Electronics Structure of Monochalcogenide Materials MX (M = Ge, Sn and Pb; X = S and Se) Buckled Square Lattice

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Electronics Structure of Monochalcogenide Materials MX (M = Ge, Sn and Pb; X = S and Se) Buckled Square Lattice

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Abstract. The electronics structure of monochalcogenide materials buckled square lattice is investigated by computation based on Density Functional Theory (DFT). The investigation shows that there is spin splitting on xy-plane at Γ point and M point as a Rashba effect. Perturbation theory **k.p** and symmetry group C_{2v} used to calculate the originates of the spin splitting. The results show that there are strong Rashba splitting for materials with center atom Pb (with Rashba parameter 5~ eVÅ). Spin orientation displayed by spin-texture and show that there is time reversal symmetry between upper band and lower band. This condition explains that monochalcogenide materials buckled square lattice as potential candidates for spintronics devices.

Keywords: electronics structure, monochalcogenides, square lattice, Rashba effect, spin texture.

1. Introduction

Material development for spintronics devices has been a concern in recent years [1–7]. Various studies to develop the spintronics devices have been carried out. Materials that can be used in spintronics devices are materials that have a spin-orbit interaction, there is spin polarization, and allows spin transportation [1]. The suitable materials generally have the Rashba effect properties. Materials with strong Rashba effects have advantages when applied in the spintronics devices. Devices can be developed smaller in size and easier in tuning electrons spin. Another advantage is that spin of the materials can be controlled by electric field [1]. In addition, the results of the study indicate that the nature of the Rashba effect applies to room temperature. This makes the materials with the Rashba effect properties very likely to be applied in devices.

One of the materials that has a potential to have a Rashba effect is monochalcogenide material [8]. In general, monochalcogenide materials have an orthorhombic structure in bulk phase and zigzag in low dimensions (2D) [9]. Based on the model, monochalcogenide materials can also be arranged into a square lattice [8]. The area of a square lattice unit cell is $a \times a$ with a is the length of the side of the unit cell. In a square lattice, there are two atoms in one unit cell. Square lattice stability occurs when there is a bend in a two-dimensional structure for monochalcogenide materials. The buckled on square lattice causes breaking symmetry in the crystals. Due to the symmetry breaking, the Rashba effect appears

because of the internal electric field. The electric field rises from electron charges. The direction of the electric field is perpendicular to the lattice plane. The Rashba effect occurs on Γ-points and M -points in Brillouin zone. The Rashba effect is a unique spin splitting that applies when energy $\varepsilon(k) = \varepsilon(-k)$ with k is wave vectors. By knowing this situation it will be possible to develop spintronics devices that can be switch by an electric field. On the other side, this research shows that the square lattice materials are possible to develop.

2. Methods

In this model, the geometry structure of monochalcogenide materials is defined as a square lattice. So that the Brillouin zone in k-space is a square [Figure 1(c)]. The side of the Brillouin zone is $a^* = 2\pi/a$. Electronic structure calculations were carried out around the high symmetry point in the first Brillouin zone. The calculations were carried out using density functional theory (DFT) within the general gradient approximation (GGA) were implemented in the OpenMX code [10]. OpenMX code is a programming package based on density functional theory (DFT) that has been accepted in publication for the entire scientific community [11]. The definition calculation system 16 × 16 × 1 k-grid and 300 K temperatures are used in the code. The material layer is modeled by giving an inter-surface vacuum of 25 A in order to avoid interaction between other layers.

3. Results and Discussion

The results showed that the square lattice structure was consistent with the model as shown in Figures 2 (a). Based on the calculation, the lattice parameter results are consistent with the results of previous calculations as shown in Table 1. In addition, the calculation shows that the bending height d_z (Figure 2.(b)) is relatively the same as previous studies [8].

Table 1. The lattice constant (*a)*, the bending height (*d_z)* and the bending angle (*θ)* for the monochalcogenide material buckled square lattice.

