LOW DIMENSIONAL
AND
CORRELATED SYSTEMS

THREE-DIMENSIONAL AND INTRINSIC PHOTOEMISSION EFFECTS IN QUASI-TWO-DIMENSIONAL MATERIALS

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Remnant interlayer interaction in the quasi-2D layered materials leads to 3D effects in their electronic structure determined by layer-perpendicular electron dispersion $E(k_\perp)$. Its investigation by photoemission (PE) spectroscopy encounters two problems: (1) The final bands, required for evaluation of the valence band $E(k_\perp)$, strongly deviate from free-electron-like dispersion; (2) The intrinsic accuracy – the shifts of PE spectral peaks from the true quasiparticle bands (peaks of the valence band spectral function) caused basically by the final state damping – is comparable with the valence band $k_\perp$-dispersion range. This requires determination of the final state dispersions and damping, which can be achieved by Very-Low-Energy Electron Diffraction (VLEED).

We report on systematic determination of the 3D effects for typical layered materials – VSe$_2$, TiS$_2$ and graphite. VLEED shows essentially 3D dispersion of the unoccupied states, but the weak interlayer interaction results in strong non-free-electron effects, including wide band gaps and multiband composition. For graphite the band gaps are particularly wide, resulting in strong electron damping. Above ~20 eV the damping sharply rises due to the plasmon excitation. Knowledge of the final states dispersion and damping has allowed us to optimize the PE experiment in the intrinsic accuracy and map consistently the valence band $k_\perp$-dispersions (Fig.1). For graphite the intrinsic shifts, particularly large, were deconvoluted using model PE calculations.
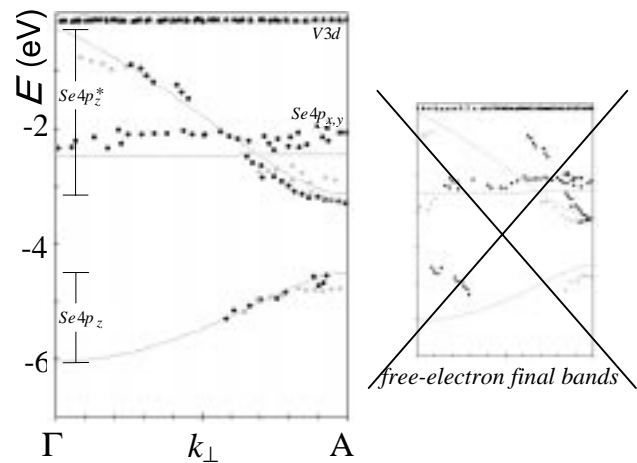

Fig.1. PE valence band of VSe$_2$: consistent determination of the $k_\perp$-dispersions is achieved if only the non-free-electron and self-energy effects in the final bands found by VLEED are taken into account; for the final states above ~20 eV the experimental points (gray) are shifted due to increase of the $k_\perp$-broadening.

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Unified theory on angle-resolved photoemission and light absorption spectra of strongly correlated electron systems

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Very recently, the angle-resolved photoemission spectrum(ARPES) of $[Ni(chxn)_2Br]Br_2$ (chxn=cyclohexanediamine), which is a typical one-dimensional(1-D) Mott insulator, has been experimentally observed[1]. The experiment has strongly suggested that the density of states of the $[Ni(chxn)_2Br]Br_2$ has quite a small gap, despite a large optical gap observed in the light absorption spectrum (LAS) [2]. In this talk, we show that the ARPES and LAS of the $[Ni(chxn)_2Br]Br_2$ are consistently explained within the framework of the 1-D extended Hubbard model. Lehmann spectra of the one-body and light absorption-type two-body Green functions are calculated by a quantum Monte Carlo method of a path-integral form. As shown in Fig.1, our theoretical results reproduce well the experimentally observed ARPES and LAS. The direct comparison of the experimental and theoretical results confirms the small one-body gap, which is double the ARPES gap, and large optical gap. The apparent difference between two gaps indicates the breakdown of a mean-filed description of the strongly correlated electron system, where the optical gap is equal to the one-body gap. We suggest that the difference is caused by the dynamical Zeeman field induced by the large quantum fluctuations.
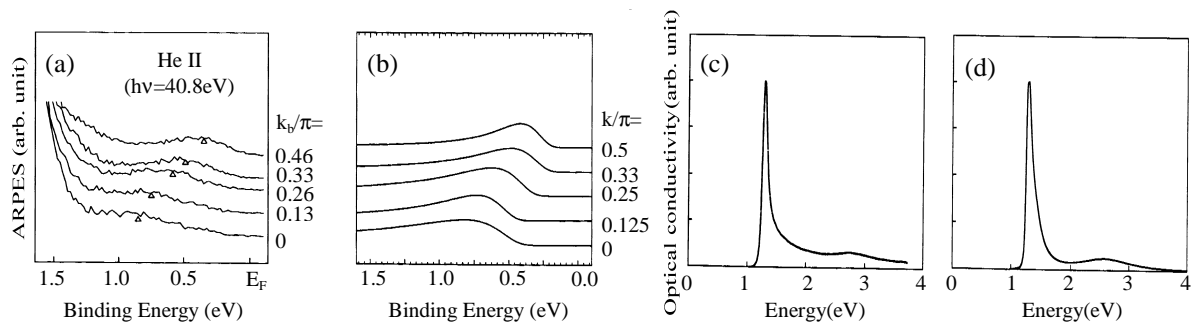

Fig.1 Observed ARPES and LAS of Ni-Br complex ((a) and (c)), and theoretical results ((b) and (d)).

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NON-LOCAL SCREENING EFFECTS ON RU 3D XPS IN SR$_2$RUO$_4$

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Sr$_2$RuO$_4$ and its family have recently attracted much attention on their superconductivity and magnetism. Core-level photoemission is one of the most powerful tools to obtain the fundamental information on the Ru 4d - O 2p valence (conduction) states. Very recently, Sekiyama has reported that the Ru 3d XPS in Sr$_2$RuO$_4$ is quite anomalous, compared with that in CeRu$_2$Si$_2$ for instance [1]. According to his results, the Ru 3d XPS in Sr$_2$RuO$_4$ consist of a weak leading peak and an intense broad satellite structure, while there is no satellite in CeRu$_2$Si$_2$. Sekiyama has suggested the possibility of **non-local screening**, in analogy to the Cu 2p XPS in low-dimensional cuprates [2]. The present study discuss the role of the non-local screening effects in Sr$_2$RuO$_4$ on basis of the exact diagonalization calculations for multi-site cluster model such as, Ru$_3$O$_{10}$ and Ru$_5$O$_{16}$.

Figure 1 is the calculated Ru 3d XPS in Ru$_5$O$_{16}$, where the Coulomb interaction strength between Ru 4d electrons (U) and that between Ru 4d and 3d electrons (Q) are varied as adjustable parameters. In this calculation, the spin-orbit splitting of Ru 3d core level is not taken into account. When U and Q are increased, several satellite peaks appears at the higher binding energy side of the leading peak. For (U, Q)=(4eV, 5eV), the total intensity of the satellites is larger than that of the leading peak. The charge distribution analysis for the XPS final states shows that the electrons on the Ru sites neighboring the core-hole site participate in the core-hole screening process quite actively, which means the importance of non-local screening. I expect that, in the limit of infinite-size cluster, those satellite lines form a continuum which corresponds to the satellite observed in the experiment.
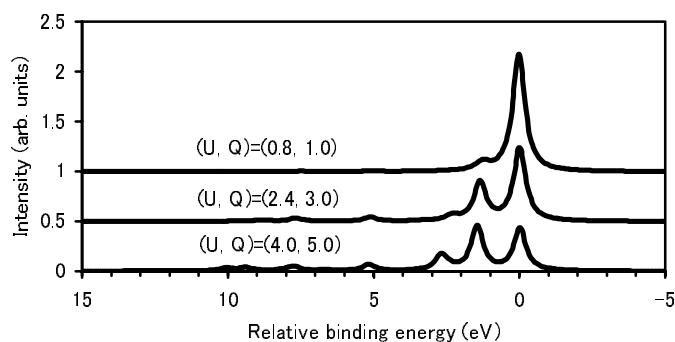

Figure 1: Ru 3d XPS calculated as functions of U and Q.

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PEIERLS FLUCTUATIONS IN THE ELECTRON SYSTEM OF A QUASI-ONE-DIMENSIONAL SOLID

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Using $NbSe_3$ as a quasi one-dimensional model system, the symmetries of the electron system were explored with angle-resolved synchrotron photoemission. Particular focus is given to precursor fluctuations [1] of the Peierls-distorted state above the actual transition temperature. The character of the electron bands is found to be largely one-dimensional, with deviations in a second dimension. The Fermi level crossings which are a prerequisite for the two charge density wave (CDW) transitions are identified. These first photoemission data on the $NbSe_3$ band structure are complemented by density functional calculations of the Fermi surface, which deliver accurate nesting conditions for both nesting vectors q_1 and q_2.

One of the two nesting vectors, q_1, is in line with the chain direction, and confirmed experimentally with high accuracy. However, in the data taken at room temperature – well above the phase transition temperature $T_1 = 145$ K – we do not observe a metallic crossing of the relevant band, but instead see a backfolding of the electron dispersion (see figure). The phenomenon is a high-temperature analogy of the effect reported by the authors for a spin density wave [2]. It implies that a supercell zone characteristic of the Peierls state is still imposed onto the electron system. To our knowledge, this is the first such direct observation of a persistent CDW symmmetry-breaking in the electron system far above the critical temperature. From the Fermi velocity of the nested band we estimate a coherence length which indicates that our observation at $T = 2.1 \times T_1$ is at the upper temperature limit where a sufficiently defined bandstructure can be seen.
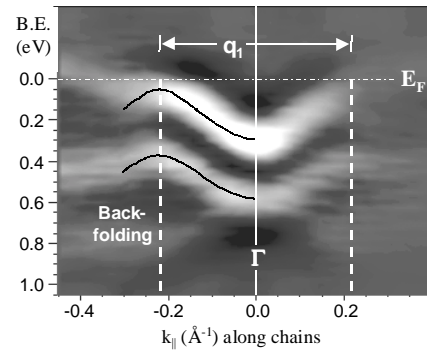

Figure: Electron bands in $NbSe_3$ near E_F satisfying the nesting condition for q_1. In the fluctuation regime at 300 K, the bands are still backfolded and obey the symmetry of the Peierls state.

