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RESEARCH ARTICLE

STRUCTURAL AND ELECTRONIC PROPERTIES OF 2D MOS_2 DOPED WITH SELECTED 3*d* TRANSITION METALS: A DFT STUDY

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Abstract

2D Molybdenum Disulfide (MoS_2) has aroused a lot of intense interest in the recent past, due to the modification capabilities in its structural and electronic properties following the substitutional doping with 3d transition metals. Limited studies exist that have explored transition metal dopants as possible optimization route towards tuning of 2D MoS_2 in order to achieve superior structural and electronic properties. In this study, Density Functional Theory has been used to investigate the structural and electronic properties of 2D MoS2 doped with Ti, Fe, Cu, Zn and Cd maintained at a concentration of 2.38% to ensure minimal distortion of structure and stability. Results show negligible changes in lattice constants after substituting the Mo atom with the 3d transitional metal dopants. Further, the energy band gap of 2D MoS_2 doped with Ti was found to widen by 6.59% compared to pristine while those doped with Cu, Zn and Cd was found to introduce new states at the edges of valence and conduction bands resulting in band gap narrowing. 2D MoS_2 doped with Fe was found to introduce metallic character. Therefore, judicious introduction of dopants in 2D MoS_2 can yield in realization of devices for wide range of applications.

Introduction:-

Molybdenum Disulfide (MoS_2) is a Transitional Metal Di-chalcogenide (TMDC) that has received extensive interest in the last few years due to its potential applications in various fields [1-4]. The 2H- phase 2D MoS_2 is a direct band gap semiconductor with an energy-gap of 1.8 eV [5]. Some studies have already shown that doping 2D MoS_2 with 3*d* transitional metals modifies its structural and electronic properties for novel applications such as photo-electrochemical (PEC) activity [6-10].

Other applications of MoS_2 include sensors, field effect transistors, lubricants, energy storage devices, catalyst in CO_2 reduction and solar cells, to mention a few [11]. 2D materials such as quantum wells, graphene and MoS_2 have enabled the design of new generation solid-state devices such as Light Emitting Diodes (LEDs), photo-detector solar cells, optical fibers, bio-sensors and they are also used in tissue engineering [12]. This has been achieved via manipulating electron concentration between the conduction and valence bands. In this approach, it has been found that doping by substitution is the best route in achieving the desired results [13, 14].

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The recent application of MoS_2 as a gate insulator in FET has re-ignited much interest in 2D MoS_2 [15, 16]. For example, Ye et al., [17] successfully used the oxygen plasma and hydrogen annealing approach to introduce a significant number of cracks and holes in 2D MoS_2, which increased the number of edges and hence, more active sites have been achieved. By doping pristine MoS_2 with Pd, Luo et al, [18] observed that it distorted the basal plane, thereby forming new states that modified hydrogen adsorption behavior on coordinated S atoms.

Anionic substitution of S atoms with O, Se and P has also been found to induce distortion in 2D MoS_2, thereby introducing regulated electronic structure with enhanced intrinsic activity [19]. Engineering 2D MoS_2 has also enhanced selectivity and sensitivity of greenhouse gases (CO_2, CH_4 and N_2O). Further, doping of MoS_2 with transition metals has been found to result not only in modification of electronic structure but also in the change from 2H to 1H, as observed by Stewart et al., [20].

There are various energy gap engineering and manipulation routes of MoS_2, that have been proposed, the facile generating 2D MoS_2 from bulk MoS_2 has a net effect of changing the band gap from indirect to direct [21]. The advantage of this approach is that electrons and holes will acquire the same crystal momentum in both conduction and valence bands and can directly emit a photon, which is not the case in an indirect band gap [22]. There is also an application of external fields, such as strain engineering, which modifies band gaps and the charge carrier's effective mass [23].

