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Doping-induce large anisotropic spin-splitting and persistent spin helix in monolayer SnSe

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Abstract

Finding persistent spin helix (PSH) materials is essential for application in energy saving spintronics. By employing first-principles calculations, we show that the PSH states are achieved on the monolayer (ML) SnSe. We find anisotropic spin splitting, which is significantly enhanced by introducing substitutional halogen doping. This spin splitting shows fully out-of-plane spin orientation, exhibiting the shift of two Fermi surface. Finally, the spin splitting, shift of the wave vector, and the wavelength of the PSH are estimated, rendering that this system is promising for spintronic applications.

1. Introduction

The recent development of spintronics relies on the new pathway for exploiting carrier spins in semiconductors by utilizing the effect of spin-orbit coupling (SOC). Here, the SOC results in momentum-dependent magnetic field $\vec{\Omega}(\vec{k})$ in term of effective SOC Hamiltonian [1]:

$$H_{SOC}(\vec{k}) = \vec{\Omega}\left(\vec{k}\right)\cdot\vec{\sigma} \qquad (1)$$

In Eq. (1), $\vec{\sigma} = \left(\sigma_x, \sigma_y, \sigma_z\right)$ is spin operator represented by Pauli matrices, and $\vec{\Omega}(\vec{k}) = \alpha\left(\vec{E}\times\vec{k}\right)$, where $\vec{E}$ is the electric field induced by crystal inversion asymmetry and $\vec{k}$ is the electron momentum.

Sinc $\vec{\Omega}(\vec{k})$ depends on the crystal symmetry; new physical phenomena may be found by controlling the crystal structures. For an instant, in the case of materials having C_{2v} symmetry, $\vec{\Omega}(\vec{k})$ can be expressed as $\vec{\Omega}_R(\vec{k}) = \alpha_R\left(-k_y, k_x, 0\right) + \beta_D\left(k_y, k_x, 0\right)$, where α_R and β_D are Rashba and Dresselhaus parameters, respectively. As a result, spin splitting in the electronic band structures is observed. Importantly, very strong anisotropic spin splitting with unidirectional $\vec{\Omega}(\vec{k})$ is achieved when $\alpha_R = \beta_D$ inducing a persistent spin helix states (PSH)[2]. When the PSH is achieved, an unusually long spin lifetime is observed, which is useful for efficient spintronic devices.

The PSH has been experimentally observed in semiconductor GaAs/AlGaAs [3] and InGaAs/InAlAs [4]. Unfortunately, achieving the PSH states requires precise control of the quantum-well with and the doping level, which is practically difficult. Recently, the PSH was also predicted for a wurtzite ZnO (10-10) surface [5] and strained $LaAlO_3/SrTiO_3$ (001) interface [6]. However, in such systems, the spin splitting is too small. Therefore, finding another class of materials exhibiting the PSH states utilizing large spin splitting is crucially important to realize spintronic devices operating at room temperatures.

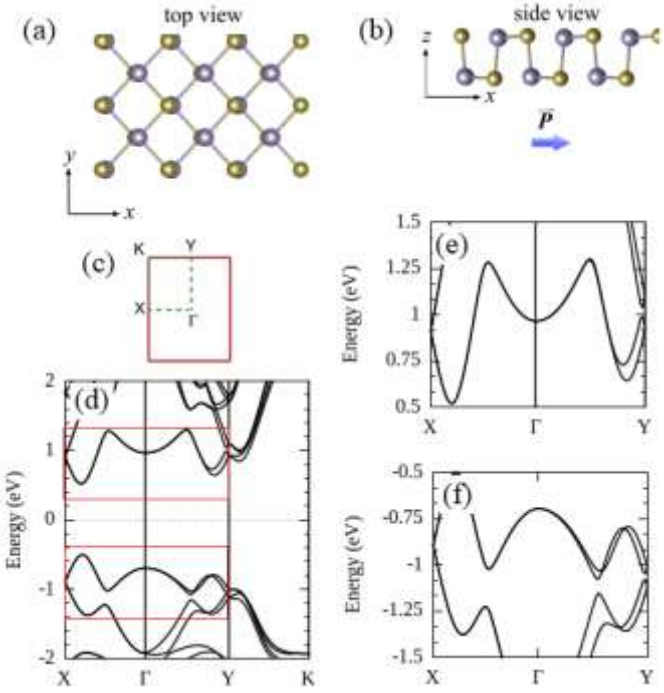

Fig. 1. Crystal structures of monolayer SnSe: (a) Top and (b) side views. (c) First Brillouin zone. (b) Electronic band structures of monolayer SnSe calculated including the effect of SOC. Spin split-bands around (e) the band minimum (CBM) and (f) valence band maximum (VBM).

In this paper, by using density-functional theory (DFT) calculations, we show that the PSH states are achieved on the monolayer (ML) SnSe. We find anisotropic spin splitting, which is significantly enhanced by introducing substitutional halogen doping. The calculated spin textures show fully out-of-plane orientation, exhibiting the shift of two Fermi surface. Finally, the spin splitting, shift of the wave vector, and the wavelength of the PSH are estimated.