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Ce $4f$ states in $CePd_2Si_2$ and $CeNi_2Si_2$ investigated by resonant photoemission spectroscopy

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$CePd_2Si_2$ and $CeNi_2Si_2$ crystallize in the $ThCr_2Si_2$-type structure. $CePd_2Si_2$ is known as an antiferromagnetic Kondo compound with the Néel temperature and the Kondo temperature (T_K) nearly equal to 10 K. $CeNi_2Si_2$ is known to be an intermediate valence (IV) compound with high T_K (500-600 K). Such phenomena are derived from a hybridization of the Ce $4f$ states with the conduction-band states. In this study, we investigate the Ce $4f$ states in $CePd_2Si_2$ and $CeNi_2Si_2$ from the valence-band spectra measured by means of high-resolution Ce $4d$-$4f$ resonant photoemission spectroscopy (RPES).

Ce $4d$-$4f$ RPES spectra were measured at BL-11D of KEK-PF. The sample temperature was set at 12 K. The sample surface was cleaned *in situ* by scraping with a diamond file. The overall energy resolution was estimated to be 65 meV at $h\nu = 122$ eV.

Figure 1 shows the Ce $4f$ spectra of $CePd_2Si_2$ and $CeNi_2Si_2$. The Ce $4f$ spectra for both materials exhibit the peak structures at 0.03, 0.28 and ~2.3 eV, which are ascribed to the $f^1_{5/2}$ (a tail of the Kondo peak), $f^1_{7/2}$ (its spin orbit partner) and f^0 final states, respectively. The intensity of the $f^1_{5/2}$ final state for $CeNi_2Si_2$ is stronger than that for $CePd_2Si_2$. This indicate that the intensity of Kondo resonance scales T_K on bulk components, although the Ce $4d$-$4f$ RPES measurements provide surface-sensitive information.

Both Ce $4f$ spectra are well fitted by the spectral calculations based on a single impurity Anderson model with considering the bulk and surface components. The parameters evaluated by the analyses for bulk components are clarified that $CePd_2Si_2$ is the nearly trivalent Kondo compound and $CeNi_2Si_2$ the IV compound. For $CeNi_2Si_2$, the hybridization of the Ce $4f$ states with the Ni $3d$ states in the next-nearest-neighboring Ni atoms around Ce also plays an important role in showing the behavior as the IV compound.
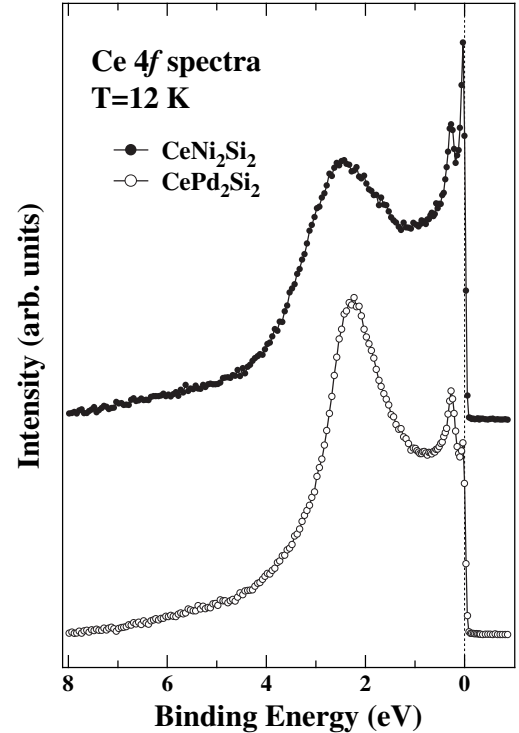

Figure 1: Ce $4f$ spectra of $CePd_2Si_2$ and $CeNi_2Si_2$. The Ce $4f$ spectra are evaluated by subtracting the off-resonance spectra taken at $h\nu = 114$ eV from the on-resonance spectra at $h\nu = 122$ eV.

High-resolution angle-resolved photoemission study of η-Mo4O11

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We have performed angle-resolved photoemission spectroscopy (ARPES) of η-Mo4O11, a quasi-two-dimensional (2D) conductor which shows charge-density-wave (CDW) transition at 109K and 35K. We found several dispersive bands across the Fermi level (E_F) which are assigned to the Mo $4d$ bands from the band structure calculation.   Although the observed width of Mo $4d$ bands is two or three times as large as the band structure calculation, we found the experimental Fermi surface (FS) shows a good agreement with the band structure calculation showing a nesting property consistent with the CDW wave vectors obtained in the X-ray diffraction experiment.   The present ARPES results indicate that the CDW instability in η-Mo4O11 is driven by " the hidden 1D FS nesting" due to the quasi-1D chains in the crystal structure.

USXES, XPS and OPTICAL PHEMONENA IN Si LOW-DIMENSIONAL STRUCTURES DEPENDENT ON MORPHOLOGY AND SILICON OXIDE COMPOSITION ON Si SURFACE

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Silicon nanocrystal systems attract scientific attention due to Si based optoelectronic devices perspective. X-ray photoelectronic spectroscopy (XPS), ultra soft X-ray emission spectroscopy (USXES), Atomic Force Microscopy (AFM), Raman scattering and photoluminescence (PL) methods have been used for the investigation PL mechanism in silicon nanocrystal structures, like porous silicon (PSi), and Si nanoparticles in silicon oxide.

We have found that PL spectra of bright red luminescence in PSi can be decomposed on two Gaussian shape elementary PL bands: A ($h\tilde{o}_m=1.70-1.85$ eV) and B ($h\tilde{o}_m=1.9-2.05$ eV). The relative intensities of these bands change with the variation of PSi preparation conditions and the temperature of measurement.

The very bright A band dominates in PL spectra of PSi samples with maximal roughness of top PSi surface and, consequently, the largest Si/SiO_x interface area. XPS results were received on different depth of PSi layer during it layer by layer Ar ion etching. XPS and USXES investigations have shown the essential quantity of silicon suboxide at Si/SiO_x interface. So, it has been found a direct correlation between suboxide concentration, the value of Si/SiO_x interface area and A elementary PL band intensity.

With increase of etching current or etching duration PSi roughness decreases. Simultaneously A band intensity decreases and B band start dominates. XPS and USXES studies have shown the Si/SiOx interface is created by silicon dioxide in this case.

The mechanisms of the both luminescence bands in PSi have been analyzed from the point of view of defect related emission centers at Si/SiOx interface, created by silicon suboxide and dioxide. The comparative investigation of the PL peculiarities of Si nanoparticles in silicon oxide films has been used for confirmation of the proposed luminescence models.

ELECTRONIC STRUCTURE OF $Sr_{2-x}La_xFeMoO_6$

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A double perovskite Sr_2FeMoO_6 is a metal ferrimagnet below $T_C = 420$ K [1]. Recently, Kobayashi *et al.* have found a fairly large magnetoresistance (MR) effect of this system at the room temperature [2]. Band-structure calculations predicted a (nearly) half-metallic nature of the system like the colossal magnetoresistive (CMR) manganites [2,3]. To elucidate the electronic structure of this system, we have performed photoemission experiments on $Sr_{2-x}La_xFeMoO_6$ (x=0.0 and 0.2). The measurements were done at the beamline 11D of the Photon Factory, using a Scienta SES-200 electron analyzer. Fresh clean surface was obtained by fracturing single crystalline samples *in situ*.

Figure 1 shows near-E_F photoemission spectra of $Sr_{2-x}La_xFeMoO_6$ at 20K. Two features at ~0.2 eV (Feature *A*) and ~1.3 eV (Feature *B*) can be observed near the Fermi level (E_F). Compared with the band-structure calculations [2,3], *A* and *B* have been interpreted to be the Fe-Mo t_{2g} down-spin band and the Fe e_g up-spin band, respectively. Upon La substitution, Feature *A* moves away from E_F by ~54 meV, reflecting electron doping. In addition, however, the intensity of *A* and *B* increases, which indicates that the carrier-doping effects are not the rigid-band type.
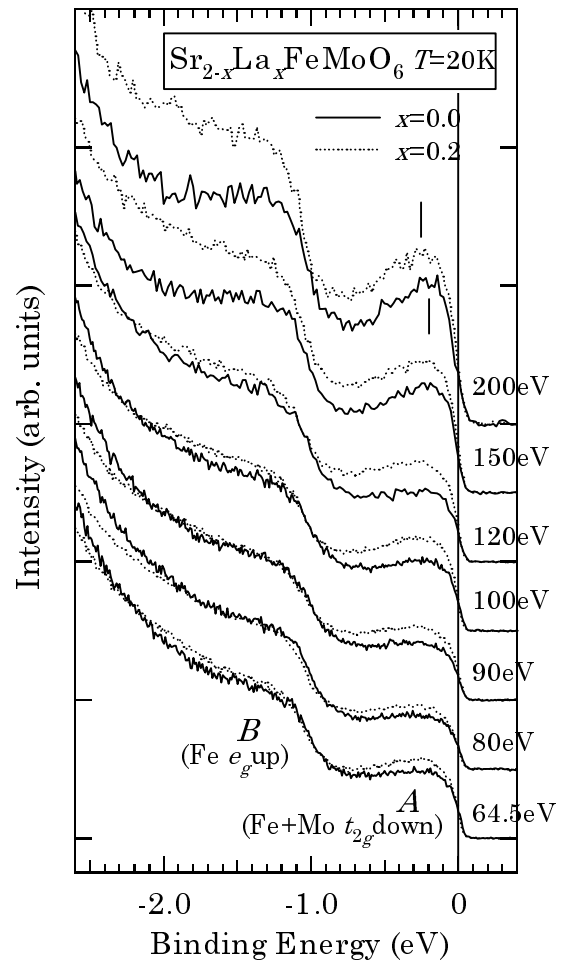

Figure 1: Near-E_F spectra of $Sr_{2-x}La_xFeMoO_6$ at 20K.

