Strain tunable structural, mechanical and electronic properties of monolayer tin dioxides and dichalcogenides SnX_2 ($\text{X}=\text{O}, \text{S}, \text{Se}, \text{Te}$)

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ABSTRACT

Based on first-principles calculations, we investigate the structural, mechanical and electronic properties of monolayer tin dioxides and dichalcogenides SnX_2 ($\text{X}=\text{O}, \text{S}, \text{Se}, \text{Te}$) under uniaxial and biaxial strains. Our results show that monolayer 1T- SnX_2 is energetically more stable than 2H- SnX_2 , while the stiffness of 2H- SnX_2 is much higher. The unstrained SnX_2 is thermodynamically and dynamically more stable than the strained ones. We also show that when external strain is applied, the band gaps of both 2H- and 1T- SnO_2 decrease linearly with increasing strain, which is contributed by the strain induced orbital redistribution of the decomposition of the p orbital of X atom and s, p orbitals of Sn atom. Notably, the slope of the band gap variation of the biaxial strained 1T- SnO_2 reaches up to -0.16 eV/1%. In our calculations, strain can result in a semiconductor-metal transition of 2H- SnX_2 , while it only affects the band gap of 1T- SnX_2 .

1. Introduction

Over the years, two dimensional (2D) layered materials like graphene, black phosphorus and MoS_2 have been intensely studied due to their intriguing electronic, optical and mechanical properties [1–5]. Particularly, they have shown many advantages in ultra-small and low-power field effect transistor, which is comparable to traditional silicon-based semiconducting technology [6,7]. Meanwhile, new 2D materials with novel structures and physical properties are still under exploring, including compounds of elements from groups III–V [7–10], II–VI [11–13], IV [14], and V [15–17]. Recently, Ataca et al [18]. have identified 52 stable monolayer transition-metal dioxides and dichalcogenides (TMOs and TMDs) which can exist in honeycomb-like structures and may provide a novel platform for practical applications of catalysis [19], energy storage [20], sensing [21], and electronic devices [22–24].

Among these materials, monolayer tin dioxides and dichalcogenides SnX_2 ($\text{X}=\text{O}, \text{S}, \text{Se}, \text{Te}$) have been attracted much attention due to their low-cost, superior electronic properties, earth-abundant and

environmentally-friendly features [25]. First-principles calculations have shown that 2D SnX_2 are semiconductors with the band gap ranging from 2.18–4.13 eV [26–28], which is helpful in photoelectric device applications [6,9,15–17]. Upon hydrogen passivation, they transfer from a metal or narrow gap semiconductor to a wide gap semiconductor [29]. Monolayer TMOs and TMDs are reported to withstand large strains [28]. SnS_2 and SnSe_2 doped with holes can exhibit strain tunable magnetism [30]. Moreover, a very recent work reported superconductivity in layered 1T- SnSe_2 using an electric-double-layer transistor gating geometry, which provides a new perspective for 2D superconductivity [31]. All these characteristics make SnX_2 potential candidate in solar-driven water splitting, gas sensing, field-effect transistor, lithium battery and electronic information storage devices [26,32–37].

However, for monolayer TMOs and TMDs, they typically crystallize in two distinct symmetries, namely the 2H (trigonal prismatic D_{3h}) and 1T (octahedral O_h) phases. Up to date, most studies of SnX_2 are mainly focused on the stable 1T phases, while the less stable 2H phase is more or less mentioned. To better understand the electronic properties of

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SnX_2 with respect to their atomic structure, it is essential to perform an extensive study on both the 1T and 2H phases. On the other hand, mechanical strain is becoming an effect way to tune the physical properties of 2D materials, while a systematic investigation of strain on the structural and electronic properties of these monolayer SnX_2 ($X = \text{O}, \text{S}, \text{Se}, \text{Te}$) is still insufficient.

In the present work, density functional theory (DFT) [38,39] calculations are conducted to investigate the effects of uniaxial and biaxial strains along the zigzag (ZZ)- and armchair (AC)-directions on the structural and electronic properties of 1T and 2H phases in the monolayer SnX_2 ($X = \text{O}, \text{S}, \text{Se}, \text{Te}$) systems. The remainder of this paper is organized as follows. In Section 2, the models and computational methods are introduced. The main results and discussions are presented in Section 3. Finally, the conclusions are reported in Section 4.

