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Giant spin–orbit splitting in ultrathin Ir(111) film

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ABSTRACT

Spin–orbit (SO) splitting in ultrathin Ir(111) film was examined on the basis of density functional theory. The states with giant SO splitting can be found in few-monolayer Ir film terminated by H atoms. They distribute in several bands. From projected wave function study, the giant SO splitting is mainly induced by the p_z and d_{yz} states. The origin of this orbital dependence is analyzed by the distribution of states on the film. The stability of states is also discussed when the Ir surface is covered with graphene or graphone (half-hydrogenated graphene). The hybridization of energy bands greatly influences the large SO splitting and the persistence of states.

1. Introduction

Spin–orbit (SO) interaction can be used to manipulate the spin of electrons even without the need of external magnetic fields [1]. It leads to many interesting effects in experiments or proposed in theories, such as spin Hall effect [2], quantum spin Hall effect [3], and topological insulating behavior [4,5]. Generally, SO strength in metal surfaces or metal films can be much larger than that in semiconductor heterostructures [6–8]. In fact, giant Rashba SO splitting [9,10] was detected in several kinds of metal surfaces or the metal films grown on certain substrates [11–13]. A giant Rashba effect on the Ir(111) surface state was also revealed by angle-resolved photoemission and by density functional theory (DFT) [14]. The Ir(111) surface state with giant Rashba splitting can persist in ambient atmosphere when the Ir surface was protected by a graphene overlayer. The persistence of the surface state in air would be helpful for the practical application of the strong SO interaction. In Ref. [14], A. Varykhalov et al. used a 15-monolayer (ML) thick Ir film to calculate the SO splitting of the Ir(111) surface state. Their density functional calculations confirmed the presence of the surface state. They also found that the Ir(111) surface state with giant SO splitting possesses p_z-like orbital character close to the Γ point and d_{yz}-like character [15] away from Γ. However, the detailed orbital character of the surface state and the origin of the orbital dependence of the giant SO splitting are unclear. In addition, more discussions are also necessary in order to clarify the reason for the persistence of the surface state under overlayer.

In the present work, we find that the giant SO splitting of the Ir(111) surface state can be also produced in the Ir film with few atomic layers, when one of the sides of the ultrathin film is terminated by H atoms. The states with giant SO splitting distribute in several bands. From projected wave function study, the giant SO splitting is mainly induced by the p_z and d_{yz} states. This orbital dependence is from the asymmetric distribution of the states on the film as the distribution of surface states. The stability of states is also discussed when the Ir surface is covered with graphene or graphone (half-hydrogenated graphene) [16]. Graphene has little influence on the SO splitting due to the weak Ir–graphene interaction. However, graphene has a substantial effect on the states, even when the layer distance is as large as 4.5 Å. The hybridization of energy bands greatly influences the large SO splitting and the persistence of states.

