Electronic Structure and Room Temperature of 2D Dilute Magnetic Semiconductors in Bilayer MoS₂-Doped Mn

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The electronic structure and magnetic properties of manganese- (Mn-) doped bilayer (BL) molybdenum disulfide (MoS₂) are studied using the density function theory (DFT) plus on-site Hubbard potential correction (U). The results show that the substitution of Mn at the Mo sites of BL MoS₂ is energetically favorable under sulfur- (S-) rich regime than Mo. The magnetic interaction between the two manganese (Mn) atoms in BL MoS₂ is always ferromagnetic (FM) irrespective of the spatial distance between them, but the strength of ferromagnetic interaction decays with atomic distance. It is also found that two dopants in different layers of BL MoS₂ communicate ferromagnetically. In addition to this, the detail investigation of BL MoS₂ and its counterpart of monolayer indicate that interlayer interaction in BL MoS₂ affects the magnetic interaction in Mn-doped BL MoS₂. The calculated Curie temperature is 324, 418, and 381 K for impurity concentration of 4%, 6.25%, and 11.11%, respectively, which is greater than room temperature, and the good dilute limit of dopant concentration is 0–6.25%. Based on the finding, it is proposed that Mn-doped BL MoS₂ are promising candidates for two-dimensional (2D) dilute magnetic semiconductor (DMS) for high-temperature spintronics applications.

1. Introduction

It is known that graphene is the most well-known member in the family of 2D materials. However, its gapless band structure has been deemed as a considerable drawback for realizing switching operation which is essential for digital logic devices [1]. On contrary to zero band gap graphene, other group of 2D materials so called transition metal dichalcogenides (TMDS) with chemical formula MX₂, where M stands for transition metals like molibdium (Mo), tung-eston (W), and so on and X stands for chalcogen atoms like selfur (S), selenium (Se), and telenium (Te), and so on are more recently discovered [2]. The experimental study reveals that the weak van der Waals forces between each 2D monolayer of which they are formed allow thin multilayers to be easily exfoliated from their bulk form [3]. Among those families, monolayer MoS₂ and few layer MoS₂ have attracted interest due to their potential application [2, 4]; for instance, the monolayer (ML) MoS₂ has emerged as a semiconductor with a large intrinsic direct band gap of approximately 1.8 eV [3], which makes it suitable for nanoelectronic and opto-electronic applications [5]. In MoS₂ materials, the electronic structure depends on the number of layers which mean that there is a gradual transition from an indirect band gap (1.3 eV) in the bulk material to a direct gap in the ML material with band gap 1.9 eV which reveals that the interlayer van der Waals (VdW) interaction may affect the electronic structure [6]. In addition, it has been reported that the electronic structure of such system depends on stacking patterns [7]. There are five different stacking configurations for the bilayer MoS₂ system [7], but the most stable one is AA’ [8].

On the contrary, during last few decades, the research in dilute magnetic semiconductors (DMSs) have attracted tremendous interest due to their great potential for different spin electronics (spintronics) applications [9]. Spintronics refers to new phenomena of electronic transport for which the electron spin plays a decisive role in contrast to
conventional electronics for which the electron spin is practically irrelevant. For a full exploitation of spintronics, one should have materials which show simultaneously semiconducting properties and ferromagnetic ordering at operational temperature [10]. In last two decades, most of DMS research has focused on the transition metal- (TM-) doped III-V and II-VI three-dimensional (3D) semiconductors. However, the ferromagnetic transition temperature in well-studied type of DMSs like Ga$_{1-x}$Mn$_x$As is less than 200 K which is far from room temperature [11]. As a result of this, the search for DMS has recently been extended to two-dimensional (2D) transition metal dichalcogenides (TMDs) like MoS$_{2-}$, MoSe$_{2-}$, and WS$_2$-doped transition metal [4]. Recent theoretical study reveals that Mn and Fe are the best candidates to generate long-range room temperature in its ML phase [4]. To date, several groups have reported experimentally [12] and theoretically the feasibility of MoS$_2$ by substitutional doping with different (TM): Mn-doped monolayer (ML) MoS$_2$ [13], iron- (Fe-) doped bilayer MoS$_2$ [14], Ni-doped ML MoS$_2$ [15], and Co-doped monolayer MoS$_2$ [16]. In addition to this, in our previous ab initio study, we have shown that V-doped ML and BL MoS$_2$ are good candidates for nearly room temperature ferromagnetism [17]. However, electronic structure and magnetic interaction in Mn-doped bilayer (BL) MoS$_2$ has not yet been studied in detail. In this current study, Mn-doped BL MoS$_2$ are studied on the basis of spin polarized (DFT + U) formalism. The relative structural stability, electronic structure, and magnetic properties of MoS$_2$-doped Mn are studied in detail. To understand magnetic ground state and the magnetic energy $\Delta E$, the energy difference between two dopants in FM and AF configurations in the ML and BL phase of MoS$_2$ was calculated for different impurity concentrations. Furthermore, based on mean field theory together with empirical correction, the Curie temperature ($T_c$) is also estimated.