2. Computational methods

First-principles calculations are carried out by using the Vienna *ab initio* Simulation Package [38–42]. The Perdew-Burke-Ernzerh (PBE) form of the generalized gradient approximation (GGA) exchange-correlation functional is applied [43]. The kinetic cutoff energy for the plane wave basis set is 450 eV and the Brillouin zone sampling is performed by using $9 \times 9 \times 1$ Monkhorst-Pack grid meshes for relaxation calculations [44]. A vacuum of 20 Å is set to prevent interactions between periodically repeated layers. The geometry of each monolayer system is relaxed at each value of strain until the forces on the atoms are less than 10^{-2} eV/Å. The total energy is converged to 10^{-5} eV. External strain is applied from -10% (compression) to 10% (tension) with an increment of 1% per step. The strength of the strain (ε) is defined as:

$$\varepsilon = \frac{L - L_0}{L_0} \quad (1)$$

where L and L_0 are the deformed (stretched or compressed) and initial equilibrium lattice constants, respectively.

3. Results and discussions

3.1. Structure and stability

The atomic structures of 2H- and 1T- SnX_2 are shown in Figs. 1 (a) and (b), respectively. The 2H phase (space group D_{6h}^4 (P6₃/mmc, No.194)) and 1T phase (space group D_{3d}^5 (P3m1, No.164)) have trigonal prismatic and octahedral coordination, respectively. The corresponding equilibrium lattice constants and atomic positions in the unit cell are given in Table 1, and the optimized lattice constants agree well with previous studies [28,29,45]. When external strain is applied, all the Sn-X bonds decrease (increase) slightly with the increasing compression

(tension) strain (left panel of Fig. 2(a) and (b)), except for the 2H SnTe_2 . Due to the Poisson effect, the corresponding distance between two adjacent X layers adjusts inversely as shown in the right panel of Fig. 2(a) and (b). For 2H- SnX_2 , the variation of the Sn-X bonds induced by uniaxial strains along the armchair and zigzag directions are isotropic, but for 1T- SnX_2 , it exhibits anisotropic statistics. Typically, the bond lengths of Sn-X change more remarkably under uniaxial strain along the zigzag direction than those in the armchair direction, though the interlayer X-X distances have the same trend. It is also found that, at each strain, both the Sn-X and X-X bonds are directly correlated with the formation of the materials with the oxides having the shortest bonds followed by the sulphides, selenides and tellurides.

The thermodynamical stabilities of both 2H- and 1T- SnX_2 monolayers are evaluated from their formation energy E_f as:

$$E_f = \frac{E_{\text{SnX}_2} - n_{\text{Sn}}\mu_{\text{Sn}} - n_{\text{X}}\mu_{\text{X}}}{n_{\text{Sn}} + n_{\text{X}}} \quad (2)$$

where E_{SnX_2} is the energy of the SnX_2 ($X = \text{O}, \text{S}, \text{Se}$ and Te) monolayers, n_{Sn} and n_{X} are the number of Sn and X atoms, respectively. For each monolayer SnX_2 , μ_{Sn} and μ_{X} are the per atom chemical potentials of Sn and X, respectively, while μ_{Sn} , μ_{O} and μ_{X} ($X = \text{S}, \text{Se}$ and Te) are calculated from bulk Sn, oxygen molecule and the crown-shaped X_8 molecules, respectively. It is found in Table 1 that the formation energies of SnO_2 , SnS_2 , SnSe_2 and SnTe_2 in 2H phase are -1.794 eV, -0.643 eV, -0.488 eV and -0.295 eV, respectively, which are higher than those (-2.288 eV, -0.930 eV, -0.754 eV and -0.485 eV) in 1T phase. So 1T- SnX_2 monolayer is more favorable in energy. Besides, SnO_2 has the lowest formation energy followed by the other three SnX_2 in the order of sulphides, selenides and tellurides, indicating that SnO_2 is thermodynamically the most stable one among all the SnX_2 monolayers (see Fig. 3(a) and (b)).