References

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Electronic Structure of $La_{1-x}Ce_xMnO_3$ by X-Ray Absorption Spectroscopy

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We report x-ray absorption near edge structure (XANES) spectra of Ce $M_{5,4}$-, Mn $L_{3,2}$-, and O K-edges of Ce doped $La_{1-x}Ce_xMnO_3$ (x = 0.2, 0.3 and 0.5) and understand their change electronic structure in terms of near-neighbor environment. No pre-edge features are observed in O K-edge spectra, which are generally present in hole-doped CMR materials implying the electron-doped nature in valence band. Intensity enhancement of all the peaks indicates that Ce $5d$ and/or Ce $4f$ states hybridization with O $2p$ states. Ce is doped into this compound in tetravalent state and not in mixed state. This study also indicates that Ce is incorporated into the lattice at La site of this material resulting in modification of Mn-O network. These changes are clearly visible in the Mn $L_{3,2}$ and O K-edges spectra. The ratio of Mn^{4+} and Mn^{3+} is changing with Ce doping and hence has direct influence on the states at the Fermi level.

Electronic Structure of Edge-Shared Chain Compounds $Ca_{2+x}M_{2-x}Cu_5O_{10}$ (M=Y, Nd, Eu, Gd) Studied by X-ray Absorption and Emission Spectroscopies

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X-ray absorption (XAS) spectroscopy near O-1s edge has been performed on polycrystalline $Ca_{2+x}M_{2-x}Cu_5O_{10}$ (M=Y, Nd, Eu, Gd; $0.0 \leq x \leq 2.0$) and single crystalline $Ca_{2+x}Y_{2-x}Cu_5O_{10}$ which contains edge-shared CuO_2 chain structure. For single crystalline samples, the occupied states of O-2p were measured by means of X-ray emission spectra (XES). All the XAS spectra of $x=0.0$ samples contain only one peak at about 530.9 eV. On the other hand, in the spectra with holes ($x>0.0$) a new characteristic peak at about 529.2 eV appears with its intensity being proportional to the hole concentration. Then, these two peaks at 529.2 eV and 530.9 eV are assigned to hole and upper Hubbard band (UHB) states, respectively. Figure 1 shows XAS spectra of single crystalline $x=0.0$ and 1.8 samples with the electric field vector, $\boldsymbol{P}$, of incident X-rays parallel to the crystalline a- and c-axes. There is no anisotropy in XAS spectra with $\boldsymbol{P}//a$- and c-axes, which means the isotropic hole distribution in the edge-shared chain structure. Figure 2 shows two XES spectra of $x=1.8$ sample with $\boldsymbol{P}//a$-axis with the excitation energies of UHB and hole states. The remarkable difference was observed between them. The difference is caused by local distortion by introducing holes constructing Zhang-Rice singlet state. There is no anisotropy between XES spectra with $\boldsymbol{P}//a$- and c-axes, which means isotropic electron distribution and is consistent with the isotropic hole distribution derived from XAS spectra. The drastic change of electronic state by introducing holes was similar to the result of spin-ladder compounds, $Sr_{14-x}Ca_xCu_{24}O_{41}$.[1]
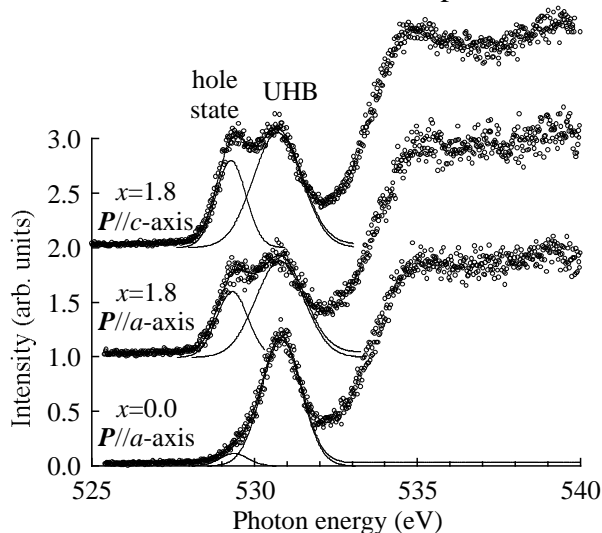

Figure 1: XAS spectra of $Ca_{2+x}Y_{2-x}Cu_5O_{10}$ single crystals.
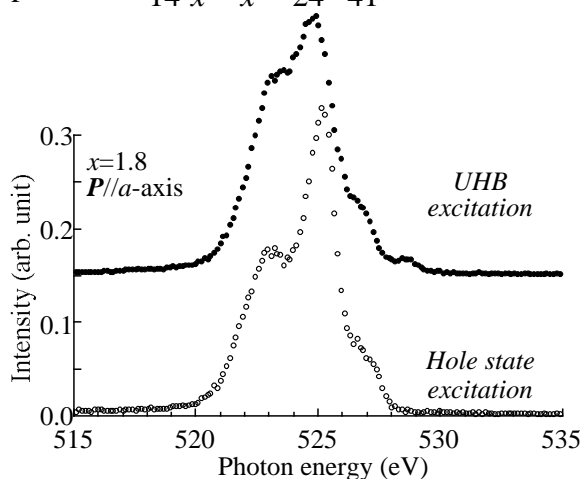
Figure 2: XES spectra of $Ca_{3.8}Y_{0.2}Cu_5O_{10}$ single crystals with $\boldsymbol{P}//a$-axis. Remarkable difference could be seen by introducing hole.

Reference
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Resonant X-ray Raman scattering spectra of Ce-compounds

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Resonant L α X-ray emission spectra (RXES) of Ce-compounds, CeF_3, CeO_2 and CeB_6 were measured around the L_{III} absorption threshold. RXES were measured at the beam line BL-7C of Photon Factory, KEK,Tsukuba. An incident photon energy was selected with Si (111)double-crystal monochromator. The emission spectra were measured by a curved Ge (400) crystal monochromator, "Escargot". The total resolution was about 1.2eV.

Figure 1 (a) shows the Ce L_{III} absorption spectrum(XAS) of CeO_2. The RXES were taken at selected incident excitation energies (ω_i) showed by vertical arrows for 1 to 19 in (a) are represented in Fig.1 (b). The emitted photon energies (ω_s) were studied across the Ce L_{III} absorption threshold as a function of the transfer energy ($\omega_i - \omega_s$). In this representation,the resonant Raman peaks C,D and E are fixed for various values of ω_i and its intensities go through a resonant maximum at spectrum No.11,No.13 and No.16, respectively. Peaks A and B are assigned to the multiplet structure correspouding to the 2p $\rightarrow$4f quadrapolar transition. Peak F indicated by dashed lines in Figure is attributed to the L α normal fluorescence line, where emitted radiation starts to grow at spectrum No.14 and its transfer energy value increases with increasing incident energy (ω_i).
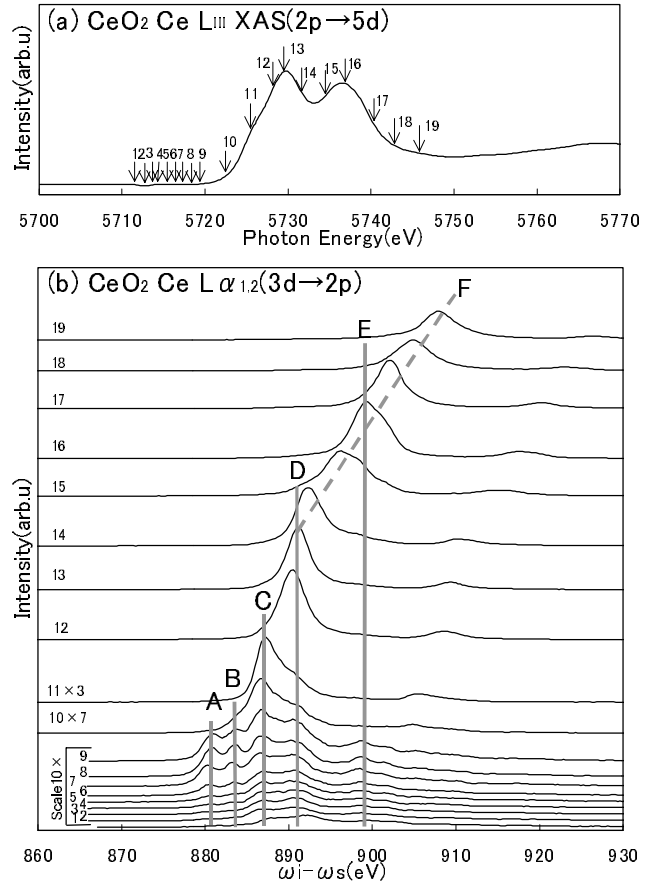
Fig.1 (a)Ce L_{III} XAS of CeO_2
(b)Ce $L\alpha_{1,2}$ resonant Raman spectra of CeO_2

