Electronic structure of iron-based superconductor Sr₄V₂O₆Fe₂As₂ revealed by angle-resolved photoemission spectroscopy

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Introduction

The discovery of iron-based high- T_c superconductors (Fe-HTSCs) generated fierce debates on the superconducting mechanism. Several theoretical and experimental investigations strongly suggest the importance of interband scattering between hole and electron pockets connected by the antiferromagnetic wave vector $Q = (\pi, \pi)$. However, the recent discovery of Sr₄V₂O₆Fe₂As₂ raises a question of the validity of this model. Most band calculations predicted that the band structure of Sr₄V₂O₆Fe₂As₂ does not satisfy the interband scattering condition [1,2]. Compared with other Fe-HTSCs, the distinct characteristic of Sr₄V₂O₆Fe₂As₂ is the presence of metallic V 3d bands. Finite hybridization between the V 3d and Fe 3d bands changes the band topology and destroys the interband scattering condition [1]. On the other hand, there is an argument that if only the Fe-derived bands are taken into account, the bare susceptibility shows a peak at (π, π) similar to other Fe-HTSCs [2]. Furthermore, it has been pointed out that strong on-site electron correlations would remove V 3d states from the Fermi level $(E_{\rm F})$ [2]. Thus, it is of particular importance to investigate the electronic structure of Sr₄V₂O₆Fe₂As₂.

Results and discussion

We have performed angle-resolved photoemission spectroscopy (ARPES) on $Sr_4V_2O_6Fe_2As_2$ ($T_c \sim 37$ K) [3]. Figures 1(a) and 1(b) show the ARPES spectra in the vicinity of E_F . We observed hole and electron bands which cross E_F centered at (0, 0) and (π , π) points, respectively. Apparently, the observed hole and electron bands are connected by $Q \sim (\pi, \pi)$, suggesting the failure of simple LDA calculations. We adopt a LDA + U approach to understand the band structure of $Sr_4V_2O_6Fe_2As_2$ and compared with the experimental band dispersion along high-symmetry lines as shown in Fig. 1(c). We found that highly dispersive bands near E_F are attributed to Fe 3*d* bands [red curves in Fig. 1(c)]. On the other hand, less dispersive bands around 1 eV correspond to V 3*d* states (white curves) that are pushed away from $E_{\rm F}$ due to the strong correlation effect. The present ARPES results combined with the LDA + U calculation suggest that the V 3*d* orbitals are in a Mott-insulating state and show an incoherent peak or lower Hubbard band at ~1 eV. The observed band dispersions near $E_{\rm F}$ are essentially similar to those in other Fe-HTSCs and suggest the importance of the interband scattering for the superconductivity in Sr₄V₂O₆Fe₂As₂.

References

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FIG. 1: (a), (b) ARPES spectra measured around (0, 0) and (π, π) points, respectively, at 40 K with hv = 80 eV. (c) Second derivative plot of ARPES intensity along high-symmetry lines together with LDA + U band calculations. Red and white curves show the bands derived from Fe 3*d* and V 3*d* states, respectively.