論文題目

Iron-Pnictide and Cuprate High-temperature Superconductors Investigated by Photoemission Spectroscopy

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In this thesis, we have investigated iron-pnictide and cuprate high-temperature superconductors by photoemission spectroscopy (PES).

Our PES data of LaFeAsO_{1-x} F_x and LaFePO_{1-x} F_x at the very early stage of iron pnictides research have answered many urgent questions and revealed many basic features of the electronic structure of these newly-discovered materials. The line shapes of the Fe 2*p* core-level spectra determined from x-ray photoemission spectroscopy (XPS), suggest an itinerant character of Fe 3*d* electrons due to the great similarity of these line shapes with those of metallic iron. Indeed, this is a major difference between pnictides and cuprates that show strong electron correlations. Using synchrotron radiation, we have studied the valence-band spectra and compared them with what is expected from LDA band-structure calculations. Interestingly, we could reproduce most of the features predicted by the

calculations and showed that the major contribution to the density of states (DOS) near the Fermi level is derived from Fe 3*d* orbitals, as illustrated in Fig. 1. These observations were a good indication that LDA is a good starting point for understanding iron pnictides.

From the resonance photoemission spectra taken in the Fe $3p \rightarrow 3d$ core-absorption region, we have obtained the experimental Fe 3d partial density of states (PDOS), and explained it in terms of a band-structure calculation with a phenomenological self-energy correction, yielding a mass renormalization factor of ~ 2 which suggests moderate electron correlation and p-d hybridization in these compounds. We also noticed that the degree of electron correlations in that $LaFeAsO_{1-x}F_x$ is stronger than in



Fig. 1. Valence-band photoemission spectra of $LaFeAsO_{1-x}F_x$ and $LaFePO_{1-x}F_x$ compared with band-structure calculations.

LaFePO_{1-x} F_x , which was expected by LDA calculations [1] and was later confirmed by angle-resolved photoemission (ARPES) results on these compounds [2].

Later we have performed an ARPES study on single crystals of another iron pnictide system, the parent compound $BaFe_2As_2$ and the electron-doped superconducting (SC) compound $BaFe_{1.86}Co_{0.14}As_2$ ($T_c=24$ K). The most interesting and influential finding of this study was the direct observation of the three-dimensional (3D) electronic structure in these compounds by ARPES. The strong photon-energy dependence of band dispersions and Fermi surfaces (FSs) around the BZ center of both the parent and SC compounds indicates the 3D electronic structure as shown in Fig. 2. However, the FS sheets at the BZ corner of both compounds show less three-dimensionality. This observation, which is in good agreement with LDA band-structure calculations [3], suggests that antiferromagnetism and superconductivity in the pnictides have to be described in terms of an orbital-dependent 3D electronic structure, where FS nesting is not necessarily strong. Moreover, these results raise many questions about the common assumption that reduced dimensionality is a prerequisite for high-T_c superconductivity which is believed to be the case of cuprates.



Fig. 2. (a) Momentum-distribution curves (MDCs) of $BaFe_2As_2$ at different photon energies (b) Fermi surface image of $BaFe_2As_2$ in the $k_{//}-k_z$ plane obtained from hv-dependent ARPES data. Black dots represent k_F points determined from MDC peak positions in (a).

In fact, it is difficult to separate the iron-pnictides research from that of cuprates. Both families have many similarities and differences and it would be always useful to make comparison between them. One common property between these two high- T_c superconductors is that superconductivity emerges from a magnetic state upon carrier doping. Therefore, investigating the relationship between superconductivity and magnetism is expected to give useful information. In this sense, we have performed ARPES studies on the

stripe-ordered system $La_{1.4-x}Nd_{0.6}Sr_xCuO_4$ with x~1/8. We have observed a normal-state gap (pseudo-gap) similar to that observed in another stripe-ordered system $La_{2-x}Ba_xCuO_4$ with x~1/8 in the normal state [4] and also similar to that observed in $La_{2-x}Sr_xCuO_4$ in the SC state [5]. These observations suggest that some pairing occurs even in the normal state in these stripe-ordered systems although the relationship between stripes and superconductivity is still not well understood.

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