	Calculation			Reference			
	a (Å)	d_z (Å)	$\theta(^o)$	*a* (Å)	d_z (Å)	$\theta(^o)$	
GeS	3.31002 ± 0.5 %	1.10868	25.35		-		This work
GeSe	3.45709 ± 0.4 %	1.18338	25.83		-		This work
SnS	3.54560 ± 0.3 %	1.18601	25.32		-		This work
SnSe	3.67610 ± 0.4 %	1.27148	26.07		-		This work
PbS	3.76372 ± 0.4 %	1.08425	22.17	3.74	1.0471	21.6	Ref [8]
PbSe	3.85410 ± 0.4 %	1.20871	23.92	3.82	1.0695	24.4	Ref [8]

The square lattice structure in the material has not been confirmed through of experiments. Some of the materials have not been studied through a computation for the square lattice model, so this research can be used as a reference. Electronics structures calculations are carried out at high symmetry points in the Brillouin one. Path selection is done by strings of X − Γ − X − Y − Γ − Y − M − Γ − X. The result of the energy for PbS shown in Figure 2(d).

The results in Figure 2(d) show that monochalcogenide materials of the lattice is semiconductor material with an indirect band gap and has the properties of the Rashba effect. The Rashba effect that occurs is anisotropic and symmetry at X − Γ − X and Y − Γ − Y directions [Figure 2(d)]. The result of calculation Rashba parameters is shown in Table 2. The Rashba parameter for PbS and PbSe square lattice relatively greater than other (more than 5 eVÅ at M-point), and it was compared with the other value research [3].

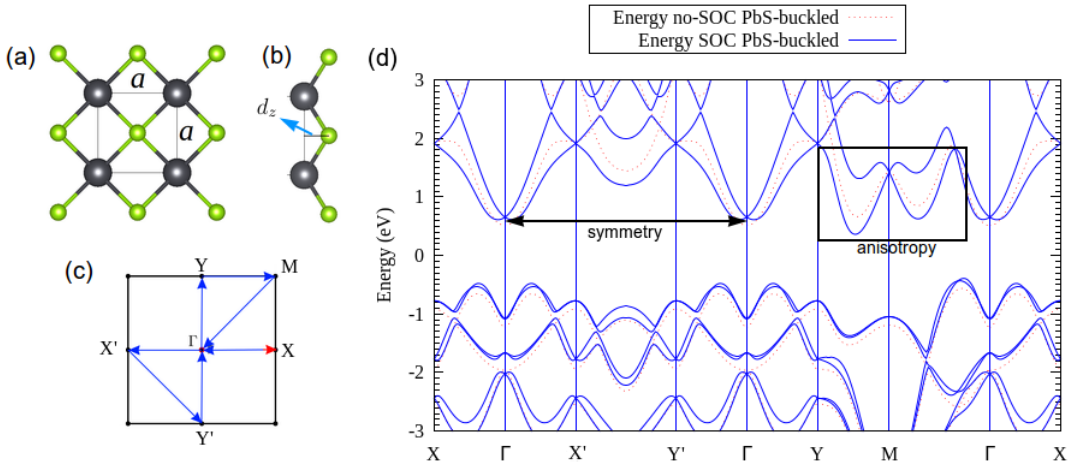

Figure 1. (a) Square lattice structure in monochalcogenide materials with lattice constant *a*. Yellow is one of the chalcogen atoms and grey is one of grup 14 atoms. (b) The form of bending seen from the side with bending height d_z, (c) The first Brillouin zone for square lattice and some high symmetry point, and (d) energy band for PbS material by path $X-\Gamma-X'-Y'-\Gamma-Y-M-\Gamma-M$

Table 2: The fittings result of Rashba parameter (α_R) for monochalcogenide materials square lattice with analysis by perturbation theory **k.p** for point group C_{2v}.

