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Tunable spin splitting and spin relaxation in polar WSTe monolayer

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Abstract

The established spin splitting with out-of-plane Zeeman-like spin textures in the monolayer (ML) of transition metal dichalcogenides (TMDs) are dictated by inversion symmetry breaking and mirror symmetry. Here, by sing density-functional theory calculations, we show that polarity-induced mirror symmetry breaking in the WSTe ML leads to large spin splitting exhibiting in-plane Rashba-like spin textures. Interplay between the out-of-plane Zeeman-like and in-plane Rashba-like spin textures plays a significant role in the spin relaxation, which is effectively tuned by the polarity, and thus useful for designing spintronic devices.

1. Introduction

Recently, monolayer (ML) of transition metal dichalcogenides (TMDs) is promising materials for spintronics because of their properties such as spin-valley coupled electronic structures [1]. The TMDs ML belongs to D_{3h} point group, and together with strong spin-orbit coupling (SOC) in the 5*d*-orbitals of transition metals atoms give rise to large spin splitting [2]. Additionally, mirror symmetry operation in the D_{3h} point group suppresses the spin splitting to exhibit fully out-of-plane spin polarization, inducing strongly enhanced spin relaxation time [2]. However, new electronic properties for spintronics may appear by breaking this mirror symmetry, which can be realized by using the polar *MXY* structures. In this paper, we proposed to use the WSTe ML to clarify the effect of the mirror symmetry breaking on the properties of spin splitting and spin relaxation.

The D_{3h} point group consists of a threefold rotations C_3 around the trigonal z axis and two mirror symmetry operations in the x-y plane ($M_{x\text{-}y}$) and y-z plane ($M_{y\text{-}z}$) [Fig. 1(a)]. In the WSTe ML, the mirror symmetry $M_{x\text{-}y}$ is broken, thus the symmetry becomes C_{3v} [Fig. 1(b)]. This mirror symmetry breaking originates from the polarity induced by out-of-plane distance difference between transition metal (W) and chalcogen (S,Te) atoms defined as $\Delta d_{\perp}=|d_{\perp\text{W-S}}-d_{\perp\text{W-Te}}|$.

We performed density-functional theory (DFT) calculations within the generalized gradient approximation and norm-conserving pseudopotentials using the OpenMX code [3]. The wave functions were expanded by linear combination of pseudoatomic orbitals (LCPAOs) specified by W7.0-$s^2p^2d^2f^1$, S9.0-$s^2p^2d^1$, and Te9.0-$s^2p^2d^2f^1$ generated using a confinement scheme [4]. The SOC was included in our DFT calculations. A slab model with vacuum layer of 25 Å was used. We find that the optimized lattice constant is 3.37 Å, which is larger than that of the WS_2 ML (3.18 Å) [2]. We characterize the degree of the polarity by evaluating $\Delta d_{\perp}$. In contrast to the WS_2 ML ($\Delta d_{\perp}$=0), we find that $\Delta d_{\perp}$=0.397 Å in the WSTe ML, indicating that this system is polar.

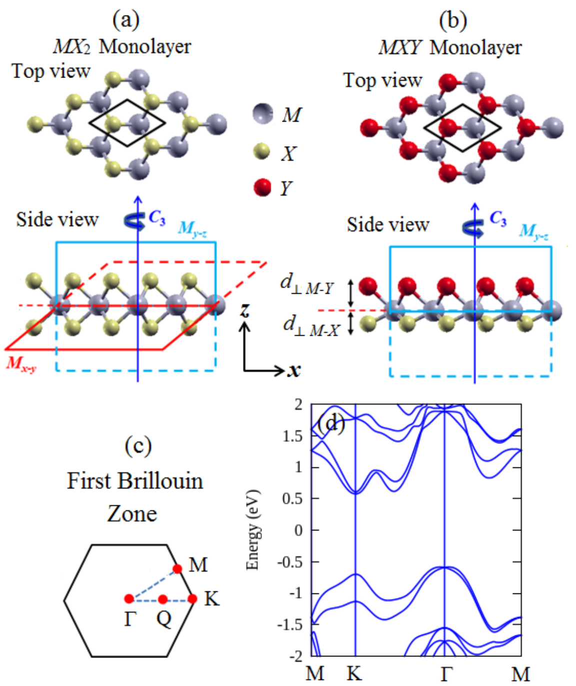

Fig. 1. Crystal structures of (a) MX_2 and (b) *MXY* monolayers. C_3 rotation and mirror symmetry [$M_{x\text{-}y}$ and $M_{y\text{-}z}$] operations are indicated. (c) The First Brillouin zone is shown. (d) The band structures of the WSTe ML with the SOC is given.

2. Results

Fig. 1(d) shows the electronic band structures of the WSTe ML along the first Brillouin zone [Fig.