2. Computational Details

DFT + $U$ calculations were performed using the plane-wave pseudopotential method with the aid of QUANTUM ESPRESSO code. On-site Hubbard parameter, $U = 4$ eV, was assigned for dopants to take into account the strong correlation in the Mn 3$d$ state [18]. Ultrasoft pseudopotentials (UPPs) were used to deal with the interaction between valence electrons and the ion core. The plane wave basis set is given a cutoff energy of 60 Ry used after performing the convergence test with respect to total energy. A unit cell with the periodic boundary condition was adopted to simulate the infinite $x$-$y$ plane. For the BL crystal, Grimmes DFT-D2 dispersion correction [19] was applied to account for the long-range van der Waals interactions between layers. The equilibrium interlayer distance was obtained by careful minimization of total energy with respect to distance between layers. To investigate the doping effects of Mn impurities on bilayer MoS$_2$, the BL MoS$_2$ was modeled by supercell of $(3 \times 3 \times 1)$, $(4 \times 4 \times 1)$, and $(5 \times 5 \times 1)$ which contains 36 S and 18 Mo, 64 S and 32 Mo, and 50 Mo and 100 S atoms, respectively. The vacuum space 20 Å thickness along the z axis was used to avoid any self-interaction of the slabs for ML (to make sure there is no interaction along the z-axis). Integrations over the Brillouin zone (BZ) were sampled based on a Monkhorst pack 2D grid [20] based on the size of supercells.

3. Result and Discussion

3.1. Defect Formation Energy and Structural Stability. To understand relative stability of dopant atom (Mn) in BL MoS$_2$, dopant formation energy ($E_{\text{form}}$) was carried out employing the following equation [17, 21]:

$$E_{\text{form}} = E(\text{Mn,MoS}_2) - E(\text{MoS}_2) - \sum_i n_i (\mu_{\text{Mn}} - \mu_{\text{Mo}}),$$

where $E(\text{Mn,MoS}_2)$ and $E(\text{MoS}_2)$ are total energy of doped and pure BL MoS$_2$, respectively, $n_i$ is the corresponding number of species that has been added to or removed from the supercell, and $\mu_{\text{Mn}}$ and $\mu_{\text{Mo}}$ are chemical potentials of Mn and Mo, respectively. Both Mo- and S-rich conditions were considered for chemical potential calculation of Mo. In the Mo-rich condition, the chemical potential for $\mu_{\text{Mo}}$ is obtained from its bulk body-centered cubic (BCC) structure of Mo [21], whereas, under the S-rich condition, $\mu_{\text{Mo}}$ is obtained from energy difference between formula unit of MoS$_2$ and ring form of sulfur molecules. The dopant formation energy calculated using equation (1) for different impurity configurations of impurity atoms is summarized in Table 1. All calculated values under the S-rich condition is negative which reveal that doping Mn under the S-rich condition of BL MoS$_2$ is favorable in comparison with the Mo-rich condition in agreement with previous theoretical report [21] and experimental result [22]. Besides to this, the least formation energy $-2.0144$ eV is obtained in doping single Mn on $4 \times 4 \times 1$ BL MoS$_2$ (6.25%) compared to $3 \times 3 \times 1$ (11.11% Mn doping) which indicates that Mn dopants are more energetically favorable to occupy the substitutional lattice site (Mo) at low impurity concentration (dilute magnetic limit) than at high concentration.