The relative stabilities of 1T SnX_2 monolayers are further confirmed by the ground state analysis, which is defined as the energy difference ΔE between two phases ($\Delta E = E_{2\text{H}} - E_{1\text{T}}$) at the equilibrium (Fig. 3(c)). Our results show that all relative energies are positive, rendering 1T phase as a ground-state structure. And ΔE decreases as the radical of X atom increases, with a maximum value up to 1.5 eV for SnO_2 . Considering that the energy difference associated with 2H-1T transition is several tenths of 1 eV in metal halides and dichalcogenides like VCl_2 , CoCl_2 , MoS_2 and WSe_2 [2], our results indicate possible phase transition from 2H to 1T in SnX_2 monolayers through external strain engineering.

To determine the dynamical stabilities of SnX_2 monolayers, we obtain the phonon spectrum of SnX_2 from the force constants calculated with density functional perturbation theory [46,47] and the PBE functional. For simplicity, here we take 2H- SnS_2 for example. The phonon spectrum of unstrained 2H- SnS_2 has been reported by Smith et al. [48], who have identified that there is no imaginary frequency, confirming the dynamical stability of unstrained 2H- SnS_2 . Mu et al.

Fig. 1. Atomic structures of 2H- and 1T- SnX_2 . (a) and (b) are the top and side views of monolayer SnX_2 ($X = \text{O}, \text{S}, \text{Se}$ and Te) in 2H and 1T phases, respectively. Yellow and green spheres represent X and Sn atoms, respectively. (c) First Brillouin zone of the hexagonal unit cell with high symmetry points. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article).

Table 1

Calculated structural parameters of SnX_2 ($\text{X}=\text{O}, \text{S}, \text{Se}, \text{Te}$) at the equilibrium: the lattice parameters (a_0 , in Å) and the atomic positions, formation energy (E_f , in eV), band gap (E_{gap} , in eV), elastic constants (C_{11} and C_{12} , in N/m), in-plane Young's modulus (Y , in N/m), the Poisson's ratio (ν).

2H structures	a_0 (Å)	Position of Sn	Position of chalcogen	E_f (eV)	E_{gap} (eV)	C_{11} (N/m)	C_{12} (N/m)	Y (N/m)	ν
SnO_2	3.090 ^a	$\left(\frac{1}{3}\frac{2}{3}\frac{1}{2}\right)^d$	$\pm\left(\frac{1}{3}\frac{2}{3}0.433\right)^d$ $\pm\left(\frac{1}{3}\frac{2}{3}0.567\right)^d$	-1.794	0.653	160.490	54.206	142.182	0.338
SnS_2	3.618 ^b	$\left(\frac{1}{3}\frac{2}{3}\frac{1}{2}\right)^d$	$\pm\left(\frac{1}{3}\frac{2}{3}0.410\right)^d$ $\pm\left(\frac{2}{3}\frac{1}{3}0.580\right)^d$	-0.643	0.787	89.681	21.817	84.373	0.243
SnSe_2	3.799 ^b	$\left(\frac{1}{3}\frac{2}{3}\frac{1}{2}\right)^d$	$\pm\left(\frac{1}{3}\frac{2}{3}0.406\right)^d$ $\pm\left(\frac{2}{3}\frac{1}{3}0.563\right)^d$	-0.488	—	67.322	22.668	59.689	0.337
SnTe_2	3.799 ^b	$\left(\frac{1}{3}\frac{2}{3}\frac{1}{2}\right)^d$	$\pm\left(\frac{1}{3}\frac{2}{3}0.383\right)^d$ $\pm\left(\frac{2}{3}\frac{1}{3}0.616\right)^d$	-0.295	—	28.493	33.116	—	—
1T structures	a_0 (Å)	Position of Sn	Position of chalcogen	E_f (eV)	E_{gap} (eV)	C_{11} (N/m)	C_{12} (N/m)	Y (N/m)	ν
SnO_2	3.220 ^a	$\left(\frac{2}{3}\frac{1}{3}\frac{1}{3}\right)^d$	$\pm(0\ 0\ 0.278)^d$ $\pm\left(\frac{1}{3}\frac{2}{3}0.389\right)^d$	-2.288	2.635	130.131	36.902	119.667	0.284
SnS_2	3.700 ^{abc}	$\left(\frac{2}{3}\frac{1}{3}\frac{1}{3}\right)^d$	$\pm(0\ 0\ 0.253)^d$ $\pm\left(\frac{1}{3}\frac{2}{3}0.414\right)^d$	-0.930	1.579	69.651	17.006	65.499	0.244
SnSe_2	3.860 ^{ac}	$\left(\frac{2}{3}\frac{1}{3}\frac{1}{3}\right)^d$	$\pm\left(\frac{1}{3}\frac{2}{3}0.247\right)^d$ $\pm(1\ 0\ 0.420)^d$	-0.754	0.784	58.165	14.114	54.740	0.242
SnTe_2	4.120 ^d	$\left(\frac{2}{3}\frac{1}{3}\frac{1}{3}\right)^d$	$\pm(0\ 0\ 0.236)^d$ $\pm\left(\frac{1}{3}\frac{2}{3}0.431\right)^d$	-0.485	—	37.037	20.542	25.643	0.554

