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Resonance photoemission study of the diluted magnetic semiconductor $Ba_{1-y}K_y(Zn_{1-x}Mn_x)_2As_2$ isostructural to Fe-based superconductors

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1 Introduction

We have studied the electronic structure and the magnetic properties of a new diluted magnetic semiconductor (DMS) $Ba_{1-x}K_x(Zn_{1-y}Mn_y)_2As_2$[1], which has the same crystal structure as those of the so-called 122-type Fe-based superconductors, by resonance photoemission spectroscopy (RPES).

2 Results and Discussion

In order to extract the local electronic structure of the doped Mn, we performed RPES experiments using photon energies around the Mn L_3 edge. In RPES, one makes use of the property that the cross-section of photoemission from an atomic orbital is enhanced by quantum-mechanical interference between direct photoemission of a *d* electron and absorption followed by a Coster-Kronig transition. This effect is useful in extracting the 3*d* partial density of states (PDOS) of a transition element in solids.

Figure 1(a) shows the valence-band spectra taken with photon energies in the Mn L_3 absorption region. Photon energies used in the measurements are shown by arrows on the XAS spectrum in panel (b). The high DOS of the Zn 3*d* states is clearly observed at ~10 eV below E_F. Photon-energy-independent peaks observed at -15 eV and -18 eV originate from the Ba 5*p* and K 3*p* orbitals, respectively. Most importantly, one can see the enhancement of spectral features in -8~0 eV as the photon energy approaches on-resonance energy at 638.5 eV and the subsequent reduction of spectral weight at higher photon energies.

In order to highlight the resonant enhancement of the Mn 3*d*-derived spectral weight, we show the on-off difference spectra in Fig. 2. The off-resonance spectrum $h\nu$ = 635 eV at the bottom of Fig. 2 (a) has been subtracted from each spectrum. The strongest enhancement around the Mn L_3 edge ($h\nu$ = 638.5 eV) is seen around -4 eV. Vertical bars indicate a constant kinetic energy characteristic of Auger emission. The absence of clear Auger peaks represents that the core hole created in the Mn 2*p* level is not efficiently screened before the Coster-Kronig decay due to the low Mn 3*d* PDOS around E_F. From this result, we see that the Mn 3*d* electrons are essentially localized and do not form band states with the As 4*p* valence band.

The Mn *3d* PDOS is obtained by subtracting the off-resonance spectrum from the on-resonance one [panel (b)]. It shows a peak around 4 eV and is relatively high between 0-2 eV below E_F with little contribution at E_F, as in the case of GaMnAs [2] [panel (c)]. This energy level below E_F creates the d^5 electron configuration on the Mn atoms with the local magnetic moment of S=5/2.

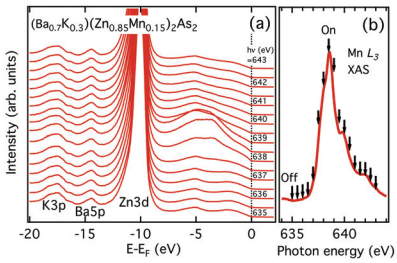

Fig. 1: Evolution of the valence-band spectra of $Ba_{1-y}K_y(Zn_{1-x}Mn_x)_2As_2$.

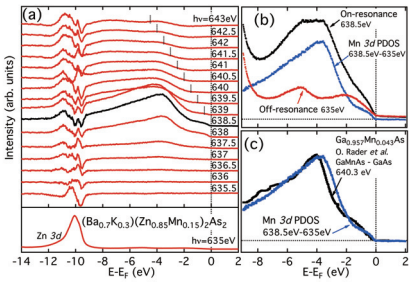

Fig. 2: (a) Evolution of photoemission difference spectra. (b) Determination of Mn 3*d* partial density of states. (c) Comparison with GaMnAs.

References

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