	Fitting result ($eVÅ$)		Reference ($eVÅ$)		
	Γ-point	M-point	Γ-point	M-point	
GeS	0.379	1.102			This work
GeSe	0.605	0.885			This work
SnS	0.810	4.49			This work
SnSe	1.036	3.30			This work
PbS	1.993	5.29	1.03	5.10	Ref [8]
PbSe	2.48	5.40			This work

The equation that used to calculate (fitting) the Rashba parameters in Table 2 is

$$(\Delta\varepsilon)^2 = 4(\alpha_1^1 k_x + \alpha_1^3 k_x^3 + \alpha_1^3 k_x k_y^2)^2 + 4(\alpha_1^2 k_y + \alpha_2^3 k_x^2 k_y + \alpha_3^4 k_y^3)^2 \quad (1)$$

where Δε is band gap between upper band and lower band, $k_x = |k|\cos\theta$ is wave number for x-axis in Brillouin zone, $k_y = |k|\sin\theta$ is wave number for y-axis in Brillouin zone and α is some constant that represents the Rashba parameter with a different order. This equation is the result of analysis perturbation theory **k.p** in group symmetry C_{2v} [5]. Equation 1 represents the third order for Hamiltonian systems. The structure of the spin orientation of the material shows that electron spin is helical, and there is a time reversal symmetry between the upper band and lower band. Spin texture shows spin orientation following a square shape. Other results Figure 2 (a) show that the spin orientation of the electrons full in plan.

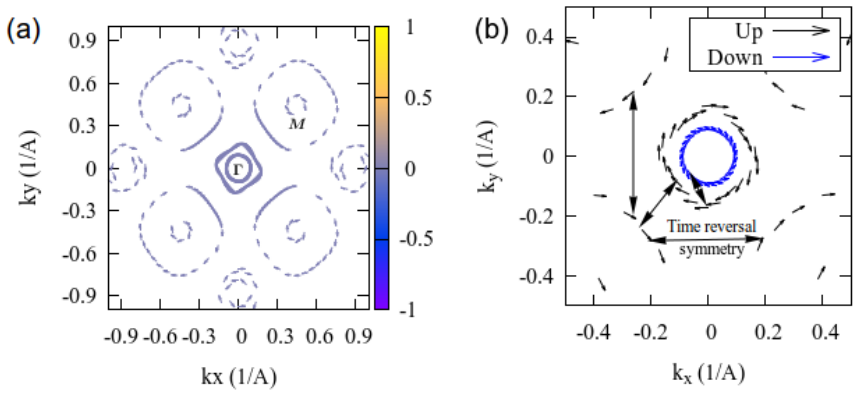

Figure 2. (a) Color represent the spin orientation of the z-axis direction and show that the orientation full in plane, and (b) shows that spin orientation between spin-up and spin-down is helical and there are times reversal symmetry around the states.

Mathematics analysis using **k.p** theory for point group $\mathbf{C_{2v}}$ [5] get the difference of eigenenergy between the lower and upper bands as shown in equation (1) for third-order Rashba parameters. By using the eigenvalue equation the wave function can be determined so that the eigenvalue for spin orientation is [12].

$$S_{\uparrow x} = -S_{\downarrow x} \tag{2}$$

$$S_{\uparrow y} = -S_{\downarrow y} \tag{3}$$

The equation (2) and equation (3) show that there is opposite direction (as time reversal symmetry) for spin orientation electron in the upper and lower bands. The result of this analysis is consistent as shown in Figure 2 (b). On the other side,

$$S_{\uparrow z} = -S_{\downarrow z} \tag{4}$$

the equation (4) shows that there is no orientation along the z-axis (it was full in the plane), this analysis confirms the result as shown in Figure 2 (a) is consistent [12]. The result of the analysis with **k.p** theory in this research is consistent compared to the analysis with tight bending as done by the previous research [8]. It shows that the monochalcogenide square lattice materials have the opportunity to develop. The development of these materials can be used in the development of spintronics devices.

4. Conclusion

The results show that there are Rashba effects on monochalcogenide materials buckled square lattice at Γ-point and M-point in the Brillouin zone. This occurs because of the Rashba properties in monochalcogenide materials have the opportunity to be used in spintronics devices. This is because it has a large Rashba parameter especially material with Pb as central atom.

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