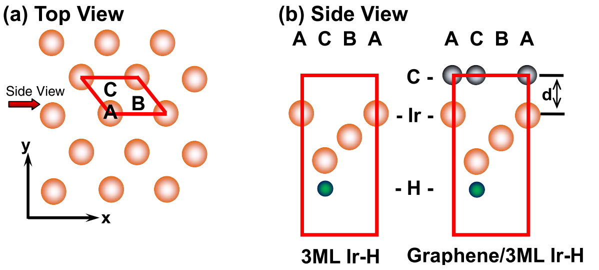

Fig. 1. (a) Top view of the Ir(111) surface. The red rhombus gives the unit cell along the surface. 'A', 'B' and 'C' represent the three stacking positions in the unit cell. (b) Side view of the H-terminated 3ML Ir(111) (left) and the H-terminated 3ML Ir(111) covered with graphene (right). The bottom of the Ir film is terminated by H atoms. The H atoms are just below the Ir atoms. The layer distance, between Ir surface and graphene, is denoted as 'd'. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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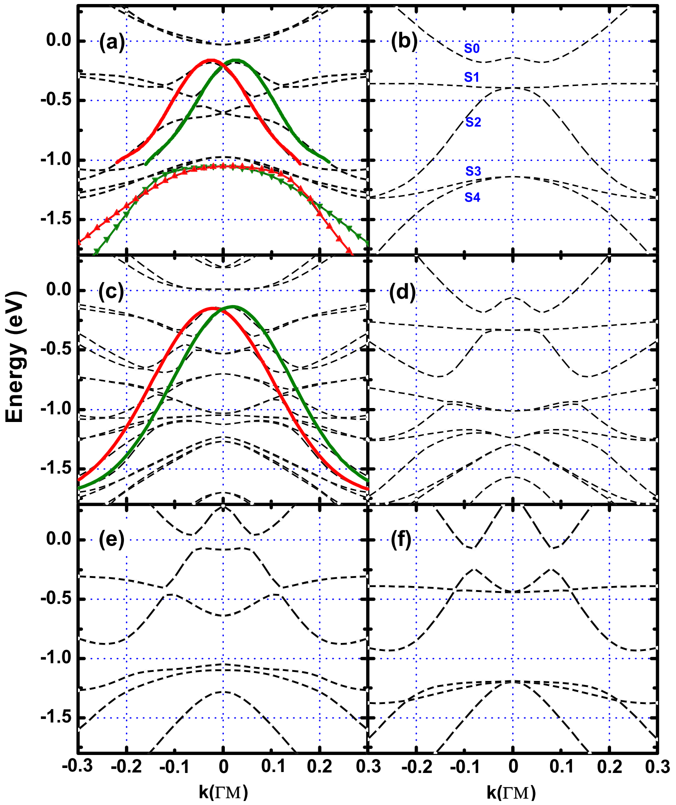

Fig. 2. The energy bands of the H-terminated 3ML Ir(111) (a, b), the H-terminated 6ML Ir(111) (c, d) and the 3ML Ir(111) without H-adsorption (e, f). The SO interaction is considered in (a), (c) and (e). The bottom of the Ir film is terminated by H atoms in (a–d). The states with giant SO splitting are marked with red and green lines in (a) and (c). The energy bands in (b) are denoted as S0–S4, respectively. The band structure is along the Γ–M direction, and the k point is in the unit of the vector ΓM. The magnitude of the unit is equal to the Γ–M distance in the Brillouin zone. The Fermi level is set to be zero.