1(c)]. Due to the absence of inversion symmetry, a substantial spin splitting is established. In contrast to the non-polar MX_2 ML [3], the spin degeneracy along the Γ-M direction is lifted due to the broken of the mirror symmetry $M_{x\text{-}y}$ [Fig. 1(d)]. We find that the spin splitting up to 0.53 eV eV is achieved at the K point in the valence band maximum (VBM), which is slightly larger than that observed on the WS_2 ML (0.43 eV) [4]. Interestingly, a large spin splitting is observed around the Γ point, referred as the Rashba-like splitting [5,6]. Because the energy level of the K and Γ points is close, interplay of their spin splitting plays an important role for controlling the spin relaxation.

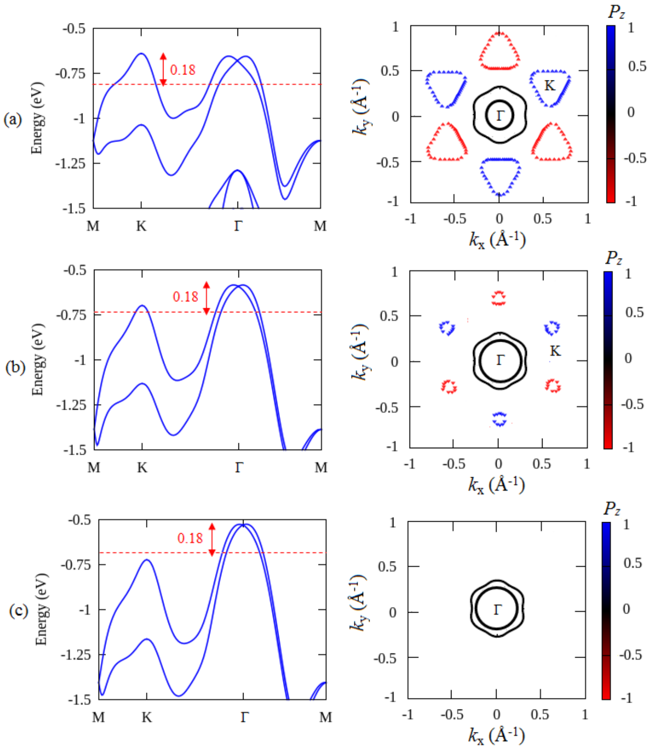

Fig. 2 Valence band maximum (VBM) and the spin textures for (a) compressive strain, (b) equilibrium, and (c) tensile strain. The colour scale in the spin textures represent the out-of-plane spin polarization (P_z).

To clarify the effect of the spin splitting on the spin relaxation, we here study the spin textures of the WSTe ML under the influence of the biaxial strain. Here, we focus on the spin splitting properties in the VBM because of the large spin splitting. As shown in Fig. 2, strong enhancement of the spin splitting is achieved around the Γ point under the compressive strain, while it is visible around the K point when the tensile strain is introduced. Importantly, these strains also shift the energy level of the VBM from the Γ to K points, which strongly modifies the features of the spin textures. By considering the spin textures located on 0.18 eV below the VBM, sixfold symmetry of spin-split hole pockets are observed in the equilibrium as well as the strained systems. In the equilibrium system, the hole pockets are characterized by out-of-plane Zeeman-like spin polarization around the K point and in-plane Rashba-like spin polarization around the Γ point [Fig. 2(b)], inducing spin-orbit field in the out-of-plane ($B_{\perp}$) and in-plane ($B_{//}$) orientations, respectively. Because the spin splitting around the Γ point is much smaller than that of the K point, small misalignment of the total spin-orbit fields (B_{tot}) from the out-of-plane orientation is achieved. Accordingly, Dyakonov-Perel mechanism implies that the spin relaxation times are much longer than that intervalley scattering times. However, the increase Rashba like spin spitting around the Γ point under compressive strain [Fig. 2(a)] enhances intervalley scattering times. Finally, the long intervalley scattering time is achieved by the tensile strain since the spin textures are dominated by the in-plane Rashba-like spin polarization [Fig. 2(c)]. Therefore, tuning the polarity by the biaxial strain in the WSTe ML is effectively controlled the spin relaxation properties, which is useful for designing future spintronic devices.

3. Conclusions

By using density-functional theory calculations, we investigate the spin splitting and spin relaxation on the WSTe ML. We find that polarity-induced mirror symmetry breaking in the WSTe monolayer induces a sizable spin splitting exhibiting in-plane Rashba-like spin textures. The interplay of the out-of-plane Zeeman-like and in-plane Rashba-like spin textures around the K and Γ points, respectively, affects the spin relaxation, which is effectively tuned by the polarity. This study clarify that the polarity-induced mirror symmetry breaking plays an important role in the spin relaxation properties of the TMDs monolayer.

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