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Hu, Fafei; Ye, Huaiyu; Tang, Hongyu; Chen, Xianping

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Modulation of Gas Adsorption on SnS by strain

Fafei Hu
College of Optoelectronic Engineering, Chongqing University
Chongqing, China
fangfei3247@126.com

Huaiyu Ye*
College of Optoelectronic Engineering, Chongqing University
Chongqing, China
huaiyuye@cqu.edu.cn

Hongyu Tang
Electronic Components, Technology and Materials, Delft University of Technology,
Delft 2628 CD, Netherlands.

Xianping Chen
College of Optoelectronic Engineering, Chongqing University
Chongqing, China

***Abstract*—SnS monolayer has sparked intensive attention due to its unique electronic and optical properties. We systemically investigate the electronic properties of SnS by first-principles calculation. Our results show that the monolayer possesses indirect bandgap. We further perform mechanical strain to adjust the electronic structure of SnS, corresponding results display an indirect-direct transition of band gap when subjected to proper external strain. Interestingly, the bandgap can be linearly increase under tensile strain from 0% to 7%, while the bandgap reduced under compressive strain. For biaxial strain, the band gap changes more remarkable compared with that under uniaxial strain (zigzag x or armchair y direction). Furthermore, we demonstrate that the gas molecules (CO_2, H_2S, C_2H_4 and NO_2) adsorption property on SnS monolayer can be modulated through biaxial strain. Especially, the NO_2 adsorption is further enhanced on the SnS monolayer under biaxial tensile strain. These results may provide guidance for fabricating SnS-based strained gas sensor.**

Keywords—first-principle; SnS; strain; gas sensors.

I. INTRODUCTION

Owing to their high carrier mobility and large surface-to-volume ratio [1], two-dimensional (2D) atomic-layer materials have great potential applications. More recently, phosphorene, with high carrier mobility (1000 $cm^2V^{-1}s^{-1}$) and band gap of 1.5 eV and thus be a good candidate for FET devices [2]. Furthermore, isoelectronic counterparts of BP such as the group-IV monochalcogenides have attracted researchers' attention [3]. Among them, tin monosulfide (SnS) is a layered semiconductor, has sparked intensive interest. Owing to its nontoxic elements and optical band gap (1.3 eV), SnS has been used as absorber material [4]. Theoretical and experimental works have reported on electronic and optical properties of few layer SnS [5]. For example, the SnS monolayer can be used as NO_2 sensor, and the outstanding sensing property is based on molecule acting as charge acceptors. External mechanical strain is one of the common methods for tuning electronic properties of 2D material. Thus it is of great significance to understand the change of SnS' electronic structure under external strain. In addition, is the adsorption properties of molecule on SnS be modulated through mechanical strain?

Here, we investigate the above problems by first-principle calculation. We further study the change of adsorption energy by gas adsorbed on the strained SnS. It is found that the electronic structure can be adjusted significantly by biaxial strain. Especially, NO_2 adsorption on the strained SnS is further enhanced under biaxial strain. Our research attempts to design an efficient methods to adjust the bandgap of SnS on a large scale, and provide guidance for designing of SnS-based nanoscale devices.

II. METHODS

All the calculations are carried out by Materials Studio software. The GGA with PBE functional are adopted. To better describe the weak van der Waals (vdW) interaction, the DFT-D proposed by Grimme is employed. The maximum displacement and maximum force was set to be 1.0×10^{-3} Å and 0.002 Ha $Å^{-1}$, respectively. A $3\times3\times1$ supercell with an adequate 20 Å vacuum region was introduced to prevent the interactions between the adjacent layers.