3.2. Electronic Structures and Magnetism of Pure and Single Mn-Doped BL MoS$_2$. The calculated equilibrium lattice constant after optimization is 3.18 Å, which is closer to the experimental value [23] and in good agreement with theoretical value 3.18 Å [24]. In addition to this, the calculated interlayer distance (the distance between two ML) of BL MoS$_2$ is found to be 6.543 Å and the band gap calculated at this interlayer distance is 1.3 eV (Figure 1) closer with the previous reported value 1.29 Å [25]. Furthermore, the band gap increases with increasing interlayer distance, as shown in Figure 1(a). To investigate the effects of single Mn doping on the electronic and magnetic properties of pure BL MoS$_2$, $4 \times 4 \times 1$ and $3 \times 3 \times 1$ BL MoS$_2$ models which result in magnetic impurity concentration of 3.125% and 5.55%, respectively, after doping a single Mn atom were considered (see Figure 2). As seen from Table 2, the total magnetic moment of the system is 1 and 1.02 $\mu_B$ after
introducing single Mn in supercell of $3 \times 3 \times 1$ and $4 \times 4 \times 1$, respectively.

To understand how the states are distributed, the total density of state (DOS) for pure and single Mn-doped BL MoS$_2$ is plotted. As shown from Figure 3(a), for the pure system, the Fermi level is located at the middle and spin up and spin down states are symmetric indicating the pure BL MoS$_2$ are nonmagnetic semiconductors. However, after introducing single Mn, the spin degeneracy of the band structure is broken and the minority of states remain semiconductors, whereas the majority (spin up state) impurity state is formed in the vicinity of the Fermi level; as a result, it behaves as metallic, leading to magnetic and half metallic behavior of the total DOS. On the contrary, with increasing concentration of Mn dopant (3.125% to 11.11%), the impurity state is broaden (moves closer to conduction band minimum (CBM)) Figures 3(b)–3(e) which reveals that the doped system behaves as the n-type of semiconductor. Furthermore, to understand the nature of band structure and defect state, the band structure of pure and single Mn doped in one of its layers is plotted. As shown from Figures 4(a) and 4(b), the pure system is nonmagnetic semiconductor with direct band gap measured to be 1.3 eV. However, in single Mn-doped system, the majority band structure and the impurity states are formed above the Fermi level (within the gap) (Figure 4(c)). But, the minority state remains semiconductor, but the band gap is suppressed by 0.1 eV compared to the pure system (Figure 4(d)), which also gives further confirmation half metallic and magnetic behavior of the doped system. On the contrary, the impurity state closer to CBM reveals that the system is more likely the n-type of semiconductor. Based on those observation, it is suggested that the origin of magnetism as an isolated Mn atom with electron configuration $[Ar]3d^54s^2$ has one more d-orbital electron than Mo (with electron configuration $[Ar]3d^44s^2$); thus, the extra one electron is responsible for the observed defect state in the gap.

### Table 1: The calculated values of formation energy ($E_{\text{form}}$(eV)) under Mo-rich and S-rich growth conditions.

| Supercell | Doping site | Mo rich ($E_{\text{form}}$(eV)) | S rich ($E_{\text{form}}$(eV)) |
|-----------|-------------|-------------------------------|-------------------------------|
| $3 \times 3 \times 1$ | 1 Mn | 1.908 | $-0.7523$ |
| $>$ | N | 3.4019 | $-1.9173$ |
| $>$ | NN | 3.7658 | $-1.5534$ |
| $>$ | NNN | 3.4027 | $-1.9184$ |
| $>$ | Updn (do) | 3.9779 | $-1.3432$ |
| $>$ | Updn (d1) | 3.9806 | $-1.3406$ |
| $4 \times 4 \times 1$ | 1 Mn | 1.8677 | $-0.7919$ |
| $>$ | N | 3.3067 | $-2.0144$ |
| $>$ | NN | 3.6618 | $-1.6580$ |
| $>$ | NNN | 3.7086 | $-1.6126$ |
| $>$ | Updn (do) | 3.7319 | $-1.5873$ |
| $>$ | Updn (d1) | 3.7381 | $-1.5811$ |