2.Method

In our DFT calculations, we used the OpenMX code [7] where the wave functions were expanded by a linear combination of pseudoatomic orbitals (LCPAOs) specified by

Sn9.0-$s^2p^2d^1$ and Se9.0-$s^2p^2d^1$ generated utilizing a confinement scheme. The crystal structures of SnSe ML is shown in Figs. 1(a) and (b), while the first Brillouin zone is given in Fig. 1(c). For doping calculation, we construct 4x4 supercell consisting of 64 atoms.

3. Results and discussion

Fig. 1(d) shows the electronic band structures of the monolayer SnSe with the SOC. We find that a substantial spin splitting is observed mainly along the Γ-Y direction, while there is no spin splitting along the Γ-X direction, indicating that this system shows the anisotropic character of the spin splitting. Here, the spin splitting is 45 meV in the valley along the Γ-Y direction in the conduction band minimum (CBM) [Fig. 1(e)], while it is 22 meV in the valence band maximum (VBM) [Fig. 1(f)].

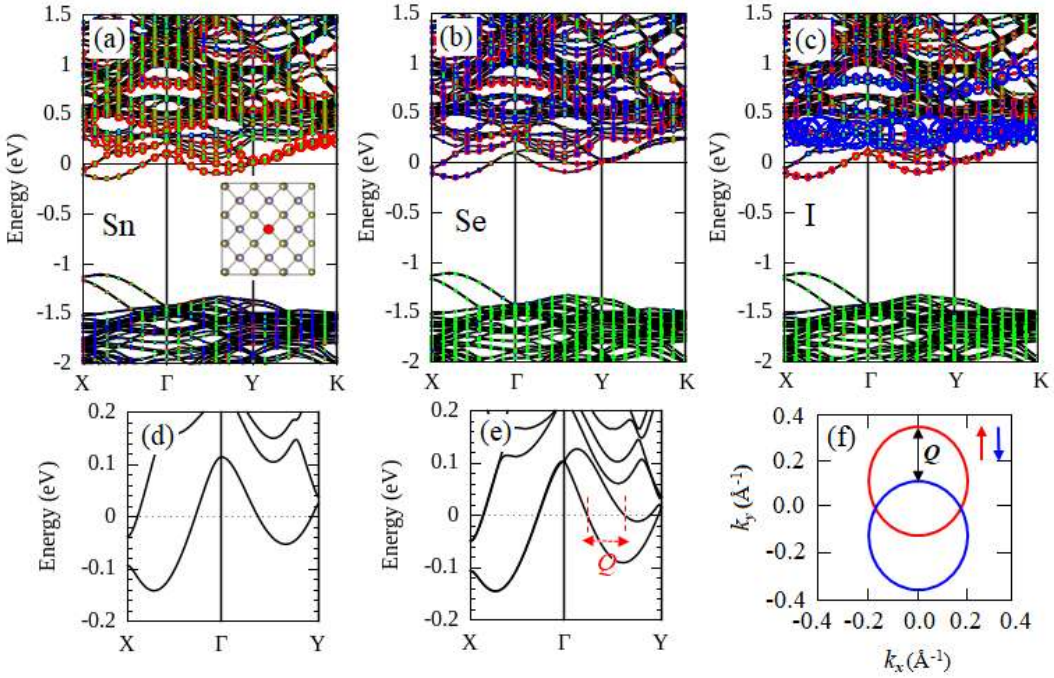

Fig. 2 Orbital-resolved electronic band structures of I-doped SnSe ML projected to: (a) Sn, (b) Se, and (c) I atoms. Red, blue, and green circles indicate *s*, *p*, and *d* orbitals, respectively. The size of the circles represents spectral weight. Electronic band structures calculated (d) without and (e) with SOC. (f) The calculated spin textures at Fermi surface. Red and blue arrows show the fully out-of-plane spin with up and down orientations, respectively.

Since the observed spin splitting is too small in the pristine system, it may limit the functionality for spintronic devices. Therefore, we introduce substitutional doping arises from halogen (Br and I) atoms. Here, we focussed on the doping located on the Se site rather than the Sn site since it has lower formation energy. Taking the I doping as a representative system, we find localized impurity states (LIS) around the Fermi level, indicating that this system is *n*-type [Figs. 2(a)-(c)]. By calculating orbital-resolved of electronic band structures projected to the atoms around the doping site, we find that the LIS at the Fermi level mainly originated from the contribution of *s* and *d* orbitals of Sn, *s* and *p* orbitals of Se, and *s* and *p* orbitals of I.

Importantly, we find large spin splitting (up to 0.14 eV) in the LIS along the Γ-Y direction at Fermi level [Figs. 2(d)-(e)]. This splitting shows a unidirectional fully-out-of plane spin textures [Fig. 2(f)], exhibiting the shift of the wave vector $\boldsymbol{Q}$ = 0.18 Å^{-1} and corresponding to the wavelength λ_{PSH} = 3.4 nm. The small λ_{PSH} and large spin splitting found in the present system is important for miniaturization of spintronic devices operating at room temperatures.

4. Conclusions

We have investigated the PSH in monolayer SnSe. We find anisotropic spin splitting, which is significantly enhanced by introducing substitutional halogen doping. We also confirmed the fully out-of-plane spin textures, exhibiting the shift of the Fermi surface. Finally, the spin splitting, shift of the wave vector, and wavelength of the PSH are estimated, rendering that this system is promising for energy saving spintronics.

Acknowledgments

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