^{bi} = +3\%$ (or $\varepsilon^{uni} = +3\%$). Therefore, under tensile strain condition, the ON-current performance increases well for same oxide dielectric, a trait beneficial for TFET application.

Finally, we wish to state that in this present case we did not contemplate the influence of phonon scattering and impurity scattering that should be considered to provide a more complete picture of a practical device model, which is well beyond the scope of this paper.

III. CONCLUSION

We have investigated the direct band-to-band tunneling current in transition-metal dichalcogenide channel based tunnel field effect transistor (TFET) by studying their complex band structures by DFT-LDA. It is observed that all the five MX_2 sheets support direct BTBT in their unstained forms. Further, it is investigated that the application of tensile strain can also favorable to increase the ON-current performances. Relatively higher tunneling current, much lower SS value and better gate controllability in MX_2 based TFETs indicate that these may become the promising channel materials for future TFET applications.

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