TT 23.23 Mo 14:00 Poster TU D

Strong spin triplet contribution of the first removal state in the insulating regime of Bi-cuprates — •R.-S. Unger[1], C. Janowitz[1], U. Seidel[1], A. Krapf[1], R. Manzke[1], V.A. Gavrichkov[2], and S.G. Ovchinnikov[2] — [1]Humboldt Universität zu Berlin, Institut für Physik, 12489 Berlin — [2]L.V.Kirensky Institute of Physics of the Sibirian Branch of the Russian Academy of Science, Krasnoyarsk, 660036, Russia

The experimental dispersion of the first removal state in the insulating regime of $Bi_2Sr_2Ca_{1-x}Y_xCu_2O_{8+\delta}$ is found to differ significantly from that of other parent materials: oxyclorides and La_2CuO_4. For Y-contents of $0.92 \geq x \geq 0.55$ the crystal lattice parameters a,b,c change very strongly. This (a,b) parameter increase and c parameter decrease results in an unconventional three peak structure at $(0,0);(\frac{\pi}{2},\frac{\pi}{2});(\pi,\pi)$ for $x = 0.92$. We can describe the experimental data only beyond the framework of the 3-band pd-model involving the representations of a new triplet counterpart for the Zhang-Rice singlet state [1]. The former results, obtained on a cuprate with two CuO_2-layers per unit cell, is found to be universal. Measurements on single layered $Bi_2Sr_{2-x}La_xCu_2O_{6+\delta}$ give similar results.
[1] JETP Lett, 80(11) in print. (2004)

TT 23.24 Mo 14:00 Poster TU D

Angular resolved photoemission on Pb-Bi2201: Doping-dependent evolution of the pseudogap in the underdoped case — •L, Dudy[1], B. Müller[1], L. Lasogga[1], A. Krapf[1], H. Dwelk[1], C. Janowitz[1], R. Manzke[1] und H. Höchst[2] — [1]Humboldt Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin — [2]Synchrotron Radiation Center (SRC), Madison/Wisconsin (USA)

In search for the pairing mechanism of the hole doped HTSCs there is still a debate about the pseudogap [1]. Some groups report a vanishing pseudogap around optimum doping [2]. Other measurements show in the overdoped region a smooth convergence of the pseudogap temperature with T_c, which gives the idea to treat the pseudogap state as a normal state precursor of the superconducting gap due to local, dynamic pairing correlations in a state without long range phase coherence[3]. An important point has been observed in the layered cuprates, which show that the pseudogap temperature T^* is almost not dependent of the number of CuO layers[4]. We focus our work on measurements of the Pb and La doped one-layer Bi2201 single crystals. Here we present temperature dependent ARPES data from the optimum doped Pb-Bi2201 ($T_c = 32K$) down to the strongly underdoped ($T_c \sim 0K$) case. The data shows the evolution of the pseudogap temperature T^* and the magnitude Δ^* with respect to doping. [1] T. Timusk et al., Rep. Prog. Phys. **62** (1999), 61-122 [2] J.L. Tallon et. al., Physica C **282-287** (1997) 236-239 [3] V.J. Emery et al., Nature **374** (1995), 434 [4] T. Honma et al., cond-mat/0309597 (2003), accepted for Phys. Rev. B

TT 23.25 Mo 14:00 Poster TU D

Four-Unit-Cell Superstructure in the Optimally Doped $YBa_2Cu_3O_{6.92}$ Superconductor — •Z. Islam[1], X. Liu[2], S.K. Sinha[2], J.C. Lang[1], S.C. Moss[3], D. Haskel[1], G. Srajer[1], P. Wochner[4], D.R. Lee[1], D.R. Haeffner[1], and U. Welp[5] — [1]Advanced Photon Source, ANL, Argonne, USA — [2]University of California, San Diego, USA — [3]University of Houston, USA — [4]MPI f. Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — [5]Materials Science Division, ANL, Argonne, USA

Diffuse x-ray scattering measurements reveal that the optimally doped $YBa_2Cu_3O_{6.92}$ superconductor is intrinsically modulated due to the formation of a kinetically limited 4-unit-cell superlattice, $q_0 = (1/4, 0, 0)$, along the shorter Cu-Cu bonds. Long-range strains emanating from these modulated regions generate an inhomogeneous lattice which may play a fundamentally important role in the electronic properties of yttrium-barium-copper-oxides.

TT 23.26 Mo 14:00 Poster TU D

Competing magnetic instabilities in 214-ruthenates — •P. Steffens[1], O. Schumann[1], O. Friedt[1], M. Braden[1], Y. Sidis[2], J. Kulda[3], S. Nakatsuji[4], N. Kikugawa[4], and Y. Maeno[4] — [1]II. Physikal. Institut, Uni Köln — [2]LLB, France — [3]ILL, France — [4]Kyoto University, Japan

We present the results of inelastic neutron scattering on pure and doped Sr_2RuO_4.

The role of magnetic excitations in the pairing mechanism of the spin-triplet superconductor Sr_2RuO_4 is still unclear. The excitation spectrum is dominated by incommensurate fluctuations (caused by Fermi-surface-nesting) at q=(0.3,0.3,q_l). We determined their anisotropy of in-plane and out-of-plane component. In addition, we found a broad ferromagnetic signal (presumably the γ-band contribution) around q=0.

On minor substitution of Ru^{4+} by Ti^{4+}, the incommensurate fluctuations get enhanced and finally condense into static order. We present first results on the excitation spectra of samples with and without order.