PHOTOEMISSION STUDY OF QUASI-ONE-DIMENSIONAL HALOGEN-BRIDGED COMPOUND [Ni(chxn)₂Br]Br₂

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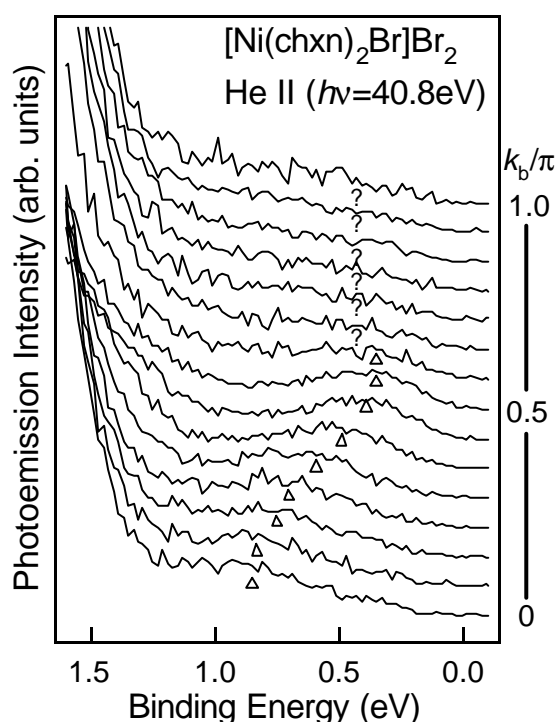[2]*Department of Physics, Graduate School of Science, University of Tokyo, Hongo 7-3-1, Tokyo 113-0033, Japan*
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The one-dimensional (1D) halogen (*X*) bridged transition-metal (*M*) compounds (*MX*-chain compounds) have been attracting much attention as a good target material to investigate the properties of the 1D electronic state under the influence of strong electron-lattice interactions and electron-electron correlations. In these compounds, the electronic structure of 1D chain is composed of half-filled d_{z2} orbitals of the metals and the filled p_z orbitals of halogens, and is considered to be a purely one-dimensional. In particular, the complex with *X*=Br and *M*=Ni, [Ni(chxn)₂Br]Br₂ (chxn=1R, 2R-cyclohexanediamine) is known to show no lattice distortions related to Peierls or Spin-Pierls transition even at low temperatures. The magnetic susceptibility *c* is described by Boner-Fisher formula with *S*=1/2 and *J*=3600K, and this material can be regarded as the 1D Heisenberg chain. In the present study, the electronic structure of this compound is studied by angle-resolved photoelectron spectroscopy. Figure shows the spectra, taken with parallel to the chain axis. The expected two dispersions, originated with spin-charge separations as have been observed in other 1D electron system, are not clearly observed in this compound. Instead, only one "band" having about 0.5eV energy dispersion, is found in the half of the Brillouin zone. These results are compared with other 1D electron system, like SrCuO₂[1] or Sr₂CuO₃[2]. In addition, *d-p* chain model calculations are employed to understand these differences.

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PHOTOEMISSION STUDY OF ONE-DIMENSIONAL GOLD CHAINS ON STEPPED SILICON SURFACES

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It is well known that low dimensional structures present different physical behaviors compared to 3D materials. A striking example is the breakdown of the Fermi-liquid description in one-dimensional metals, which are described by the Luttinger liquid formalism, where quasiparticles are replaced by distinct collective excitations involving spin and charge, called spinons and holons, respectively.

In a previous study, a double peak in photoemission spectra has been observed on the Au/Si-(5x1) surface [1]. This double peak has been interpreted as spin-charge separation in a Luttinger Liquid. This is now a matter of debate, since new studies seem to demonstrate that the band splitting does not vanish at the Fermi level, in contradiction with the spinon-holon interpretation of this spectral feature [2].

In an attempt to clarify the real nature of the studied system, we present new photoemission measurements of Au/Si-(5x1). We compare them to the former studies [1, 2], and to measurements of a new system, the Au/Si-(3x1) surface, which, to our knowledge, has not been measured yet.

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INDIUM CHAINS ON SI(111): A PEIERLS TRANSITION ?

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Self-assembled one-dimensional (1D) chains received much attraction both in the development of nano-scale devices, and also in testing the theories describing their electronic structure, which differs significantly from that of conventional 3D Fermi liquid systems. 1D Luttinger liquid-type chains, however, may become unstable due to fluctuations at finite temperature and, hence, become susceptible to metal-insulator transitions such as, e.g., the Peierls textbook example for quasi-1D chains.

Recently, quasi-1D Indium chains on vicinal Si(111) have been found to exhibit a metal-insulator transition upon cooling [1], but the temperature and character of this transition was not investigated in great detail. Although the geometric structure of Indium chains on vicinal Si(111) seems to be explained now [2], the detailed electronic band structure near the Fermi surface (FS) as a function of temperature, and consequently the nature of the transition remain quite unclear.

The existence of three surface state bands induced by the (4x1) reconstruction has been established [3]. What concerns the nature of the transition, a simple FS nesting picture for only one of those Indium induced surface state bands has been proposed, based on FS mapping experiments with moderate resolution[1].

We examined in detail the geometric and electronic structure of thin Indium chains on Si(111) surfaces by means of low energy electron diffraction (LEED) and ultrahigh-resolution photoemission (ARPES) as a function of temperature. Our data reveal a transition around 115 K from a high temperature (4x1)- to a low temperature (8x2)-phase being reversible with a small hysteresis of the order of 10 K. ARPES spectra exhibit clearly important concomitant changes in the electronic band structure near the Fermi surfaces and at the border of the surface Brillouin zones [4]. We derive the dispersive behavior of the bands involved in the transition in detail and demonstrate that at least two surface state bands show the opening of a pseudo energy gap on the Fermi surface leaving small but finite spectral weight in the low-temperature state. We conclude that this transition is probably driven by a similar but more complex mechanism than in a conventional Peierls transition. Furthermore, we evidence a strong influence of matrix element effects, as we observe considerable spectral weight of the same bands in different Brillouin zones.

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PHOTOEMISSION ON TWO-DIMENSIONAL ELECTRON SYSTEMS

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Photoelectron spectroscopy in the VUV region is a powerful tool to investigate low-dimensional electron systems. Here we report on the electronic behavior of the two-dimensional electron gas (2DEG) on an InAs(110) surface being induced by adsorption of Nb and Fe in the submonolayer regime. This is of great importance for the understanding of different aspects in the field of, e.g., spin electronics and the quantum Hall effect. Additionally, the 2DEG can be used for fundamental investigations in the photoemission process due to its relatively large intrinsic life time and its spatial confinement. The n-InAs(110) crystals were cleaved in-situ ($N_D = 1 \times 10^{16} cm^{-3}$). A calibrated electron beam evaporator enables the adsorption of metals in the submonolayer regime with a high accuracy. This investigation was carried out at two different beamlines at HASYLAB/DESY (Hamburg). The former one allows an overall energy resolution of 50meV and an angular resolution of about 1°, the latter one of 10meV and 0.3°, resp.

Figure 1 exemplarily shows the determination of the coverage dependent surface band bending and the increasing intensity of the corresponding 2DEG peak. In this experiment Nb was evaporated at room temperature. Obviously, the growing intensity with increasing coverage is directly correlated with the increasing electron density of the 2DEG. Figure 1c demonstrates a dispersion effect showing the angular dependence of the 2DEG peak. The peak maximum slightly shifts to higher energies with increasing detection angle.
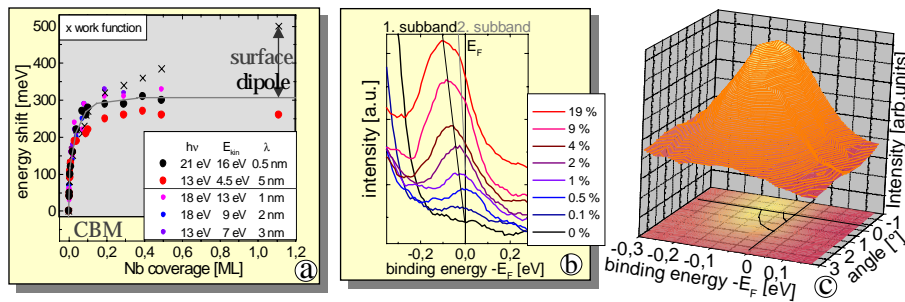
Figure 1: (a) Energetic shift of the valence band peak on the InAs spectrum as a function of the Nb coverage. The corresponding excitation energy (hν), kinetic energy of the photoelectrons (E_{kin}) and the estimated escape depth (λ) are given. The solid line marks the resulting surface band bending. (b) The 2DEG peak measured at hν = 13eV and different Nb coverages. The expected subband energies are marked as lines. (c) Angular dependence of the 2DEG peak at hν = 13eV for 8% Nb coverage. In the x-y-plane the expected dispersion of both subbands are given.

SOFT X-RAY ABSORPTION SPECTROSCOPY (Mn-L$_{2,3}$, O-K) IN MIXED VALENCE MANGANITES.

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In mixed valence materials, like $RE_{1-x}A_xMnO_3$ (RE being a trivalent rare-earth cation and A a divalent cation), the extra charges induced by partial substitution of the rare-earth site are expected to go to states of mixed transition-metal 3d-oxygen 2p character, within the framework of the Zaanen-Sawatzky-Allen model [1]. The purpose of this work was to check the validity of this model in a wide range of doped manganites by means of X-ray absorption spectroscopy at both, Mn-L$_{2,3}$ and O-K edges.