3.3. Magnetic Interaction between Dopants in Monolayer (ML) and Bilayer (BL) MoS$_2$ Doped with a Pair of Mn Atoms. The magnetic interaction between dopants in doped ML and BL MoS$_2$ systems is studied by calculating the total energy difference between FM and AF configurations at the same impurity separation [17]. The magnetic energy ($\Delta E$) is given by

$$\Delta E = E_{\text{FM}} - E_{\text{AF}},$$

where $E_{\text{FM}}$ and $E_{\text{AF}}$ are the total energies of the supercell in FM and AF states, respectively. Employing model supercells, $5 \times 5 \times 1$, $4 \times 4 \times 1$, and $3 \times 3 \times 1$ MoS$_2$ result in doping concentrations 4%, 6.25%, and 11.11%, respectively. Five configurations with different dopant-dopant (Mn-Mn) separations were considered: nearest-neighbor (N) configuration in which the two Mn atoms are in the nearest neighboring position with Mn-Mn distance of 3.4 Å, the second nearest-neighbor (NN) configurations in which the two Mn atoms are in the next nearest-neighboring position with Mn-Mn distance of 5.4 Å, and the third nearest-neighbor (NNN) configuration in which the distance between the two doped Mn atoms are 6.4 Å; two Mn atoms in different layers of BL MoS$_2$ are separated by interlayer distance (updn(d$_0$) = 6.53 Å), and two Mn atoms in different layers of BL MoS$_2$ are separated by interlayer distance (updn(d$_1$) = 7.8 Å) results summarized in Tables 2 and 3. As can be seen from Tables 2 and 3, the calculated $\Delta E$ for all impurity configurations are negative which show that FM interaction is favorable for all concentrations of impurity in agreement with previous study in ML MoS$_2$-doped Mn [26]. In addition to that, the strength of FM interaction decays from N to NNN for all concentrations of impurity. Furthermore, in order to get insights into FM interaction between the two nearest neighbor (N) Mn dopants, the total density of states (DOS) are plotted as shown in Figures 3(e) and 3(e); the dopants are ferromagnetically interacting, and the impurity states push towards the CBM with increasing impurity concentration (6.25–11.11%), which is in broad agreement with dilute magnetic semiconductor properties [11]. We further extend our investigation by doping two Mn in different layers of BL MoS$_2$, as seen in the input structure in Figure 2(d) and Table 4, and $\Delta E = -0.006$ and $-0.0025$ eV when two dopants are separated by $d_0$ = 6.53 Å (at equilibrium interlayer distance) and $d = 7.8$ Å, respectively. Interestingly, the result reveals that two dopants in different layers can interact ferromagnetically, and the strength of ferromagnetism suppresses with atomic distance and impurity concentration. This is also seen in the DOS plot in Figure 3(e), where spin degeneracy of spin up and spin down is breaking and system becomes ferromagnetic. For further information, the electronic band structure is drawn, as shown from the band plot for those system seen in Figures 4(e) and 4(f), the system becomes magnetic even when two dopants are in different layers, and this makes the physics of system under investigation more interesting that how two dopants in different layers are communicating. On the contrary, understanding mechanism of exchange interaction in magnetic system is another issue. Good enough – Kanamori–Anderson rules which state that the magnetic ion-ligand-magnetic ion angle is 180° of two magnetic ions with partially filled d shells is strongly antiferromagnetic, whereas the magnetic ion-ligand–magnetic ion angle is 90° and is ferromagnetic super exchange.
bond angle (Mn-S-Mn) is calculated as 93° which is closer to 90° and ensures that FM super exchange is primarily response for magnetic interaction in nearest neighbor dopants, in other words, Mn 3d orbital electrons interact antiferromagnetically with one of sulfur (S) 3p electrons then this state further interacts with other Mn 3d electrons; in this way, the two Mn atoms communicate ferromagnetically indirectly with aid of sulfur 3p state. We now turn to investigate the role of interlayer interaction in BL MoS2, and we make magnetic energy, ΔE, comparison between pair of Mn-doped MoS2 ML with BL MoS2 using a 5 × 5 × 1, 4 × 4 × 1, and 3 × 3 × 1 supercells, and the results are listed