Tuning structural and electronic properties of 2D MoS_2 significantly enhances its function in the visible spectrum [24]. This happens by substitutional doping where 3*d* transitional metal dopants substitute the molybdenum atom (Mo) in a 2D MoS_2 system. The 3*d* transitional metal dopants exhibit different oxidation states and are therefore considered ideal candidates in manipulating the energy band gap. Throughout this study, a dopant concentration of 2.38% has been used to ensure minimal strain and also reduce any likelihood of phase transition occurring.

In this study, we examine the impact of selected 3*d* transition metals (Ti, Fe, Cu, Zn, and Cd) on the structural and electronic properties of 2D MoS_2, aiming to assess the suitability of these dopants for enhancing the various application of 2D MoS_2-based devices that include energy and enviroment [2, 4, 6, 7]. The selected 3*d* transitional metal dopants (Ti, Cu, Fe, Zn, and Cd) have more or less comparable atomic radii with Mo thus ensuring negligible structural distortions [25]. Using Density functional theory as implemented in Quantum Espresso (QE) code that employs pseudopotentials, we systematically examine these dopants. Unlike previous studies that have often employed different codes, pseudopotentials, all-electron potential or only a limited selection of dopants (one or two), our work considers five different dopants to identify potential trends. We evaluated dopant concentrations 2.38%, in line with available experimental data that have shown such concentrations induce negligible structural strain and the hexagonal structure is conserved.

Computational Details: -

This study used DFT approximations implemented in quantum Espresso code to perform all the calculations reported in this work [27]. It is performed using the self-consistent plane wave pseudo-potential total energy method. It has been used to study the structural and electronic properties of the 2D MoS_2 material [28]. The exchange and correlation potential's generalized gradient approximation (GGA) was employed using Perdew-Wang functional [29]. All the structures used here were relaxed until forces on atoms were smaller than 0.02 eV/ Å. Electronic wave functions (charge density) were expanded in plane wave basis with an energy cut off of 50 Ry (500Ry for charge density). As described by Vanderbilt's formulations, co-electrons were replaced with ultra-soft pseudo-potential [30]. The integration over Brillouin zone (BZ) was performed on (12×12×1) k-point Monk-horst pack grid [31].

2D MoS_2 surface was modeled using a supercell consisting of 24 Mo atoms and 24 S atoms. Mo atoms were substituted with dopants (Ti, Fe, Cu, Zn and Cd) and geometry optimization was performed using a conjugate gradient algorithm until all residual forces were lower than 0.01eV/Å, with an electronic energy convergence of 10^{-8}eV between two successive self-consistent steps. A vacuum of 15 Å in a perpendicular direction was introduced to avoid interaction between successive layers. In addition, to ensure that Vander Waals interactions were fully described, the Grimme –term was added to the calculation [32].

Results and Discussion:-

Structural Properties:-

Figures 1(a) and 1(b) show the top view and the side view of the optimized structure of 2D MoS_2 doped with selected 3*d* transitional metals. 2D MoS_2 doped with Ti, Fe, Cu, Zn, and Cd were found to maintain their hexagonal structures with the lattice constants **a** and**c** showing minimal changes. This suggests that the dopants did not significantly distort the structure. In the case of Ti and Fe dopants, the bond lengths of Ti-S and Fe-S were found to contract by 0.81% and 5.7% respectively, while Cu, Zn, and Cd-induced elongation of 1.6 %, 3.6 %, and 8.6 % respectively. Such a change in bond lengths indicates a decrease in bond energy, which implies a decrease in bond strength and can be attributed to the fact that the bond order increases. Our calculated values for **a** and**c** for both pristine and doped systems were in good agreement with available theoretical and experimental studies as shown in Table 1.

Table 1:- Lattice constants **a** and **c** bond lengths and bond angles of pristine and doped $MoS_2$for 2.38 % concentration.