XANES spectra of REMnO$_3$, $RE_{1-x}Ca_xMnO_3$ (RE=La, Tb) and $RE_{0.5}A_{0.5}MnO_3$ (RE-A= LaCa, TbCa, PrCa, PrSr) were measured at the beamline ID12B at ESRF, by recording the total electron yield. Experiments were carried out as a function of temperature up to room temperature. The Mn 2p spectra shift towards higher energies with increasing the formal valence of the sample, as it occurs for the Mn K-edge XANES spectra [2]. Moreover, the spectral shape change slightly with both, the doping rate and the different rare-earth cations. However, the O 1s spectra are much more sensitive to the variations in the rare-earth atoms. The spectra at the O K-edge show a prepeak at the Fermi energy corresponded to empty states in the O-2p band. This prepeak shifts to lower energies and increases the intensity with the divalent metal content. A double structure is observed for this prepeak in REMnO$_3$ samples. Similarly to the Mn K-edge results [2], neither the O-K edge nor the Mn-L$_{2,3}$ edge XANES spectra of the intermediate compounds cannot be reproduced by a weighted linear combination of the REMnO$_3$ and CaMnO$_3$ ones.

Finally, a comparison between the O K-edge and the Mn K-edge spectra indicates that the first excited states in these systems are mainly of 2p oxygen character, strongly hybridized with the Mn 3d states, so the conduction electrons move in the oxygen 2p band. Therefore, new models based on many-body interaction effects are needed for well understanding these results.

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Temperature-Dependent High-Resolution Photoemission Spectroscopy of $YbMCu_4$ (M=In, Cd, Mg)

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We have investigated the electronic structure near the Fermi level (E_F) of $YbMCu_4$ (M=In, Cd, Mg) from 10 K to room temperature (RT) by means of the high-resolution (~5 meV) photo-emission spectroscopy (UPS) with an excitation photon energy $h\nu$=21.22 eV. The Yb 4d x-ray photoemission (XPS) experiments with an Al K_α line were also carried out in order to investigate the valence of the Yb atom. Among three compounds, $YbInCu_4$ exhibits a first order valence transition at T_v=42 K where the Yb changes from a nearly trivalent at high temperature to a mixed valent state (z~2.8) at low temperature [1].

For $YbInCu_4$ and $YbCdCu_4$, the prominent peak due to the Yb^{2+} $4f_{7/2}$ states are clearly observed near E_F at 10 K in the UPS spectra. The energy positions of the Yb^{2+} $4f_{7/2}$ peaks of $YbInCu_4$ and $YbCdCu_4$ are 46 and 31 meV, respectively. A deeper binding energy for $YbInCu_4$ qualitatively corresponds to the higher Kondo temperature (~430 K for $YbInCu_4$ [2] and ~220 K for $YbCdCu_4$ [3]). These peaks almost disappear at RT for both compounds. With the decrease of temperature from RT to 50 K, the peaks gradually gain intensity and their energy positions shift toward E_F side, which is similar to the result for $YbAgCu_4$ [4]. From 50 to 10 K, the peak intensity of $YbInCu_4$ becomes drastically high and the energy position shifts toward the deeper side. On the other hand, the peak of $YbCdCu_4$ shows the monotonous temperature dependence like from RT to 50 K. The drastic change of the Yb^{2+} $4f_{7/2}$ peak of $YbInCu_4$ suggests that the electronic structure changes due to the valence transition at T_v. For $YbMgCu_4$, the Yb^{2+} $4f_{7/2}$ states appear as a broad structure in the UPS spectra and the spectra show few temperature dependence, which means the Yb 4f states only in $YbMgCu_4$ is different from those in $YbInCu_4$ and $YbCdCu_4$.

In the Yb 4d XPS spectra of $YbInCu_4$ and $YbCdCu_4$, the structures due to the Yb^{2+} and Yb^{3+} states are observed. For both compounds, the Yb^{2+} exist even at RT and with the decrease of temperature, the structure due to Yb^{2+} states gradually grows in intensity, while the intensity of the Yb^{3+} structure decreases. Drastic change caused by the valence transition of $YbInCu_4$ has been not clearly been observed. On the other hand, the Yb in $YbMgCu_4$ is almost divalent states.

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ANGLE-RESOLVED PHOTOEMISSION STUDY OF CHARGE-DENSITY-WAVE STATES IN 1T-TaS$_x$Se$_{2-x}$

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We have investigated the electronic structures of metal-to-insulator transitions due to charge-density-wave (CDW) phase transitions in 1T-TaS$_x$Se$_{2-x}$ by angle-resolved photoemission spectroscopy.

In the insulating phase of the sample with x=1.5, we observe a gap formation caused by a phase transition from nearly-commensurate CDW to commensurate CDW. On the other hand, in the metallic phase of the sample with x=1.2, we don't observe a drastic change in the spectra between at room temperature and at low temperature. These results agree with the physical properties such as electrical resistivities [1].

In the sample with x=1.5, we observe the lower Hubbard band which is also observed in 1T-TaS$_2$ [2]. In the metallic phase of the sample with x=1.2, the peak intensity is smaller and the peak energy shifts to E$_F$, but the peak still remains. These electronic structures are comparable to those of strongly correlated materials [3]. From these results, it is confirmed experimentally that the metal-to-insulator transition of 1T-TaS$_x$Se$_{2-x}$ is due to the Mott localization.
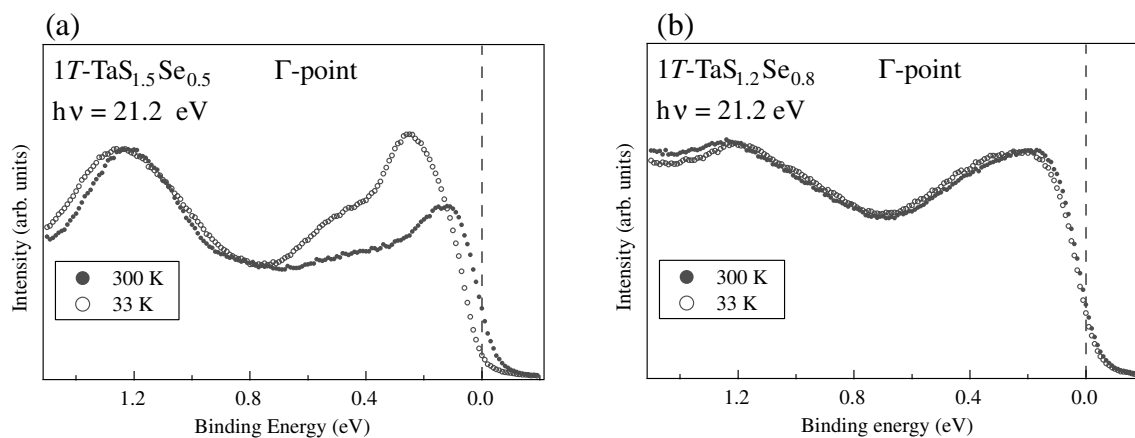
Figure 1: Γ-point photoemission spectra at room temperature (300 K) and low temperature (33 K) for (a) 1T-TaS$_{1.5}$Se$_{0.5}$ and (b) 1T-TaS$_{1.2}$Se$_{0.8}$.

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TIME RESOLVED PHOTOLUMINESCENCE INNER CORE EXCITATION IN ZnCdSe MQWs

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The core hole generation in quantum confinement structures gives rise to several interesting physical problems such as 1)hetero interface core excitons, 2)competition between core hole potential and quantum confinement potential, and 3)core hole decay dynamics in the confinement structures.
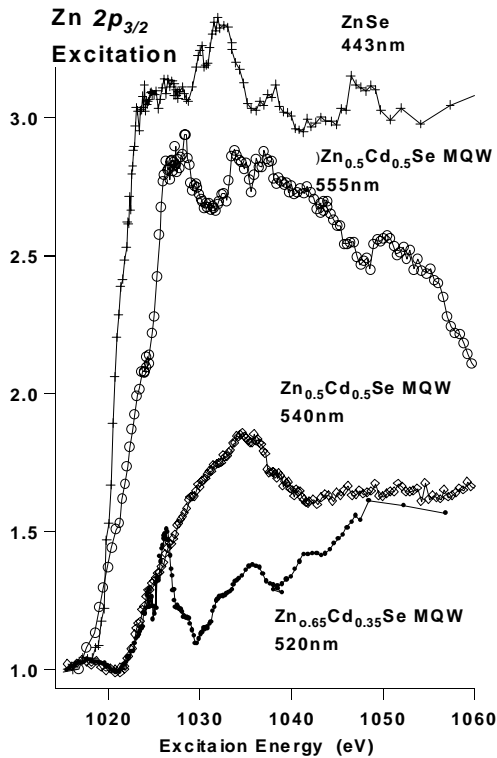
We have applied photoluminescence inner core excitation (PLICE) as a local probe for these problems in several semiconductor quantum structures[1]. The results strongly suggest that the excitation spectra probe the buried quantum structures, however, they still provide no sound evidence that proves the degree of local sensitivity. Inevitable involvement of hot electron-hole pair generation due to Auger decay of core holes, and their diffusion are thought to degrade the local sensitivity in the steady state measurements.

Here we report our recent time resolved (tr) PLICE measurements, which we performed to improve the local sensitivity of the method, in ZnSe single crystal thin layers and ZnCdSe multi quantum wells (MQW) on GaAs substrates. The experiments were done at BL19B of Photon Factory, KEK. The photoluminescence (PL) fundamental band peaks at around 443nm in ZnSe. In case of MQWs, it peaks in the range of 520nm-555nm, corresponding to the degree of confinement. These bands show a very fast component, of which profile is determined by SR bunch profile, and two delayed components with latent time of 0.3nsec and 1nsec. The excitation spectra of integrated fast PL bands in the Zn 2p excitation regime is shown in the figure. The results clearly indicate that the confinement potential drastically affects the core absorption in the quantum structures, and that tr-PLICE has high local sensitivity for the study of the problems mentioned above.