| Supercell | Distance (d) | Impurity (%) | ΔE (eV) | μm |
|-----------|--------------|--------------|---------|----|
| 3 × 3 × 1 | Single       | 11.11        | —       | 1.0 |
| >>        | N            | 22.22        | -0.18444| 2.32|
| >>        | NN           | 22.22        | -0.212240| 2.00|
| >>        | NNN          | 22.22        | -0.132042| 2.74|
| 4 × 4 × 1 | Single       | 6.250        | —       | 1.00|
| >>        | N            | 12.50        | -0.21007 | 2.07|
| >>        | NN           | 12.50        | -0.177582| 2.00|
| >>        | NNN          | 12.50        | -0.0849 | 2.00|
| 5 × 5 × 1 | N            | 8.00         | -0.1636 | 2.46|

Figure 1: The calculated interlayer distance-dependent band structure of BL MoS2: the band structure calculated at (a) equilibrium interlayer distance (6.53 Å) and (b) interlayer distance (d = 6.65 Å).

Figure 2: Optimized input structures of 4 × 4 × 1 BL MoS2: (a) top view for pure BL MoS2; (b) top view for one Mn-doped BL MoS2; (c) top view for two Mn-doped BL MoS2; (d) side view for two Mn-doped BL MoS2

Table 2: The calculated magnetic energy (ΔE = E_{FM} - E_{AF}) and magnetic moment (μ_m) for ML MoS2-doped Mn.
Figure 3: Total density of states (DOS) for $4 \times 4 \times 1$ BL MoS$_2$ (a) pure, (b) one Mn doped $4 \times 4 \times 1$ MoS$_2$ BL, (c) two Mn doped (in the same layer) $4 \times 4 \times 1$ BL MoS$_2$, (d) two Mn (one in the upper layer and the other in the lower layer) doped $4 \times 4 \times 1$ BL MoS$_2$, and (e) two Mn (in the same layer) doped $3 \times 3 \times 1$ BL MoS$_2$. The blue and red lines represent the spin-up and spin-down components, respectively; the vertical thin line indicates the Fermi level.
in Tables 3 and 4, respectively. For instance, the calculated \( \Delta E \) are \(-0.1636\), \(-0.2107\), and \(-0.1844\) eV for a pair of Mn doping in the first nearest neighbor \((N)\) configurations in \(5 \times 5 \times 1\), \(4 \times 4 \times 1\), and \(3 \times 3 \times 1\) in ML supercell, respectively, whereas \(-0.1666\), \(-0.2137\), and \(-0.1920\) eV for a pair of Mn doped in nearest neighbor configuration \((N)\) in \(5 \times 5 \times 1\), \(4 \times 4 \times 1\), and \(3 \times 3 \times 1\) BL MoS\(_2\) supercells, respectively. The result show that ferromagnetism is more stable in Mn-doped BL MoS\(_2\) than Mn-doped BL MoS\(_2\). The origin of discrepancy between BL and ML MoS\(_2\) in magnetic energy, \( \Delta E \) seems to be from interlayer interaction in BL MoS\(_2\). Therefore, we report that interlayer interaction in Mn-doped BL MoS\(_2\) system can affect its magnetic interaction, and similar finding was recently reported in iron-doped BL MoS\(_2\) [14].