III. RESULTS AND DISSCUSION

The SnS monolayer has an orthorhombic structure with one unit composed by 4 Sn and S atoms (see Fig.1 (a)). Energy band calculation (Fig.1(b)) shows that SnS monolayer has an indirect band gap of 0.968 eV with the conduction band minimum (CBM) lies between Γ and M while the valence band maximum (VBM) sitting between Γ and G points. Furthermore, it is found that the pristine SnS is a *p*-type semiconductor. Furthermore, as shown in Fig.1(c), the PDOS analysis suggesting that the valence bands near the Fermi level is contributed by the Sn s, Sn p and S p orbitals, while the conduction band only originates from Sn p orbitals. Besides, we note that the Sn s and Sn p orbitals has partial overlapped in the valence band, indicating the occurrence of orbital hybridization.

External mechanical strain can modulate and optimize the optoelectronic properties of 2D materials. For example, applying biaxial tensile strain along the

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layer stacking direction to bulk SnS can tailor the optoelectronic properties [6]. We next investigate the modulation of band structure by applying strain. Applying strain in zigzag (x) and armchair (y) directions. The strain is carried out by fixing one lattice constant and changing the other.

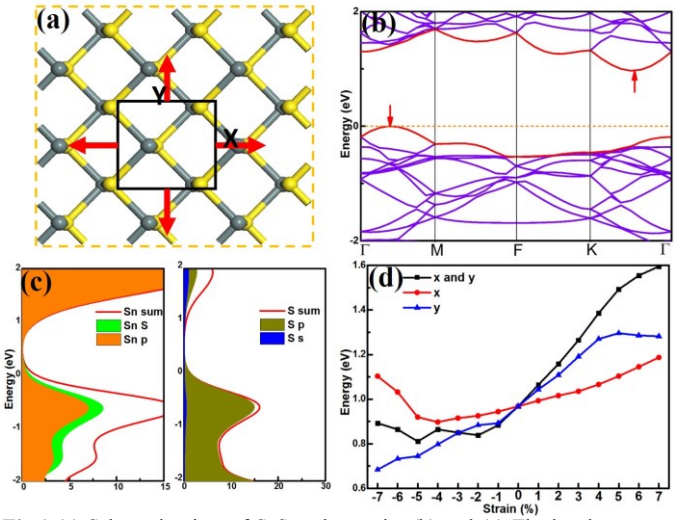

Fig.1 (a) Schematic view of SnS under strain. (b) and (c) The band structure and density of state (DOS) of SnS. (d) Band gap of SnS under strain.

The band structure is shown in Fig. 1d, it can be seen the electronic structures vary significantly by strain. For strain applied to the x direction, the bandgap linearly increases when strain increases from 0 to 7%; for compressive strain, the bandgap linearly decreases when compression ratio increases from 0 to -4%, then increases. When the compressive ratio reaches to -7%, the electronic bandgap increases to 1.103 eV, which increases by 0.135 eV as compared with the freestanding SnS. Similarily, we also applying uniaxial strain to the y direction. The results exhibit that bandgap linearly decreases when the compressive strain increases from 0 to -7% and linearly increases for tensile strain increases from 0% to 5%. When the strain is 5%, band gap is 1.296 eV, however, the bandgap decreases to 1.286 eV at the stretch ratio of 6%. In the case of biaxial tensile strain, increases linearly in bandgap can be observed. However, the bandgap decreases at first then increases at the critical compressive strain of -5%.

Better understanding the variations in the bandgap of SnS by biaxial strain, some typical electronic structures under biaxial strain are plotted. As shown in Fig. 2, when the compression strain is -5%, the electronic bandgap decreases to 0.810 eV. However, when the compressive ratio increases to -7%, the bandgap increases to 0.892 eV, which decreases by 0.076 eV compared with the freestanding one. For biaxial tensile strain, when the strain is 5%, the bandgap increases to 1.493 eV, indicating the indirect characteristic is robust. However, when the stretch radio increases to 6%，the VBM and CBM locate on the same G-Z path, suggesting the direct electronic structure with bandgap of 1.555 eV. When the compressive strain is 7%, the bandgap is up to maximum value, 1.596 eV. Therefore, we find that SnS experiences indirect-direct transition under a small critical strain.