^aRef. [28].^bRef. [29].^cRef. [45].^dOptimized.

Fig. 2. Variation of bond lengths of 2H- and 1T- SnX_2 ($\text{X}=\text{O}, \text{S}, \text{Se}$ and Te) under strain. X–X refers to the distance between two adjacent X layers in SnX_2 . The solid, hollow and crossing circles indicate strain along the zigzag, arm-chair and biaxial directions, respectively.

have successfully fabricated stable SnS_2 . Experiments indicate that the unstrained SnS_2 has very good lattice dynamical stability [49]. The phonon spectrum of 2H- SnS_2 under uniaxial and biaxial strains have been calculated, as shown in supporting information Figures S1(a)–(f). Here, we take 2H- SnS_2 with strain of -10% and 10% for example. Our results show that the strained 2H- SnS_2 are dynamically unstable as obvious imaginary frequencies exist. The appearance of imaginary frequency indicates that 2H- SnS_2 is dynamically unstable to the lattice distortion.

3.2. Mechanical properties

The mechanical properties of both 2H- and 1T- SnX_2 monolayers are studied by the in-plane Young's modulus (Y) and the Poisson's ratio (ν) analysis at the equilibrium, which are defined as $Y = (C_{11}^2 - C_{12}^2)/C_{11}$ and $\nu = C_{12}/C_{11}$ by two independent elastic constants C_{11} and C_{12} , respectively. The calculated values of C_{11} and C_{12} are listed in Table 1 and both of them are positive, which are in good agreement with previous report [50]. Besides, they meet the Born stability criteria, i.e., $C_{11} > 0$

Fig. 3. Relative stability of 2H- and 1T-SnX₂. (a) and (b) are formation energies E_f as a function of strain in 2H and 1T phases, respectively. The solid, hollow and crossing circles indicate strain along the zigzag, armchair and biaxial directions, respectively. (c) is the energy difference of monolayer SnX₂ between 2H and 1T phases. The energies are computed at the equilibrium for each phase.

Fig. 4. Band gap of SnO_2 as a function of strain along the zigzag (black), armchair (red) and biaxial (blue) directions, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article).

and $C_{11} - |C_{12}| > 0$ [51], though SnX_2 has a much smaller in-plane Young's modulus compared to two-dimensional graphene and hBN [5,52]. For each phase (2H or 1T), monolayer SnO_2 has the maximum Y value followed by SnS_2 , SnSe_2 , and SnTe_2 , indicating a softness of monolayer SnX_2 from SnO_2 to SnTe_2 . On the other hand, one can see from Table 1 that, for most SnX_2 monolayers, the in-plane stiffness in 2H phase is higher than that in 1T phase. This can be attributed to the weaker ionic bonds in 1T phase compared to those in 2H phase.

3.3. Electronic properties

The fundamental electronic properties of monolayer SnX_2 are studied by calculating the band structures along high-symmetry K points of both the 2H and 1T phases. Our results show that the 2H- SnO_2 , 2H- SnS_2 , 1T- SnO_2 , 1T- SnS_2 and 1T- SnSe_2 are semiconductors with the energy gap ranging from 0.653 eV to 2.635 eV, while 2H- SnSe_2 , 2H- SnTe_2 and 1T- SnTe_2 are metals, which are consistent with previous

Fig. 5. Band structures and PDOS of 2H and 1T-SnO₂ under biaxial strain. The red, blue and magenta lines indicate the oxygen 2p-states, Sn 3s-states and Sn 3p-states, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article).

theoretical investigations [29]. Considering that SnO₂ is not only the most energetically favorable but the stiffest monolayer, for the sake of simplicity, we will take monolayer SnO₂ as a theoretical model in the following. And relevant discussions on other SnX₂ can be found in the supporting information Figures S2-S7.