Structure	Lattice parameter (Å)	Bond length (Å) (This work)	Bond length (Å) (Other works)	Bond angle (°)
MoS_2	a=3.22 c=6.45	Mo-S=2.44	Mo-S=2.42 [33]	S-Mo-S=82.71
MoS_2-Ti	a=3.19 c=6.45	Ti-S=2.42	Ti-S=2.42 [34]	S-Ti-S=82.34
MoS_2-Fe	a=3.22 c=6.44	Fe-S=2.30	Fe-S=2.30 [35]	S-Fe-S=82.62
MoS_2-Cu	a=3.23 c=6.45	Cu-S=2.48	Cu-S=2.48 [36]	S-Cu-S=84.28
MoS_2-Zn	a=3.24 c=6.45	Zn-S=2.53	Zn-S=2.53 [37]	S-Zn-S=84.98
MoS_2-Cd	a=3.25 c=6.45	Cd-S=2.65	Cd-S=2.65 [38]	S-Cd-S=86.27

The bond angle S-Mo-S of pristine 2D MoS_2 was found to be 82.71° while those of S-Ti-S and S-Fe-S decreased to 82.34° (0.45 %) and 82.62° (0.34 %) respectively, compared to pristine 2D MoS_2. Those of S-Cu-S, S-Zn-S and S-Cd-S were found to increase to 84.28° (2.36 %), 84.98° (3.21 %), and 86.27° (4.78 %) respectively, compared to pristine 2D MoS_2. Bond angles for pristine Mo-S-Mo and S-Mo-S are 81.55° and 82.71° meaning that the introduction of the dopants slightly alters the structure though not enough to distort it from that of pristine MoS_2. Introduction of the larger atoms i.e. Cu, Zn and Cd created a relatively larger modification of the bond angles as compared to the smaller Ti and Fe atoms.

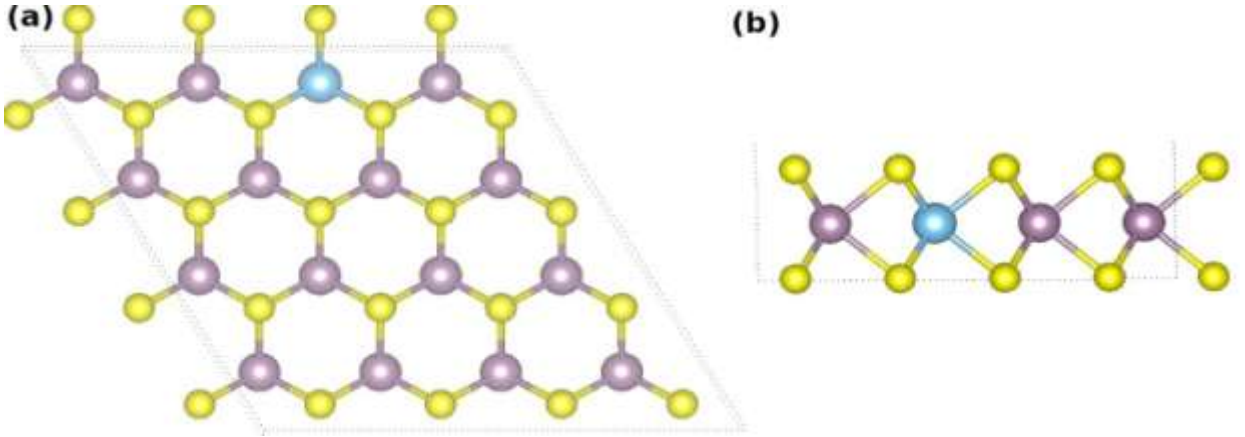

Figure 1:- Optimized 2D MoS_2 doped with selected 3d TM (a) top view, (b) side view.Ball and stick representation of atoms (in color), brown, yellow and blue represent Mo, S, and TM atom dopants respectively.