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Electronic Structure of oxidic Perovskites:
X-ray Fluorescence Measurements on $KTaO_3$, $KNbO_3$ and Sr_2FeMoO_6

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Oxidic perovskites, commonly described as ABO_3, exhibit a huge variety of possible applications. Ferroelectric materials with perovskite structure like $KTaO_3$ and $KNbO_3$ are of great interest in modern technology like optical signal processing, holographic storage and phase conjugation [1]. Another class of oxidic perovskites are materials with odered double-perovskite ($A_2BB'O_6$) structure. Some of them show a colossal magnetorestance (CMR) effect. This effect is attracting interest from both fundamental and practical point of view. The CMR effect in Sr_2FeMoO_6 has been reported recently and is quite peculiar since it is a high temperature and low field MR linked to the half-metalllic state of the compound [2,3].

The electronic structure of the investigated perovskites is quite different, but some similarities can be observed: The valence band is formed by oxygen 2p states hybridized with the metal nd states (metal on the B-site) while the A-site metal has no contribution to the valence band [2,3,4]. In order to measure the partial density of states (pDOS) of each relevant state we used synchrotron radiation at the ALS Beamline 8.0.1 for excitation and the University of Tennessee's fluorescence spectrometer for monitoring the photon emission process.

To check the O 2p contribution to the empty states we first measured the absorption spectra at the O Kα -edge. Furthermore we measured the emission spectra at various excitation energies below, at and above the absorption edge. In case of $KTaO_3$ and Sr_2FeMoO_6 , no excitation energy dependence could be observed while in $KNbO_3$ the position of the emission maximum shifted slightly with excitation energy. The emission spectra taken at the Ta N_{III} – edge (Ta 5d $\rightarrow$ 4p) in $KTaO_3$ show a strong dependence on the excitation energy. This behaviour can be explained by the transition out of different states in the valence band: at excitation energies just above the absorption threshold an emission from the bottom of the valence band can be found whereas at higher excitation energies an emission from the middle of the valence band is observed. Fe $L_{2,3}$ and Mo $M_{2,3}$ in Sr_2FeMoO_6 show a similar behaviour. In $KNbO_3$ the contribution of the 5p states to the valence band was investigated via the energy dependent Nb $M_{4,5}$ emission. The shape of all absorption and emission spectra are compared with calculations done on the basis of the all-electron full-potential linearized augmented plain-wave method (FLAPW), convoluted with the experimental resolution and lifetime broadening.

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PHOTOEMISSION STUDIES OF STRONGLY CORRELATED NICKEL COMPOUNDS

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High resolution core level photoelectron spectra and resonant photoemission detected in the valence band spectra of strongly correlated materials can reveal the extent of electronic correlations in these compounds [1]. Recently, a systematic investigation of Ni compounds has been reported with the aim to relate the lineshape of Ni 2p core lines to the Ni-O coordination [2]. We present photoemission data from NiO single crystals and compare them to the results obtained from several divalent nickel compounds with the aim to show the effect of ligand on the satellite features observed both in core level and valence band spectra. In the case of NiO, we show that the giant resonant features observed in the valence band spectra collected at the Ni 2p-3d absorption threshold can be consistently interpreted on the basis of an impurity cluster calculation where the multiplet splitting is fully accounted for by using a configuration interaction scheme.

These results are compared to those obtained from the analysis of K_2NiF_4 [3] and NiS_2 [4]. While NiO is an insulator, NiS_2 is a semiconductor and K_2NiF_4 is a strongly insulating layered perovskite. The differences observed in the satellite features of both valence band and Ni 2p core level data can be ascribed to differences in the Ni-ligand bond, which ultimately affect the energy gap of these compounds. An estimate of the ligand-metal charge transfer energy, calculated on the basis of the impurity cluster model, is given, which scales with the energy gap of these materials.

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Fermi surface of Bi-cuprates

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The topology of the Fermi surface is one of the most important normal state properties of the HTSC's. Its exact determination is the input for predictions of the physical properties of the HTSC's. Over the last years, about all information about the Fermi surface topology has been derived from ARPES studies on Bi-2212, namely $Bi_2Sr_2CaCu_2O_8$. Besides sample quality leading to scattering and therewith broadening furthermore the magnitude of the bilayer splitting for n=2 compounds [1,2] makes it difficult to determine the exact shape of the Fermi surface. In the case of $Bi_2Sr_{2-x}La_xCuO_6$ with different doping levels and only one CuO_2 layer per unit cell a number of these parameters can be controlled in a way that the intrinsic linewidth and dispersion can be determined more unequivocally. In this contribution we investigate the Fermi surface of n=1 material at various photon energies and polarization geometries by angle resolved photoemission with very high energy and momentum resolution. Our results show the importance of matrix element effects in ARPES for determining the exact shape of the Fermi surface. Additionally we report ARPES measurements for various doping levels of the system $Bi_2Sr_{2-x}La_xCuO_6$. In the context of the current debate on the overall Fermi surface topology our results confirm the view of a hole like Fermi surface for n=1 material over a wide doping range. Furthermore a small splitting of the Zhang-Rice singlet near E_F could be resolved and traced along major symmetry lines in accordance to recent findings [3]. It will be discussed in the context of the results of Feng [1] and Chuang [2] and its relation to current theoretical models of the spectral function of HTSC's. Finally the results from Fermi surface mapping of triple layered $Bi_2Sr_2Ca_2Cu_3O_{10}$ will be presented.

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OVERDOPED CUPRATES AS QUASIPARTICLE LIQUIDS

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The question as to whether the Fermi Liquid model is a valid description of the electronic state of the cuprate superconductors is one of the central questions in condensed matter physics. It is generally believed that the underdoped cuprates are not Fermi liquids while samples that are overdoped enough probably are, though there is little data to this effect. This presentation describes extensive Angular Resolved Photoemission (ARPES) measurements on highly overdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ samples with T_C as low as 51K. The results are analyzed with respect to previous work on under and optimally doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ as well as ARPES of metal surface states. We find that several features of the ARPES data favour a quasiparticle description of the single electron excitations. Among these are that the self energy is only weakly **k** dependent and transport is simply related to the quasiparticle lifetime. Also, the single electron excitation is well defined for a wider range of **k** values and energies than for the lesser-doped cuprates but not so well defined as in metals. Sample data illustrating this point are shown in the figure below, with data for the overdoped sample, an optimally doped cuprate [1], and a Mo surface state [2]. The detailed behaviour of these quasiparticles is not described by a simple Fermi Liquid description nor is it similar to regular metallic states where electron-phonon interactions dominate for most temperatures of interest. We are thus led to believe that the overdoped cuprates form a quasiparticle liquid, but that the dominant interactions for the electrons in this system are similar to but weaker than those found at lower doping levels.
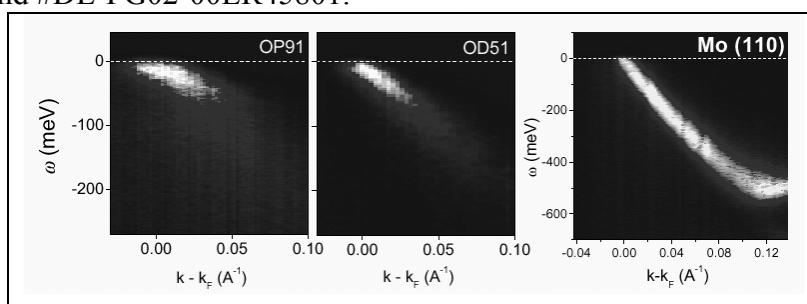
Figure 1: Intensity (by colour) versus energy and momentum for three samples. Left to right they are an optimally doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ sample [1], the overdoped sample, and a Mo (110) surface state [2].

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X-ray emission and absorption spectra and electronic structure of MgB_2

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The results of measurements of soft X-ray emission spectra of constituents of new superconductor MgB_2 (T_c=39 K) [1-2] are presented. B K-emission and absorption and Mg L-emission and absorption spectra are measured using sintered powder samples of MgB_2. According to dipole selection rules these spectra probe the distribution of B 2p and Mg 3s-states, respectively. The spectra are converted to the binding energy scale with help of additional XPS B 1s and Mg 2p measurements. The obtained results are compared with first principles band structure calculations [3]. The experimental spectra are found in a good agreement with partial density of states and theoretical X-ray spectra which are calculated taking into account the matrix element of transition probability.

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RESONANT INELASTIC SOFT X-RAY SCATTERING OF INSULATING CUPRATES

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The low energy excitations of cuprates are receiving considerable attention in current literature. It would be particularly interesting to establish a relationship between the behavior of these excitations and the manifold of low temperature phase transitions found in cuprates. Several insulating cuprates are parent compounds of a family of superconductors when doped, such as the antiferromagnetic La_2CuO_4 and the $La_{1-x}Sr_xCuO_4$ high-temperature superconductor family. $CuGeO_3$, another insulating cuprate shows an unusual Spin-Peierls transition at low temperature.

We have studied La_2CuO_4, $SrCuO_2$, CuO, and $CuGeO_3$ using resonant soft x-ray emission spectroscopy (RSXES). The features in the RSXES spectra excited at the Cu 3p- and 3s-resonance disperse linearly with incident x-ray energy and can be understood as resonant inelastic x-ray scattering (RIXS) as described by the Kramers-Heisenberg formula. The energy loss of the scattering corresponds to the excitation energy of this structure, which can be easily obtained by taking the difference of elastic and inelastic peak energy. In an ionic picture, we are dealing with crystal field or dd-excitations of the Cu^{2+}-ion. With our method we can establish the excitation energy with high precision (better than ±0.1eV) and good signal-to-noise ratio.

On the other hand, the RSXES spectra excited at the O1s-resonance must be interpreted as consisting of one part that reflects the partial density of states and another part that is due to a local excitation [1]. The RIXS energy loss shows an interesting variation between the different compounds and varies between 1.6 eV for $CuGeO_3$ and 2.3 eV for La_2CuO_4. This cannot easily be reconciled with theoretical expectations for the excitation energies of dd-excitations. We therefore attribute some of the structures to the formation of a Zhang-Rice singlet (ZRS) [2]. A ZRS is an excitation that involves a charge transfer from a Cu to an O-atom and is considered as the lowest ionization state. Although it is very prominent in the RIXS spectra of insulating cuprates, ZRS are difficult to observe in valence band photoemission.