3.4. Ferromagnetic Transition Temperature \( (T_c) \). By mapping Heisenberg Hamiltonian together with mean field approximation, the Curie temperature \( \left( T_c \right) \) below which the system develops a long-range ferromagnetic ordering can be found as follows [27]:

\[
\frac{3}{2} k_B T_c = -\frac{\Delta E}{N},
\]

where \( \Delta E = E_{\text{FM}} - E_{\text{AF}} \) is the magnetic energy obtained from the first principle spin polarized DFT calculation and \( N \) is the number of dopants in supercell. Using the value \( \Delta E \) for first nearest neighbor impurity configurations \((N)\) in Table 3 and \( N = 2 \), we have calculated ferromagnetic transition \( T_c \) for Mn-doped BL MoS\(_2\). However, it is well known that the magnetic ordering in the doped system is strongly

Figure 4: Band structures of \( 4 \times 4 \times 1 \) bilayer MoS\(_2\): (a) and (b) pure MoS\(_2\); (c) and (d) one Mn-doped in the upper layer of MoS\(_2\) bilayer; (e) and (f) two Mn-doped MoS\(_2\) bilayer (in different layers). The blue and red lines represent the spin-up and spin-down components, respectively. The zero energy represents the Fermi level.
Table 3: The calculated magnetic energy (ΔE = E FM − E AF ) and magnetic moment (μ m ) for BL MoS 2-doped Mn.

| Supercell | Distance (d) | Impurity (%) | ΔE (eV) | μ m |
|-----------|-------------|--------------|---------|-----|
| 3 × 3 × 1 | Single      | N            | 5.55    | 1.00|
| >>        | N           | 11.11        | −0.192  | 2.13|
| >>        | NN          | 11.11        | −0.232  | 2.00|
| >>        | NNN         | 11.11        | −1.30A6 | 1.83|
| >>        | updn(d0)    | 11.11        | −0.085  | 2.00|
| >>        | updn(d1)    | 11.11        | −0.033  | 2.00|
| 4 × 4 × 1 | Single      | N            | 3.125   | 1.02|
| >>        | NN          | 6.25         | −0.21A7 | 2.03|
| >>        | NNN         | 6.25         | −0.169  | 2.00|
| >>        | updn(d0)    | 6.25         | −0.082  | 2.06|
| >>        | updn(d1)    | 6.25         | −0.005  | 2.00|
| 5 × 5 × 1 | N           | 4.00         | −0.166  | 2.46|

The data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that there are no conflicts of interest.

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In conclusion, Mn dopant in BL MoS 2 are energetically favorable to occupy the substitutional lattice site (Mo) under sulfur- (S-) rich regime than Mo. The magnetic interaction between dopants in Mn-doped BL MoS 2 is always ferromagnetic. Moreover, the strength of ferromagnetism decays with atomic distance. Interlayer interaction in Mn-doped BL MoS 2 affects its magnetic properties. Super exchange mechanism is primarily responsible for ferromagnetic interaction between a pair of dopants. The calculated T c shows that good dilute limit of dopant concentration is 0 − 6.25%, and further increasing dopant concentration results in FM instability. Based on the result, it is suggested that Mn-doped BL MoS 2 are promising candidates for 2D dilute magnetic superconductors for high-temperature spintronics applications.


data availability

The authors acknowledge financial support from the Center for Science and Technology of the Non-Aligned and Other Developing Countries (NAM S & T Center), Supercomputer Education and Research Center (SERC) at Indian Institute of Sciences (IISc) for providing the computational facilities, and Arba Minch University, Arba Minch, Ethiopia.

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4. Conclusion

In conclusion, Mn dopant in BL MoS 2 are energetically favorable to occupy the substitutional lattice site (Mo) under sulfur- (S-) rich regime than Mo. The magnetic interaction between dopants in Mn-doped BL MoS 2 is always ferromagnetic. Moreover, the strength of ferromagnetism decays with atomic distance. Interlayer interaction in Mn-doped BL MoS 2 affects its magnetic properties. Super exchange mechanism is primarily responsible for ferromagnetic interaction between a pair of dopants. The calculated T c shows that good dilute limit of dopant concentration is 0 − 6.25%, and further increasing dopant concentration results in FM instability. Based on the result, it is suggested that Mn-doped BL MoS 2 are promising candidates for 2D dilute magnetic superconductors for high-temperature spintronics applications.
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