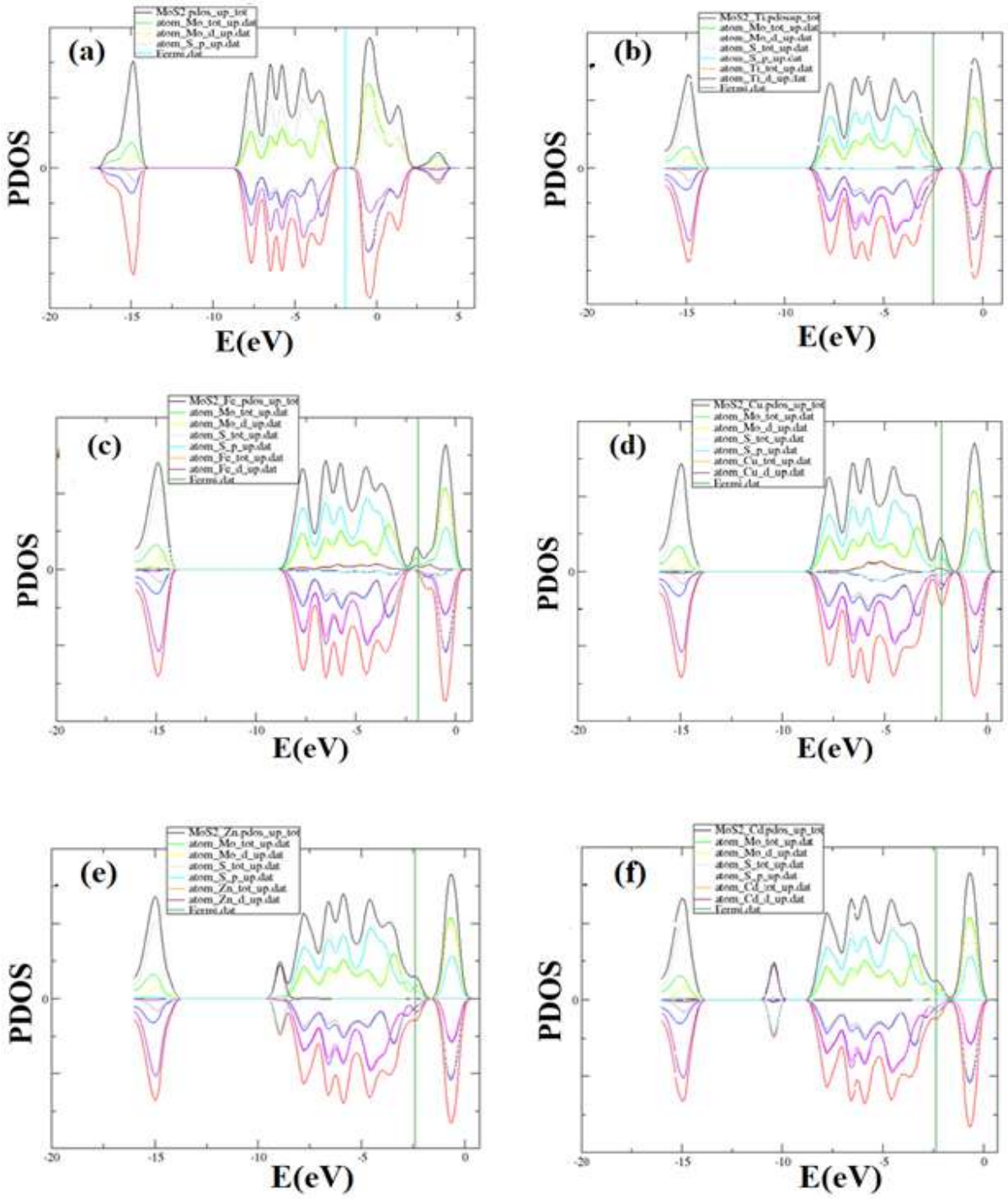

Figure 2:- PDOS of (a) pristine 2D-MOS_2, (b) Ti doped 2D-MoS_2, (c) Fe doped 2D-MoS_2, (d) Cu doped 2D-MoS_2, (e) Zn doped 2D-MoS_2 and (f) Cd doped 2D-MoS_2.

Electronic Properties

The chemical reactivity of a structure is determined by the Highest Occupied Molecular Orbital (HOMO) and Lowest Occupied Molecular Orbital (LUMO) which is a parameter that shows electrical transport characteristics and therefore dictates the electron conductivity.