First theoretical discussions and model calculations have recently been published by Okada et al. [3] and corroborate our interpretation of the O1s-RIXS structures in cuprates. We conclude that further investigation of these excitations with RIXS can provide valuable new insight into the low energy excitations of cuprates.

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SYNCHROTRON-LIGHT ABSORPTION SPECTROSCOPY STUDY OF MAGNETIC HIGH TEMPERATURE SUPERCONDUCTORS

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Synchrotron-light absorption spectroscopy was used to study a new, recently discovered class of magnetic high temperature superconductors. These compounds are based on BiPbSrCaCuO single crystals which are made magnetic (paramagnetic and ferromagnetic) by doping with rare earth atoms. Their superconducting and magnetic properties as well as other characteristics were intensively investigated with a variety of techniques including crystallography, infrared spectroscopy, transport measurements, SQUID measurements, chemical microprobe analysis and others. The results clearly demonstrated the coexistence of magnetism and superconductivity in the same phase.[1] However, these data do not elucidate the electronic structure nor the origin of this exotic and interesting phenomenon.

The present study provides valuable information on the unresolved issues, based on absorption data taken at the O1s and Cu 2p absorption edges. Data obtained with high energy resolution explored the effects of doping on the electronic structure. The possible implications on the coexistence of two seemingly antagonistic phenomena—ferromagnetism and superconductivity—will be discussed.

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Quantization of electronic states in an ultrathin rare-earth film: Gd/W(110)

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In recent years quantized electronic states have been identified by photoelectron spectroscopy in several noble-metal and transition-metal systems [1]. For magnetism, these observations were particularly interesting since the observation of quantized states could be related to long-range magnetic coupling effects, for instance in the giant-magnetoresistance system Co/Cu/Co(100) [2]. In this case, the s,p conduction electrons in the Cu mediate the long-range magnetic coupling between the ferromagnetic Co layers. In this respect the Cu interlayer acts analogously to the noble-metal host in a spin glass: the s,p conduction electrons mediate the oscillatory magnetic coupling between the localized moments of the dilute transition metal, the so-called RKKY interaction

In rare-earth metals the localized 4f magnetic moments also interact in the same way. In this case the delocalized 5d6s electrons are magnetically polarized by the 4f electrons and mediate the long range order of the 4f moments. Despite a large amount of photoemission studies on rare-earth thin films, quantization effects in the electronic structure have to date not been reported.

We report on normal-emission photoemission spectra of Gd films on W(110) for various thicknesses. The spectral features show a strong dependence on the deposited Gd mass up to at least 4 monolayers (ML). Strong changes occur in the whole spectrum upon increasing the thickness from 1 to 2 ML. Around 3 ML, the spectra change again. In particular, individual peaks in the energy range around 3 eV binding energy can be distinguished and assigned to the formation of quantum-well states confined through the existence of a W bulk band gap extending from about 6 eV to about 2 eV binding energy.

In the energy range near the Fermi level, on the other hand, particularly sharp peaks develop from about 2 ML Gd on. These peaks cannot be assinged to a parent Gd bulk band. We present a simple interpretation of these features on the basis of Gd quantum-well states in resonance with W substrate-derived electronic states. In brief, the states formed are similar to image-potential states but shifted towards lower energies due to a resonant interaction with the W substrate.

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High-resolution ARPES investigation of the quasiparticle scattering processes in a Model Fermi liquid: 1T-TiTe$_2$

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We performed high resolution ARPES and resistivity measurements on the metallic quasi-2D system TiTe2. We found that the quasi-particle lifetime is in excellent agreement with transport relaxation time. Moreover we characterize and separately evaluate the effect of electron-electron, electron-phonon, and electron-defect interactions on the experimental lineshape. A residual low temperature spectral linewidth (Γ_0=17 meV) indicates that the three dimensional nature of the electronic states cannot be neglected even in this quasi-2D material.

Strongly correlated normal state and the peierls transition in 1D charge-density-wave systems

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We have studied by high-resolution ARPES the metallic normal states and the insulating CDW phases of the typical quasi-1D Peierls system $(TaSe_4)_2I$. In the normal state we observe quasiparticles heavily dressed by phonons. The large spectral weight renormalization is at the origin of a deep pseudogap around the Fermi level. Remarkably, most of the spectral weight is distributed along the calculated one-particle bands, notwithstanding the largely renormalized mass. The temperature-dependent ARPES spectra illustrate the opening of real gaps below the Peierls transition temperature. In contrast with conventional scenarios, the gap energy is not directly related to the binding energy of the main dispersing spectral feature.

Competing periodic potentials: energy eigenvalues and spectral weight

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Translational symmetry is a key ingredient for the description of the electronic structure of solids. The dispersion of the electronic states, and ultimately, the physical properties of a material, reflect the periodicity of the lattice potential. When the electrons feel two competing periodicities, the band structure may be deeply modified. This situation is actually realized in low-dimensional charge-density-wave (CDW) systems, because the periodicity of the CDW is not directly related to the lattice parameter. Incommensurate potentials are expected to yield localized wavefunctions and a fractal spectrum. We used ARPES to investigate this effect in the 1D system $(TaSe_4)_2I$. We show that while the energy eigenvalues may indeed have a fractal structure, the spectral weight, measured by ARPES, is non-uniform, and exhibits signatures of both periodicities. Model calculations highlight the importance of the relative strength of the two potentials.

PHOTOEMISSION STUDIES OF $R_{1-x}Ca_xBa_2Cu_3O_{6+d}$ (R=Y, Eu) IN THE INSULATOR TO METAL TRANSITION

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The valence band and core level states of $R_{1-x}Ca_xBa_2Cu_3O_{6+d}$ (R=Y, Eu) were studied by means of angle integrated photoemission. Changes of the electronic structure in the insulator to metal transition as an effect of doping were examined. Studies have been performed for deoxygenated $YBa_2Cu_3O_{6.16}$, $EuBa_2Cu_3O_{6.06}$, $Y_{0.84}Ca_{0.16}Ba_2Cu_3O_{6.09}$, $Eu_{0.85}Ca_{0.15}Ba_2Cu_3O_{6.18}$, $Y_{0.7}Ca_{0.3}Ba_2Cu_3O_{6.12}$ and $Eu_{0.7}Ca_{0.3}Ba_2Cu_3O_{6.13}$ as well as for high T_c samples $YBa_2Cu_3O_{6.91}$ and $EuBa_2Cu_3O_{6.93}$. The last two were superconducting below 91.4 K and 93.3 K respectively. The deoxygenated samples with Ca content of 0.3 were superconducting below approximately 20 K.

The valence band studies reveal that a peak appears at 2.4 eV below the Fermi level and grows systematically with hole doping (Figure 1). This feature is characteristic of a metal-insulator transition and is common for both calcium and oxygen doping. This structure is interpreted to originate from the Zhang-Rice singlets. The Cu 3d level spectra confirm a higher population of the $3d^9\underline{L}$ states in the oxygenated samples. An additional doublet in the Ba 4d level appears for oxygenated samples, what proves that oxygen doping also affects the electronic structure of Ba. No changes in Y 3d level were observed.
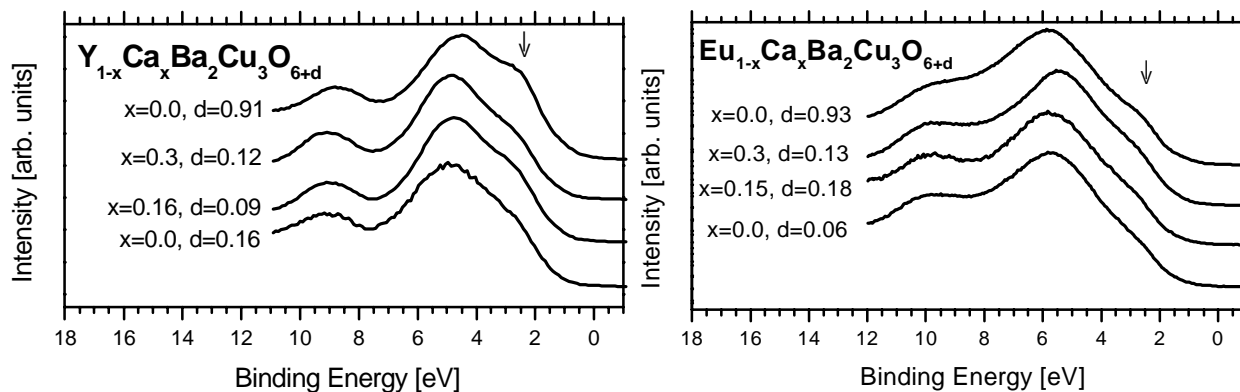

Figure 1: The valence band spectra measured with He-I radiation

The parameters of the electronic structure were determined by the cluster model calculations [1] and are listed as follows: the charge transfer energy between Cu 3d and O 2p states $\Delta \sim 1$ to 2 eV, the hopping integral between Cu 2p and Cu 3d states $T \sim 2.5$ to 3.5 eV and the onsite Coulomb repulsion in the 3d Cu states $U_{dd} \sim 6.5$ eV.

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ANALYSIS OF THE ELECTRONIC STRUCTURE IN K-DOPED AND NON-DOPED QUASI-ONE-DIMENSIONAL MONOPHOSPHATE TUNGSTEN BRONZES

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The monophosphate tungsten bronzes (MPTB) exhibit quasi-low-dimensional structural and electronic-transport properties similar to those observed in the molybdenum bronzes [1,2]. Their structure is characterized by ReO_3-type slabs of WO_6 octahedra connected by PO_4 tetrahedra that form tunnels between the W-O layers. There are different MPTB structures, corresponding to the non-doped and doped compounds. In both cases, the crystalline structures are quite similar, but in the non-doped ones the tunnels are pentagonal ($MPTB_p$) while in the doped ones they are hexagonal ($MPTB_h$), due to the placement of the doping atoms in these channels [3]. Theoretical calculations show that the electronic structure of both compounds exhibits 1D and 2D-like bands. It is suggested that the existence of a Charge Density Wave (CDW) [4] is due to the 1D nested Fermi surface [5].