The energy gap of SnO₂ under external strain is shown in Fig. 4. For 2H-SnO₂ (Fig. 4(a)), the energy gap decreases monotonically with the uniaxial and biaxial strains varying from -10% to 10%. It is also notable that its energy gap becomes zero when a tension strain of 5% is applied, indicating a semiconductor to metal transition. Slightly different, the energy gap of 1T-SnO₂ first reaches the maximum of 3.86 eV at $\varepsilon = -8\%$ and decreases linearly when the strain is applied from -8% to 10% (Fig. 4(b)). A sharp modulation of the energy gap with the slope is estimated to be -0.13 eV/1% (-0.16 eV/1%) for biaxial strained 2H-SnO₂ (1T-SnO₂). On the other hand, the modulation induced by uniaxial strain is much smaller than that by biaxial strain.

To further understand how the electronic properties of SnX₂ are modulated by the strain, we plot the band structures and projected density of states (PDOS) in Fig. 5. Our calculations show that both unstrained 2H- and 1T-SnO₂ monolayers are indirect gap semiconductors. The conduction band minimum (CBM) and the valence band maximum (VBM) of 2H-SnX₂ are situated at the high symmetric Γ and K points, respectively, and those of 1T-SnX₂ are located at Γ point and slightly away from K point. When external strain is applied, the CBM of 2H-SnX₂ is pulled down with the increasing tension, and finally crosses the Fermi level and overlaps with the VBM at $\varepsilon = 5\%$ (Fig. 5), becoming a metal. During this process, the momentums of the CBM and VBM keep the same, so the energy gap modulation can be seen as an example within the deformation potential theory. On the contrary, when a biaxial strain of -8% is applied on 1T-SnO₂, the VBM is replaced by the momentum at Γ point, inducing an indirect-to-direct band gap transition. The energy gap modulation of SnO₂ is further explained by analyzing the PDOS. As shown in Fig. 5, the low-energy region band is mainly attributed to the decomposition of the 2p orbital of O atom and 3s, 3p orbitals of Sn atom. When the interlayer O-Sn distance is increased by tensile strain, the hopping between the in-plane s, p_x and p_y will decrease, resulting in the narrowing of band gap.

Our DFT results show that the linear energy gap modulation by strain is not general for all the SnX₂ (X=S, Se, Te) as shown in the supporting information Figure S8. The slopes for 2H-SnS₂, 1T-SnS₂ and 1T-SnSe₂ are calculated to be 0.06 eV/1%, 0.06 eV/1% and 0.08 eV/1% for biaxial negative strains and -0.10 eV/1%, -0.16 eV/1% and -0.04 eV/1% for positive strains, respectively, leading band gap increases (decreases) accordingly. The results are helpful in representing monolayer SnX₂ as an ideal elastic material for the nanoscale electro-mechanical devices, such as sensors, field-effect transistors and switches et al.

4. Conclusion

By performing first-principles calculations, we have investigated the strain-dependent structural, mechanical and electronic properties of 2H- and 1T-SnX₂ (X=O, S, Se, Te). Our results show that the 1T-SnX₂ monolayers are energetically more stable. Good agreement with experiment is obtained, confirming the unstrained SnX₂ is thermodynamically and dynamically stable. The calculated bond length and formation energy of SnO₂ have the minimum values followed by SnS₂, SnSe₂, and SnTe₂, but the order of Young's modulus is reversed. When external strain is applied, the energy gap of 1T-SnO₂ decreases linearly with a slope up to -0.16 eV/1%. And we contribute the energy gap modulation to the strain induced orbital redistribution of the decomposition of the p orbital of X atom and s, p orbitals of Sn atom. Moreover, the SnX₂ undergoes a semiconductor-metal transition within elastic deformation region in this study. Our results reveal that the structural and electronic properties of Sn-based materials could be modulated effectively by external strain, which may have great potential applications in elastic devices.

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Appendix A. Supplementary data

Supplementary material related to this article can be found, in the online version, at doi:<https://doi.org/10.1016/j.materresbull.2019.110533>.

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