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Photoemission and X-ray absorption spectroscopy study of $Ba(Fe_{1-x}Mn_x)_2As_2$

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Introduction

Superconductivity in iron-based materials is induced either by hole or electron doping into the parent antiferromagnetic metal. For example, electron doping can be achieved by Co substitution for Fe in $BaFe_2As_2$. Hole doping in $BaFe_2As_2$ by Mn, however, does not induce superconductivity. In addition, the remaining antiferromagnetic metallic phase is reported to be quite peculiar [1]. In order to elucidate the pairing mechanism in iron-pnictide systems, the absence of superconductivity for Mn doping could give useful insight. We have performed a photoemission and X-ray absorption spectroscopy (XAS) study of the iron-pnictide material $Ba(Fe_{1-x}Mn_x)_2As_2$ (Mn-Ba122, x=0.08) at beamlines 28A and 2C, respectively. XAS spectra have made clear that the dopant Mn atoms take a strongly hybridized ground state. We have also deduced the partial density of states (PDOS) of Mn *3d* orbitals by resonant photoemission spectroscopy. The data indicate that the Mn *3d* PDOS is distributed at E_B~1-10eV but not near E_F.

X-ray absorption spectroscopy

Figure 1 shows X-ray absorption spectra at the Mn and Fe *L*-edges. The line shapes of the Mn $L_{2,3}$-edges of $Ba(Fe_{0.92}Mn_{0.08})_2As_2$ resemble those of Mn metal and to some extent $Ga_{1-x}Mn_xAs$. The dopant Mn is tetrahedrally coordinated by As atoms both in Mn-Ba122 and $Ga_{1-x}Mn_xAs$, and, therefore the lineshapes resemble each other in that there is no multiplet structure unlike MnO. The L_3 line shape of $LaMnO_3$ has its weight at higher photon energies (~642eV) than that of Mn-Ba122. These results suggest that the doped Mn atoms take Mn^{2+} state and are strongly hybridized with As *4p* orbitals.

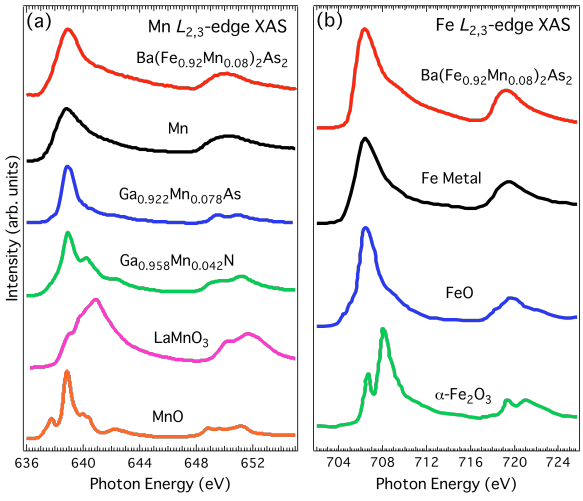

Figure 1: XAS spectra of Mn (left) and Fe (right) *L*-edges.

The peak positions of Fe $L_{2,3}$-edges in $Ba(Fe_{0.92}Mn_{0.08})_2As_2$ are also close to those of FeO. The line shapes those of Fe metal. These results confirm that Fe atoms in the parent compound have the valence 2+ and are in the strongly hybridized ground state.

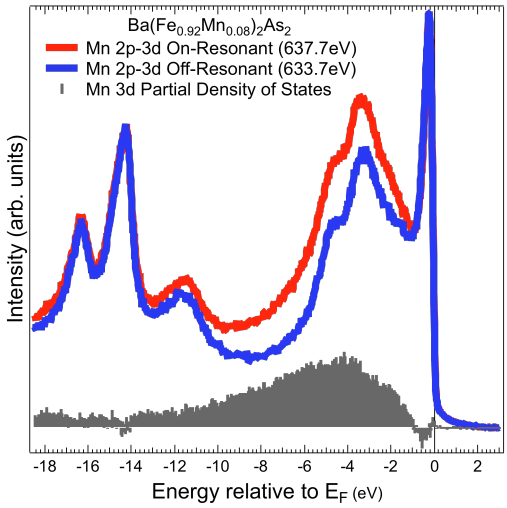

Figure 2: Valence-band spectra taken with Mn *2p-3d* on-resonant (637.7eV, red) and off-resonant (633.7eV, blue) photons. The bottom curve shows the Mn *3d* PDOS.

Resonant photoemission spectroscopy

Resonant photoemission spectroscopy is a useful tool to investigate the partial density of states of a specific element in solids. Figure 1 shows the valence-band spectra taken with Mn *2p-3d* on-resonant and off-resonant photons. The difference in the spectral weight corresponds to the partial density of states of the dopant Mn. This result show that the Mn *3d* PDOS is located at 1-10eV below the Fermi level and that there is little Mn *3d* PDOS at. EF, suggesting that the Mn *3d* electrons are localized at the dopant site.

References

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