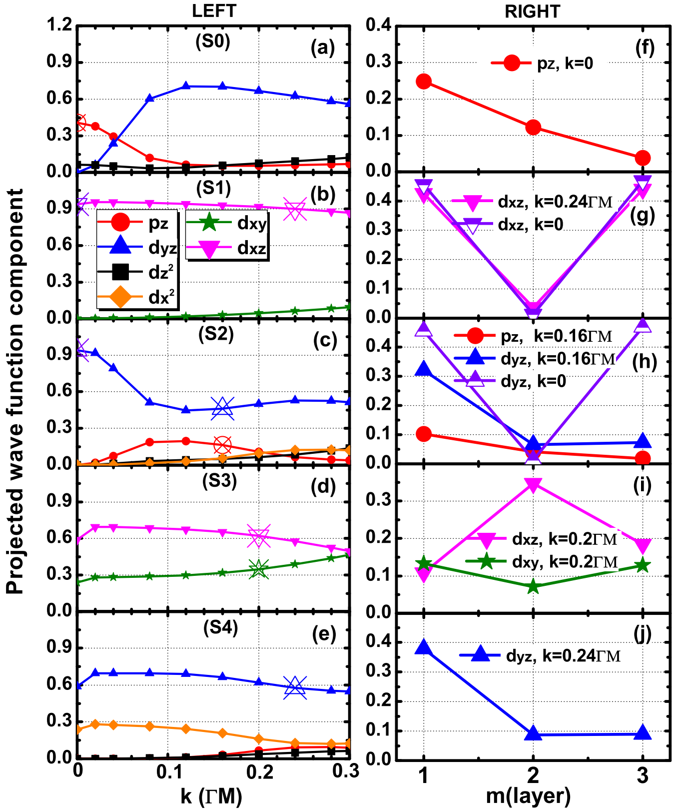

Fig. 3. LEFT (a–e) The projected wave function components of the S0–S4 bands in Fig. 2(b). The k point is in the unit of the vector ΓM. The magnitude of the unit is equal to the Γ–M distance in the Brillouin zone. RIGHT (f–j) The distribution of states on the Ir film. The states are marked in LEFT accordingly. The first layer is the top layer, while the third layer is the H-terminated Ir atomic layer.

2. Method and computational details

The calculations were performed by using DFT on the basis of the projector-augmented wave (PAW) formalism [17]. Local spin-density approximation (LSDA) was employed to describe the exchange–correlation interaction [18]. An energy cutoff of 400 eV for the plane-wave expansion of the PAWs is used, and the Brillouin zone is sampled by using a 31 × 31 × 1 Γ-centered k-point grid. The total-energy convergence was better than 10^{-5} eV. The structure relaxations were carried out until the forces of atoms were less than 0.02 eV/Å. A vacuum layer of at least 10 Å was used in the direction perpendicular to the Ir surface, representing the isolated slab boundary condition in z-direction. The lattice constant in plane was set to be 2.715 Å. The atomic structures are shown in Fig. 1. The SO interaction takes the form of $H_{so} = \frac{\hbar}{4m^2c^2}(\nabla V_{eff} \times \vec{p}) \cdot \vec{\sigma}$, where V_{eff} is the effective potential of electrons, $\vec{p}$ is the momentum operator, and $\vec{\sigma} \equiv (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices. In the traditional two-dimensional electron gases (2DEGs), it can be simplified to the Rashba SO interaction, $H_R = \alpha_R(p_x\sigma_y - p_y\sigma_x)$, where the Rashba strength α_R depends on the gradient of the potential along the direction perpendicular to the 2DEG plane [9].

3. Results and discussion

Although the SO interaction in H atoms is very weak, H–Ir interaction can induce a giant Rashba SO splitting in ultrathin Ir films by breaking the inversion symmetry of the metal films. The giant SO splitting is mainly from the Vacuum/Ir inversion asymmetry. The detailed discussion on the mechanism and the function of H-adsorption can be found in Ref. [19]. Therefore, the SO effect can be studied in detail since the influence of the bulk states are reduced in the ultrathin films.

The energy bands of the H-terminated 3ML Ir(111) with and without SO interaction are shown in Figs. 2(a) and 2(b), respectively. The giant SO splitting is consistent with the detected result of the Ir(111) surface state in experiment [14]. The states with giant SO splitting are marked with red and green lines in Fig. 2. They distribute in several bands. For the sake of analysis, the energy bands without SO interaction in Fig. 2(b) are denoted as S0–S4, respectively. The S0–S2 bands are near the Fermi level ($E = 0$), while the S3 and S4 bands are located under −1.0 eV. These bands have different SO effect. The SO strength in the S1 and S3 bands is weaker than that in the S2 and S4 bands. Around Γ point, the hybridization of the S0–S2 bands leads to a relatively complicated band structure after including SO interaction. It may be directly related to the presence of a kink in the SO splitting of Ir(111) surface state [14].

As a comparison, the band structures of the H-terminated 6ML Ir(111) and the 3ML Ir(111) without H-adsorption are shown in Fig. 2(c–f). The giant SO splitting can also be produced in the H-terminated 6ML Ir(111). It is not sensitive to the thickness of the film. However, the thicker film has the more bands, which overlap the states with giant SO splitting in energy, or even in real space. It is unfavorable for the discussion of the SO effect. In the 3ML Ir(111) without H-adsorption, the states symmetrically distribute on the entire film as quantum well states, greatly different with the surface states. Comparing with the bands of the H-terminated 3ML Ir(111), the location and the shape of bands are changed greatly. Especially, the top of the parabolic band is above