Thesis Summary

Electronic structure of Kondo insulator $Yb_{1-x}Zr_xB_{12}$ and Kondo lattice $Yb_2Pt_6X_{15}$ (X=Al, Ga) studied by photoemission spectroscopy

(光電子分光による近藤絶縁体 $Yb_{1-x}Zr_xB_{12}$ および近藤格子 $Yb_2Pt_6X_{15}$(X=Al, Ga)の電子状態の研究)

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In my doctoral work, electronic structures of Zr, Y and Lu-doped Kondo insulator YbB_{12} and Kondo lattices $Yb_2Pt_6X_{15}$ (X=Al, Ga) and $YbNi_2X'_2$ (X′=Si, Ge) were studied by means of hard x-ray photoemission spectroscopy (HAXPES) with hω=5.95 keV, low-energy photoemission spectroscopy (LEPES) with hω=7 eV, vacuum ultraviolet photoemission spectroscopy (VUVPES) with hω=182 eV and angle-resolved photoemission spectroscopy (ARPES) with hω=35 eV.

The electronic structure of Kondo insulators $Yb_{1-x}Zr_xB_{12}$ were investigated by means of HAXPES and LEPES. In the Yb 3*d* HAXPES spectra, both Yb^{2+} and Yb^{3+} derived structures were clearly seen for $0 \leq x \leq 0.875$, indicating valence fluctuation. The Yb valence decreases with Zr substitution and on cooling. The valence at 300 K changes from 2.93 for YbB_{12} (x=0) to 2.83 for $Yb_{0.125}Zr_{0.875}B_{12}$ (x=0.875). The Yb^{3+} 4*f* multiplet structures in the valence-band spectra shifts to the deeper binding energy (E_B) with Zr substitution, reflecting that the Yb^{3+} 4*f* hole level becomes closer to Fermi level (E_F). The energy shifts of the B 1*s* and Zr $3d_{5/2}$ peaks toward deeper E_B, which is understood as a result that the supplied electrons by Zr substitution push E_F to higher energy of the conduction-band DOS. The detailed gap formation at E_F were clearly observed by LEPES. In YbB_{12}, the pseudo gap at 18 meV starts to open from 130 K. The *c*-*f* hybridization and Yb $4f_{7/2}$ peaks are observed at 15 and 45 meV, respectively. With Zr-doping, the *c*-*f* hybridization peak disappears and the spectral weight at E_F is gradually recovered by Zr substitution and the pseudo gap is closed.

The electronic structure of $Yb_{1-x}R_xB_{12}$ (R=Y, Lu) were also studied by means of HAXPES and LEPES for comparison with the results of $Yb_{1-x}R_xB_{12}$. Both Yb^{2+} and Yb^{3+} derived structures clearly seen in the Yb 3*d* HAXPES spectra and the intensity of Yb^{2+} components gradually increases while that of Yb^{3+} gradually decreases with increasing R-concentration. The Yb 3*d* spectra of $Yb_{0.125}Y_{0.875}B_{12}$ shows temperature dependence on cooling, and the Yb valence is ~2.88 at 300 K and gradually decreases to 2.84 at 20 K. In the valence-band HAXPES spectra at 300 K, the Yb^{2+} 4*f* and Yb^{3+} 4*f* derived structures are observed near E_F and at 6 -12 eV, respectively. With R-doping the Yb^{3+} 4*f* multiplet structures gradually shifts to higher E_B side and the Yb 4*f* hole level gradually closer to E_F. In the B 1*s* spectra, the energy shifts toward higher E_B side with R-doping are also observed. The chemical shifts in the core level suggest that the conduction electron is transferred mainly from B site to Yb site, inducing the decrease of the Yb valence. Temperature dependent LEPES was also performed for $Yb_{1-x}R_xB_{12}$. We clearly observed the pseudo gap is still opens in $Yb_{0.5}Y_{0.5}B_{12}$ and $Yb_{0.5}Lu_{0.5}B_{12}$ in contrast to $Yb_{0.5}Zr_{0.5}B_{12}$, where the pseudo gap is already closed. The gap is closed in $Yb_{0.125}Y_{0.875}B_{12}$. These results suggest that the electron doping plays significant role in the pseudo gap closing. The large change in the maximal value of in the magnetic susceptibility (T_{max}) observed only in the Zr-doping system $Yb_{1-x}Zr_xB_{12}$ is also originated from the electron doping system.

The electronic structures of Kondo lattices $Yb_2Pt_6X_{15}$ were investigated by means of HAXPES, LEPES, VUVPES and ARPES. In the Yb 3*d* HAXPES spectra, the both Yb^{2+} and Yb^{3+} derived structures were clearly observed. The intensity of the Yb^{2+} (Yb^{3+}) structures for $Yb_2Pt_6Al_{15}$ gradually increases (decreases) on cooling, showing significant valence fluctuation. The estimated Yb valence of $Yb_2Pt_6Al_{15}$ is 2.89 at 250 K gradually decreases to 2.83 at 20 K. On the other hand, the Yb 3*d* spectra for $Yb_2Pt_6Ga_{15}$ show almost temperature-independent with the Yb valence of 2.34. The Energy shifts toward lower E_B by ~0.3 eV was observed in the Pt 4*f* states on going from X=Al to Ga. At the same time, in the valence-band HAXPES and VUVPES spectra, we found the energy shift toward deeper E_B in the Yb^{3+} 4*f* multiplet structures. These results compared with the Kondo lattices $YbNi_3X_9$. In these system, $YbNi_3Al_9$ has antiferromagnetic ground state and Yb valence close to 3+. On the other hand, $YbNi_3Ga_9$ exhibits a typical valence fluctuation behavior. We compared the valence-band and core level spectra of both $Yb_2Pt_6X_{15}$ and $YbNi_3X_9$ systems, and proposed a common electronic model. We described the enhanced *c*-*f* hybridization and T_K in $Yb_2Pt_6X_{15}$ based on the Pt-derived DOS at E_F and the Yb^{3+} 4*f* hole level relative to E_F together with results from $YbNi_3X_9$. We also conclude that the larger conduction-band DOS of Pt at E_F compare to that of Ni at E_F is a main reason for their different physical properties. The same trend is observed between $YbNi_2Si_2$ with low T_K and $YbNi_2Ge_2$ with high T_K. The similarity suggests that the characteristic universalities in the electronic structure when the compounds with the same crystal structure and similar conduction electron states move from non-magnetic to magnetic regions in the Doniach phase diagram. We performed ARPES measurements on $Yb_2Pt_6X_{15}$ and the results show very clear Fermi surface structure and *c*-*f* hybridization band structures. Base on periodic Anderson model without the 4*f*-4*f* Coulomb interaction energy, we fitted the *c*-*f* hybridization band structures and estimated the effective mass enhancement factor and hybridization energy are 1.18 and ~0.0008 eV for $Yb_2Pt_6Al_{15}$, and those are ~1.59 and 0.13 eV for $Yb_2Pt_6Ga_{15}$.