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Unidirectional out-of-plane spin textures in two-dimensional group-IV monochalcogenide *MX* monolayer for persistent spin helix

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Abstract

Spin textures in the momentum *k*-space induced by spin-orbit coupling (SOC) plays an important role for inducing spin precession and spin-polarized currents in the spintronic devices. However, the *k*-dependent of the spin textures causes decoherence of electron spins in nonbalistic transport, making spin lifetimes too short for practical purposes. Here, we show from first-principle calculations that two-dimensional group-IV monochalcogenide *MX* monolayer having in-plane ferroelectricity can host persistent spin textures in the out-of-plane orientations, where spin configurations are independent from the *k*, potentially ensuring an extremely long spin lifetime in this materials. Finally, the spin-orbit strength parameters and wavelength of the spin-polarization are estimated, rendering that these systems are promising for spintronics.

1. Introduction

Recently, development of spintronics relies on the new pathway for exploiting carrier spins in semiconductors by utilizing the effect of spin-orbit coupling (SOC). However, in a system with lack of inversion symmetry, the SOC induces momentum *k*-dependent of the spin textures and breaks spin rotation symmetry, implying to the fast spin decoherence through Dyakonov-Perel spin relaxation mechanism [1]. As a result, the spin lifetime significantly decreases, playing a detrimental role in losing spin information. To overcome this problem, finding a novel structures supporting an extended spin lifetime is important task, which is achievable by using persistent spin helix (PSH) materials [2].

The key concept of the PSH is to render the total effective magnetic field induced by the SOC aligning along a particular direction for the all-electron's wave vectors, and thus resulting in *k*-independent spin configuration, known as the persistent spin textures (PST) [3]. As a result, spin conservation is preserved, which is robust against both spin-independent disorders arising from impurities, defects, and Coulomb interactions [3]. The PSH has been widely studied on various quantum well systems [4,5,6,7]. However, it requires the stringent condition for fine tuning the Rashba and Dresselhauss SOC, which is practically nontrivial. In this paper, we show that the PSH can be intrinsically achieved on a two dimensional group-IV monochalcogenide *MX* monolayer, a new class of the noncentrosymmetric materials having in-plane ferroelctricity [8]. We observed the PST with unidirectional out-of-plane spin orientations having large spin-orbit parameters, suggesting that the present systems are promising for spintronic applications.

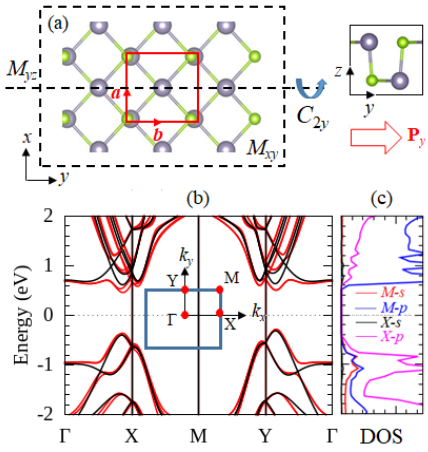

Fig. 1. (a) Crystal structures of the *MX* monolayer SnSe. Symmetry operations in the unit crystal are indicated by twofold screw rotation $\bar{C}_{2y}$; glide reflection $\bar{M}_{xy}$; and reflection M_{yz}. (b) The calculated electronic band structures of monolayer SnTe calculated without (black) and with (red) the SOC. (c) The calculated density of states projected to the atomic orbitals are shown.

2.Method

In our DFT calculations, we used the OpenMX code [9] where the wave functions were expanded by a linear combination of pseudoatomic orbitals (LCPAOs) utilizing a confinement scheme. The black phosporene-type structures is used for the *MX* monolayer with symmetry operations are shown in Fig. 1(a). Here, the symmetry group is isomorphic to C_{2v}^{7} or $Pmn2_1$ space group [8].

3. Results and discussion

Fig. 1(b) shows band structures of SnTe monolayer as a representative example of the *MX* monolayer. There are two equivalent extrema valleys characterizing valence band maximum (VBM) and conduction band minimum (CBM) located at the points that are not time reversal invariant. The VBM is mainly contributed from the Sn-*s* and Te-*p* orbitals, while the CBM originates from the Sn-*p* and Te-*s* orbitals [Fig. 1(c). Importantly, we observed a sizable spin splitting of the band dispersions when the SOC is turn on. However, there are special high-symmetry lines and points in the first Brillouin zone, where the splitting is absence. In particular, the case for Γ-Y line, where the wave vector ***k*** is parallel to the ferroelectric polarization along the *y* direction.