To study the impact of biaxial strain on adsorption properties, the adsorption energy of gas molecule on strained SnS (biaxial compressive (-7%) and tensile (7%)) were examined and contrast with the results of pristine one (Fig. 3a). Note that NO_2 adsorption shows highly sensitive to strained SnS. Under the compressive strain, the adsorption energy decreases significantly, while adsorption energy increases dramatically under tensile strain. For CO_2, H_2S, and C_2H_4, the adsorption energy enhanced under strain. This phenomenon of the NO_2 toward strain is ascribed to the adsorption configurations..

Fig.3(b) presents the adsorption energy of NO_2 changes with biaxial tensile strain from -7% to 7%. It is worth noting that biaxial strain results in a gradual decrease in adsorption energy. In contrast, application of biaxial compressive strain will enhance NO_2 adsorption, which is manifested by the increase in adsorption energy. Therefore, we conclude that NO_2 adsorption is dependent on strain. These findings will provide theoretical guidance for fabricating strain gas sensor.

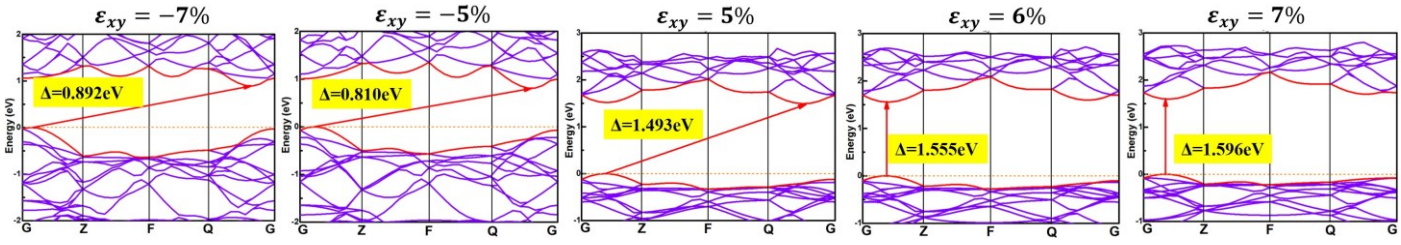

Fig.2 Electronic structure of SnS under -7%, -5%, 5%, 6% and 7% biaxial strain.

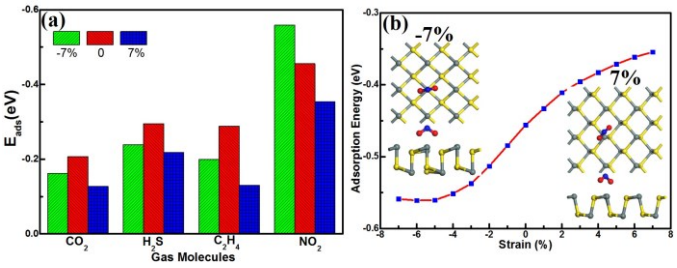

Fig.3 (a) Adsorption energy of CO_2, H_2S, C_2H_4 and NO_2 gas molecules on strained SnS (-7%, 0, and 7%). (b) Change of adsorption energy as a function of strained SnS. Inset shows the adsorption configuration of NO_2-adsorbed SnS system under -7% and 7%.

IV. CONCLUSION

In this work, we perform systemically a first-principles study on the electronic properties of SnS monolayer. It is found that SnS has an indirect band gap of 0.968 eV. In addition, we preform mechanical strain to adjust the electronic structure of SnS, corresponding results display an indirect-direct transition. In addition, the adsorption properties of gas molecule on SnS can be significantly enhanced by biaxial strain. And NO_2 adsorption is highly dependent on biaxial strain. Our theoretical study found that strained SnS monolayer is a good candidate for gas sensing. Our work offers a valuable reference for fabricating SnS-based strain gas sensors.

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