Sign Change of the Spin Hall Effect Due to Electron Correlation in CuIr Alloys

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Spintronics is a rich research field, not only for the wide applications of low energy consumption and energy transformation devices, but also for the new physics with the interplays among charge, spin, orbital, heat and so on. The spin Hall effect (SHE), which converts the injected longitudinal charge current into the transverse spin current via the spin-orbit interactions, is crucial for the development of spintronic devices. The SHE is characterized by the ratio between the transverse and the longitudinal resistivities, called spin Hall angle (SHA). The magnitude of SHA describes conversion efficiency between the charge current and the spin current, while the sign distinguishes the scattering direction of electrons, i.e., clockwise or anticlockwise into the transverse direction.

In the experiment of the CuIr alloys, the dominant contribution to the SHE was verified to be an extrinsic skew scattering mechanism and the SHA was measured to be positive 2.1% [1].

The skew scattering arises from the interference between the scatterings of the *d*-wave and the *p*-wave described by the phase shifts. The phase shift of *p* orbitals is calculated to be -0.05 by the density functional theory (DFT), which means the electron number of the partially filled p orbitals of the Ir impurity is slightly smaller than that of the Cu host. Since the phase shift of *p* orbitals is small, the SHA is approximately proportional to it, and it gives SHA=-1.0% [2].

Such a negative SHA is opposite in sign with the experiment. We argue that such a discrepancy is highly non-trivial, which inspires us to find out the key physics decisive on the sign of SHA. Based on the Anderson model [3], it indicates that the local correlation effects in the *5d* orbitals will raise the *5d* state of the Ir impurities, so that the electron number of the 5d orbitals of Ir will decrease, as sketched in Fig. 1 [2]. In a metal the net charge of the impurity must vanish, thus the decrease of *5d* electrons is partially balanced by the increase of *6p* electrons of Ir. This may change the phase shift of *p* orbitals from small negative to positive, and the sign of SHA from negative to positive correspondingly, which sheds light on removing the discrepancy between theory and experiment in sign.

To simulate the local correlation effects numerically, we develop two specific combined methods of DFT+QMC (quantum Monte Carlo algorithm) and DFT+HF (Hartree-Fock approximation) [2, 4]. By both of the two methods, as the local correlation parameter *U* increases from 0, the sign of SHA changes from negative to positive as expected, giving a positive SHA at the realistic value of *U*=0.5 eV, as shown in Fig. 2 [2]. These theoretical results are consistent with the experiment in quality, revealing the key physics that the local correlation effects are decisive on the sign of SHA in the CuIr alloys.

Furthermore, such a sign of SHA of CuIr is sensitive to perturbation of the local correlations, which is favorable to prospects of controlling the sign of the transverse spin Hall voltage, as illustrated in Fig. 3. This may open up a way to devise a spin current switch or a spin current diode.

References

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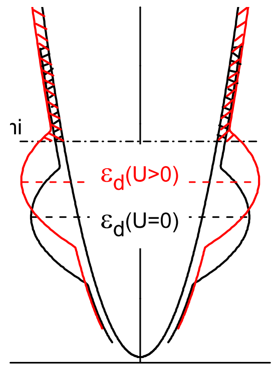

Fig. 1 Schematic picture of the density of states (DOS) of the nonmagnetic CuIr alloys with the *5d* orbitals of Ir including the local correlation *U*, based on the Anderson model [2, 3].

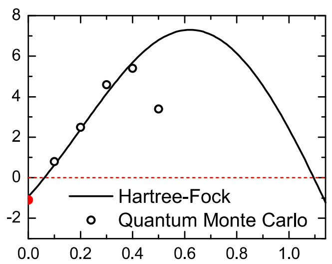

Fig. 2 SHA of the CuIr alloys by DFT under *U*=0 (red dot), by quantum Monte Carlo (black circles) and Hartree-Fock approximation (black line) under *U*>0 for the *5d* orbitals of Ir [2].

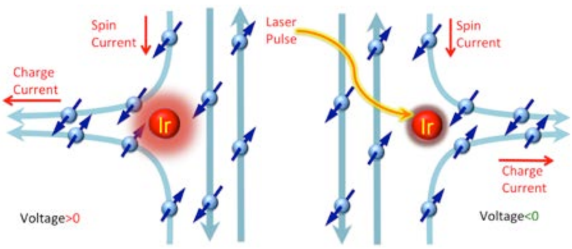

Fig. 3 Schematic picture about the external control of the sign of SHE in CuIr alloys.

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