Table 2 shows the calculated energy gaps for pristine 2D MoS_2 and 2D MoS_2 doped with Ti, Fe, Zn, Cu and Cd.

Table 2:- Calculated band energy for pristine and doped MoS_2

Structure	Energy gaps (eV)	Other works (eV)	
		Theory	Experimental
MoS_2	0.91	1.8 [5]	1.69 [39]
MoS_2 – Ti	0.97	1.0 [40]	
MoS_2 – Cu	0.24	0.51 [41]	
MoS_2 – Zn	0.26		1.29 [42]
MoS_2 – Cd	0.13		

The calculated band gap energies were found to be in good agreement with existing theoretical and experimental works as shown in Table 2, although these values are underestimated due to the use of DFT which tends to predict lower values of the bandgap.

Figure 3(a) shows theProjected Density of States (PDOS) of pristine 2D MoS_2 with an equal number of electrons and holes implying that pristine MoS_2 is a semiconductor.

The Highest Occupied Molecular Orbital (HOMO) of pristine 2D MoS_2 can be attributed to d orbitals of the Mo atom. The calculated energy band gap is 0.91eV which is lower than 1.69eV [39] due to the underestimation attributed to DFT. Ti-doped 2D MoS_2 has its Fermi level shifted to the left compared to that of pristine structure, suggesting that it remains a semiconductor even though with reduced carrier concentration compared to pristine 2D MoS_2. The introduction of substitutional Ti at 2.38% concentration induces a widening of the energy band gap by 6.59 %, as shown in Figure 3(b), compared to the pristine MoS_2 structure. A closer look at the PDOS shows that there are no symmetric peaks on the Fermi level on both spins and it maintains zero density of states thereby confirming that it is indeed a semi-conductor.

Fe doping of 2D MoS_2 has states due to Fe-d orbitals located in the band gap, therefore introducing metallic character in the system, as shown in Figure 3. This is in the agreement with the works of Huang et al [44]. The fermi level is shifted to the right clearly indicating that it turns out to be metallic.

Cu doped 2D MoS_2 was found to reduce band-gap to 0.24 eV compared to the pristine structure as seen in figure 3(d). This is confirmed by introduction of new states on top of the HOMO. In the conduction bands of new system there is hybridization of Mo d-orbitals and S p-orbital giving rise to strong Mo-S bond. The contribution of Cu-d orbitals to the system is more significant compared to Cu s and Cu p orbitals.

Doping 2D MoS_2 with Zn and Cd resulted in narrowing the energy band gap to 0.26eV and 0.13 eV respectively compared to 0.91eV for pristine 2D MoS_2. Thus, theZn and Cd dopants effectively reduce the pristine MoS_2 band gap energy to levels comparable to the redox potentials of H_2O/H_2. This band gap tuning indicates that Zn and Cd dopants could significantly enhance the material's PEC activity, making it more suitable for applications such as water splitting. In contrast, Fe dopants induce semi-metallic character in 2D MoS_2 making it undesirable for PEC water-splitting as shown in Figures 3.

Conclusions:-

The bond lengths of Ti and Fe doped 2D MoS_2 decreased while those of Cu, Zn and Cd doped 2D MoS_2were found to increase marginally. This indicates a decrease in bond energy that showed there is a decrease in bond strength. The bond angles aroud the dopants were also found to vary slightly and therefore no structure modification was established.

2D MoS_2 doped with Ti widened the band gap and shifted its fermi level to the left indicating that it remained a semiconductor. Fe doping of 2D MoS_2 introduced a metallic character as it shifted its Fermi level to the right and also introduced Fe d-orbitals which hybridizes to form a hoping site on the spin up state. 2D MoS_2 doped with Cu, Zn and Cd was found to exhibit reduced band gap therefore,these are considered ideal for PEC activity such as water splitting among other applications.

This study has shown that tuning a photocatalyst such as 2D MoS_2 by doping can lead to a superior photocatalyst which is useful in enhancing PEC activity. It modifies the band gap by introducing new states within it which can be responsible for carrier concentration.

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