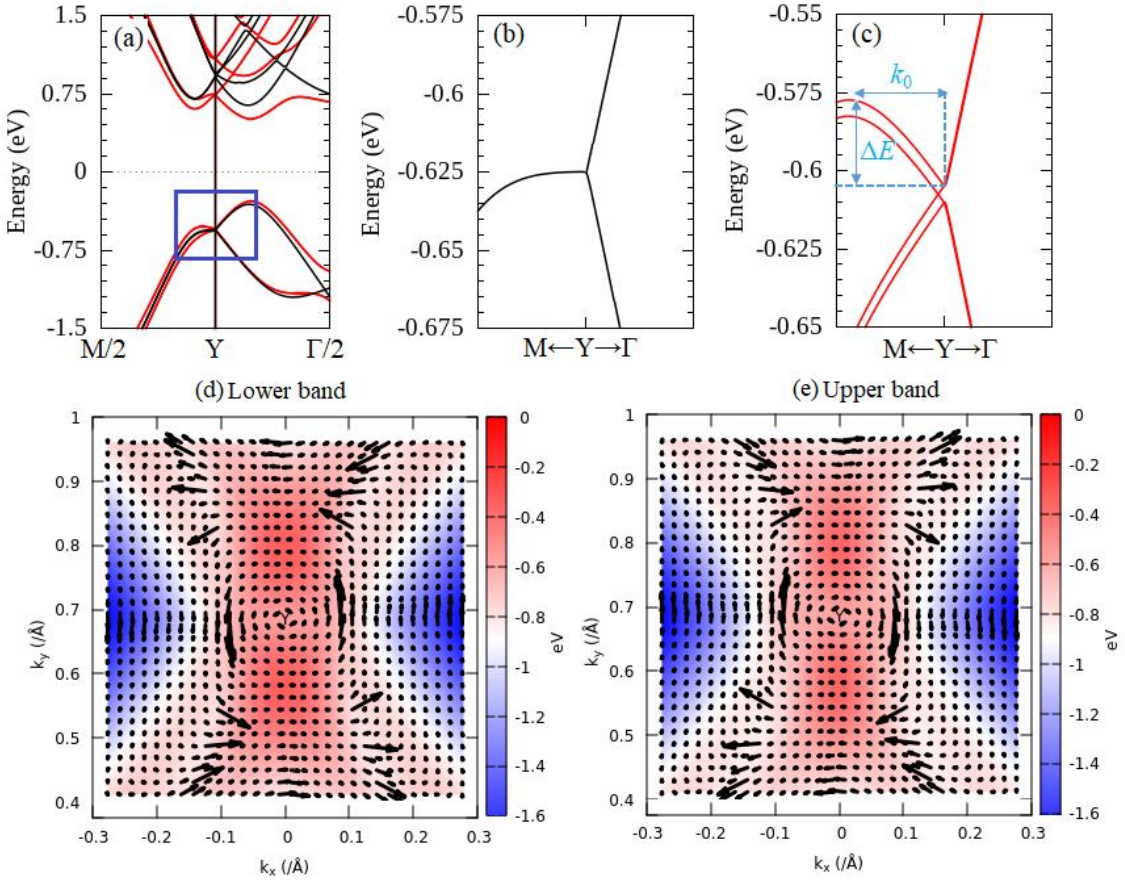

Fig. 2 (a) Spin-split bands of SnTe monolayer along the M-Y-Γ lines. Black and red lines indicate the band structures calculated without and with the SOC, respectively. Spin-split bands close to the Y point calculated (b) without and (c) with the SOC are shown. The spin split bands are characterized by (i) splitting energy (ΔE), i.e., different energy between the VBM and the energy level at the Y point in the valence band, and (ii) momentum offset (k_0). The calculated spin textures around the Y point near the valence band maximum for (d) lower and (e) upper bands. Color scale indicates the energy of the bands.

Now, we focus our attention on the VBM (including spin) around the Y point as highlighted in Fig. 3(a). Without the SOC, it is evident from the band dispersion that fourfold degenerate state appears at Y point [Fig. 3(b)]. Taking into account the SOC, this degeneracy splits into two pair doublets with the splitting energy of ΔE_Y = 9.2 meV [Fig. 3(c)]. These doublets remain unchanged for the $\boldsymbol{k}$ along the Γ-Y line, while they split into a singlet when the $\boldsymbol{k}$ moves away along the Y -M line, thus inducing a highly anisotropic spin splitting. Our spin textures calculations at the VBM around the Y point confirmed that unidirectional out-of-plane spin configurations are observed [see the red region in Fig. 2(d)-(e)], indicating that that the PST is achieved, which is expectable to induce long spin lifetime through PSH mechanism [2]. By analyzing the band splitting along the Y-M line [Fig. 2(c)], we estimated the spin-orbit parameter α using the formula: $\alpha = 2E_R / k_0$, and find that α=1.2 eVÅ. The large value of α is important for operation of spintronic devices at room temperatures.

4. Conclusions

We have investigated the spin-splitting properties of the *MX* monolayer by using DFT calculations. We find strongly anisotropic spin splitting in the VBM, preserving the PST in the out-of-plane orientations. Our study clarify that the *MX* monolayer can be used as an ideal PSH material, potentially ensuring a very long spin lifetime, thus promising for energy spintronic applications.

Acknowledgments

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