In this work, we report synchrotron-radiation excited Angle Resolved Photoemission measurements of the MPTBp and K-doped MPTBh compounds, above the critical temperature. The experiments were done at the SU8 beamline at LURE. One of the main characteristics of this experimental set up is that it is designed in such a way that it is possible to distinguish the symmetry of the initial states. The electronic band structure of $MPTB_p$ and $MPTB_h$ was measured along different high symmetry directions within the two symmetry detections. The 1D and 2D conduction contributions have been identified. The experimental Fermi surface (FS) was also obtained. The analysis reveals the existence of some parallel portions, typical of nesting.

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Electronic changes related to the metal to insulator phase transition in RNiO$_3$

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The transition metal oxides exhibit a fascinating variety of physical properties ranging from high-T_C superconductivity to colossal magnetoresistance. In particular, rare earth (R) nickel oxide perovskites (nikelates, RNiO$_3$) show, except for LaNiO$_3$, metal-insulator (MI) phase transition as temperature decreases. The transition temperature (T_{MI}) increases, as the R-ion becomes smaller [1]. These nickelates present also, at low temperatures, a complex antiferromagnetic order. For light R-ions (e.g. Pr and Nd), the antiferromagnetic transition temperature (T_N) coincides with T_{MI}. However, for heavy R-ions (e.g. Eu, Sm), T_{MI} and T_N are very far apart, suggesting that the magnetic and electronic behaviors are not directly coupled.
Nickelates crystallize in a distorted perovskite structure, where the NiO$_6$ octahedra tilt and rotate to fill the empty space left around the R-ion. The degree of distortion, measured by the angle Ni-O-Ni, increases as the size of R becomes smaller, i.e., for heavier R-ions. Obviously, one can correlate the degree of distortion with T_{MI} and the electronic properties of these systems.
In the framework of the Zaanen-Sawatsky-Allen scheme [2], the electronic structure of transition metal compounds is classified either into the Mott-Hubbard or charge transfer regime. In the Mott-Hubbard regime the Coulomb repulsion energy U is smaller than the ligand-to-metal charge-transfer energy Δ, and the gap is controlled by U. In the charge transfer regime, $\Delta<U$ and the gap is controlled by Δ. RNiO$_3$ perovskites are placed in the boundary of these two regimes. However, there are several evidences [3] pointing to a charge transfer gap, mainly controlled by Δ, and then strongly dependent on hybridization.
This question motivated us to study RNiO$_3$ systems using Ni L-edge absorption spectroscopy (transition $2p\rightarrow3d$). This technique gives direct information on the density of Ni $3d$ empty states, in particular on the multiplet splitting and on the hybridization between Ni$3d$ and O$2p$ bands. Measurements were performed at SXS beam line in LNLS, Brazil. The Ni L$_{III}$ and L$_{II}$ absorption edges were measured for PrNiO$_3$, NdNiO$_3$ and EuNiO$_3$ (T_{MI} = 135, 200 and 480K). At room temperature, dramatic differences are observed between EuNiO$_3$ (insulating) and the other two samples (metallic). Normalized spectra give evidence for a higher density of 3d unoccupied states and a larger multiplet splitting in the insulating compound. Both effects might be correlated to a decreasing hybridization. The same behavior is observed for NdNiO$_3$ in the insulating phase (at T<200K), showing that the opening of the gap is directly related to the degree of hybridization.

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X-RAY PHOTOELECTRON DETERMINATION OF THE Ln5p,4f – ELECTRONIC STATE DENSITY OF LANTHANIDES IN OXIDES

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Earlier the Ln4f electrons before chemical bond formation were traditionally suggested to be promoted to, for instance, the Ln5d atomic orbitals. The calculation results show that the Ln4f atomic shells can participate directly in the formation of molecular orbitals in lanthanide compounds. This important fact needs experimental corroboration. Another important phenomenon we have thoroughly studied recently is effective participation of the filled inner valence Ln5p atomic shells in formation of the outer (OVMO) and inner (IVMO) valence molecular orbitals. The comparability of the experimental and theoretical partial Ln4f and Ln5p electron densities can serve a criterion of correctness of the electronic structure calculation of lanthanide compounds. The present work analyses the fine structure of the low-energy ($0 - 50$ eV E_b) X-ray photoelectron spectra of lanthanide (La through Lu excepted for Pm) oxides, and compares it with the non-relativistic X_α- Discrete Variation calculation results for the clusters reflecting the close environment of lanthanides in oxides.

The obtained results show that the $Ln4f^n$- electrons of lanthanides in oxides by their spectral parameters have much in common with the M3d- electrons in oxides of the 3d-transition metals, in whose compounds the M3d atomic orbitals take an active part in formation of the molecular orbitals. According to these data, the Ln4f shell in lanthanides is rather outer and can participate in formation of molecular orbitals in compounds. The XPS data at least do not contradict the theoretical suggestion about the significant participation of the Ln4f- electrons in formation of the molecular orbitals in the studied materials. Indeed, the noticeable difference between the experimental and theoretical Ln4f relative line intensities is in agreement with the fact that the atomic wave functions for the Ln4f- electrons can differ from those for the lanthanide ions in compounds. A significant growth of the 4f line intensity (photoemission cross-section) while going from Lu (Z=71) to Hf (Z=72), Ta (Z=73), W (Z=74) and further proves that the Ln4f- electrons in lanthanide oxides are significantly more delocalized than in the further elements.

The spectra in the Ln5p – O2s binding energy region of the studied lanthanide oxides were found to exhibit the complicated structure instead of detached peaks due to the electrons of the $Ln5p_{3/2,5/2}$ and O2s atomic shells. Taking into account the energy differences between the inner (Ln3d) and outer (Ln5p) electronic shells for some metallic lanthanides and their oxides, the Ln5p atomic shells were shown to participate in the formation of the inner valence molecular orbitals. That agrees qualitatively with the calculation results.

XPS STUDY OF $Pr_{1-X}R(Sm, Dy, Tm)_X Ba_2 Cu_3 O_{7-Y}$ TO INVESTIGATE HOW Pr SUBSTITUTION FOR Y AFFECTS SUPERCONDUCTIVITY IN THE $YBa_2 Cu_3 O_{7-Y}$ SYSTEM

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Effect of substituting Pr for Y in the $YBa_2 Cu_3 O_{7-y}$ system still continues to sustain interest for lack of unanimity on how or whether it always quenches superconductivity in it. We have studied the Cu 2p and Ba 3d spectra on four different *in situ* scraped samples to throw further light on this issue. Our study differs from the earlier ones in the sense that hitherto in most studies Y had been partly or wholly replaced only by either Pr or any other rare-earth(R) cation. We, instead, compare the behaviour of a pure $PrBa_2 Cu_3 O_{7-y}$ system with those in which 80% of the Pr is replaced by Sm or Dy or Tm. All the samples were prepared and well characterised in our lab.

The Cu 2p lines can be fit into two components pertaining to the presence of the Cu $3d^9$ and the Cu $3d^9\underline{L}$ states, $\underline{L}$ representing a hole in the ligand. A comparison of their relative intensities that the holes appear to decrease in the order Sm>Dy>Tm. The satellite intensity also shows the same behaviour indicating that the superconducting fraction may also be decreasing in that order. Similarly, the Ba 3d lines are also resolvable into two components corresponding probably to the presence of orthorhombic and tetragonal phases in the samples and their relative intensities also showing that the orthorhombic phase is maximum in the Pr/Sm sample followed by the Pr/Dy and then by the Pr/Tm sample. While the ionic radius of the Sm ion happens to be intermediate between those of Pr and Y, that of Dy nearly equal to that of Y and Tm much smaller than that, it is the Pr/Sm sample that shows the best superconducting attributes and not the Pr/Dy one. The c-axis length also tends to be different in each of the four samples. We take all these aspects into account to present our version of how and when Pr behaves like it does under different conditions and raise a question if the Cu 3d–O 2p hybridization the sole reason for quenching of superconductivity in the $YBa_2 Cu_3 O_{7-y}$ system when Y is replaced by Pr.

High-resolution angle-resolved photoemission study of BaCo$_{1-x}$Ni$_x$S$_2$

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We have performed angle-resolved photoemission spectroscopy (ARPES) on a layered Mott system BaCo$_{1-x}$Ni$_x$S$_2$ across the phase transition from antiferromagnetic insulator to anomalous metal. We found that the valence-band dispersion shows a systematic change as a function of Ni content (x). Overall features of the valence band are well reproduced by the LDA band calculation. Photon-energy-dependent measurement shows the two-dimensional nature of this compound. In the anomalous metallic phase (x=0.28), we found a large Fermi surface centered at M(A) point in good agreement with the band calculation, which predicts the dominant Co (Ni) $3d_{3z^2-r^2}$ character. Comparison between the metallic and insulating (x=0.18) phases indicates that the Hubbard bands in the insulating phase has a remnant of Fermi surface in the metallic phase and gradually evolves into metallic dispersive bands upon carrier doping. We discuss the present results in comparison with high-T_c cuprates.

Ultrasoft X-Ray Spectra of Magnesium Diboride

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At ultrasoft X-ray spectrometer with high resolution the following spectra of MgB_2 were studied: emission K-spectrum of boron, quantum yield spectrum in the range of K-edge of absorption of boron and emission $L_{2,3}$-band of Mg. These spectra are compared with the corresponding spectra of pure boron and metal magnesium.

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