Doping with La increases the number of electrons, and the shift of the nesting signal indicates that the filling occurs predominantly in the one-dimensional bands.

Especially interesting is the phase diagram created by substitution of Sr by Ca. The compounds near $Ca_{1.5}Sr_{0.5}RuO_4$ show almost ferromagnetic behaviour. In contrast to Sr_2RuO_4, the excitation spectrum is dominated by fluctuations at (0.22,0,0). At low energy and temperature the spectrum becomes ferromagnetic.

TT 23.27 Mo 14:00 Poster TU D

Renormalization group studies of pairing mechanism and order parameter symmetry in Sr2RuO4 — •Andrey Katanin[1,2], Arno Kampf[3], and Ivan Leonov[3] — [1]Max-Planck-Institut fuer Festkoerperforschung, 70569 Stuttgart, Germany — [2]Institute of Metal Physics, 620219 Ekaterinburg, Russia — [3]Institut fuer Physik, Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Universitaet Augsburg, 86135 Augsburg, Germany

We study superconducting pairing in Sr2RuO4 by application of the functional renormalization group method combined with the Bethe-Salpeter analysis to realistic 3-band Hubbard model, which describes this compound. The competition of singlet and triplet pairings with different symmetries is investigated within this model. The results are compared to earliar proposals on the mechanism of triplet pairing in Sr2RuO4.

TT 23.28 Mo 14:00 Poster TU D

Magnetic quantum oscillations in the normal and superconducting state of YNi_2B_2C — •O. Ignatchik[1], J. Wosnitza[1], M. Jäckel[1], D. Souptel[2], G. Behr[2], and P. Canfield[3] — [1]Institut für Festkörperphysik, TU Dresden, D-01062 Dresden, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW), D-01069 Dresden, Germany — [3]Ames Laboratory, Iowa State University, Ames, Iowa 50011, USA

The de Haas–van Alphen (dHvA) effect, or quantum oscillations of the magnetization, is the most direct method to study Fermi-surface properties in metals. It is remarkable, that these magnetic quantum oscillations persist deep into the vortex state of many type-II superconductors. The damping of the oscillation amplitude below the upper critical field can be related to the magnitude of the superconducting gap. For YNi_2B_2C, however, quite controversial results for the dHvA signal in the superconducting state have been reported. We will present dHvA measurements of YNi_2B_2C single crystals prepared by different methods. The flux-grown crystals exhibit dHvA oscillation in the superconducting state down to 3 T as reported in literature. However, we observed an unexpectedly sudden vanishing of the dHvA signal in the mixed state for crystals grown by a zone-melting method. The very quick disappearance of the oscillating signal below B_{c2} suggests an unexpected fast opening of a large superconducting gap. At high magnetic fields six different dHvA frequencies could be detected.

TT 23.29 Mo 14:00 Poster TU D

Lattice dynamics and electron-phonon coupling in $YBa_2Cu_4O_8$ — •V. Pankoke[1], R. Heid[2] und K.-P. Bohnen[2] — [1]Forschungszentrum Karlsruhe, Institut für Wissenschaftliches Rechnen, P.O.B. 3640, D-76021 Karlsruhe — [2]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, P.O.B. 3640, D-76021 Karlsruhe

The superconducting properties of YBaCuO depend strongly on the oxygen content thus it is of crucial importance to understand the lattice dynamics and the electron-phonon coupling as function of doping. While it has been possible to investigate these quantities recently with modern ab-initio methods [1] studying doping effects is a much more difficult task due to the loss of translational invariance. Fortunately, some ordered structures exist which can be treated rigorously with moddern density functional methods. Among these $YBa_2Cu_4O_8$ plays a special role due to the fact that this compound contains double Cu-O chains a structural building block which is very rare in the high-T_c ccompounds. Using the density functional perturbation approach we have studied the lattice dynamics and electron-phonon coupling of $YBa_2Cu_4O_8$. Results will be compared with available experimental data. Good agreement between

calculated and measured vibration frequencies was obtained however eigenvectors inferred from experiments differ in some cases substantially from the calculated ones. These differences will also be discussed.
[1] K.-P. Bohnen, R. Heid, M. Krauss, Europhys. Lett. **64**, 104 (2003)

TT 23.30 Mo 14:00 Poster TU D

Electronic structure and weak electron-phonon coupling in TiB_2 — •Eugenio Forzani[1] and Helge Rosner[2] — [1]I. Physikalisches Institut, Universität Göttingen — [2]MPI for Chemical Physics of Solids, Dresden

The Fermi surface of TiB_2 was studied with the de Haas-van Alphen (dHvA) effect in order to clarify the electronic analogies with the previously investigated ZrB_2 [1]. This effort intends to revise a past work [2], which accused sample limitations, and to extend the investigation of the transition metal diborides of the fourth group. For a definite assignment of all the dHvA frequencies the angular dependencies of the extremal cross-section areas are estimated from full-potential band structure calculations [3]. In order to explain the absence of conventional superconductivity also in this diboride compound, the electron-phonon coupling constants are deduced from the experimental and theoretical datas. Developments of the measurement technique and new goals are discussed.
[1] S.L. Drechsler et al., J. of Low Temp. Phys. 131, 5/6 (2003)
[2] T. Tanaka and Y. Ishizawa, J. Phys. C: Solid St. Phys. 13, 6671-6 (1980)
[3] H. Rosner et al., Phys. Rev. B66, 024521 (2002)
*With grant of the Göttingen Graduate School of Physics

TT 23.31 Mo 14:00 Poster TU D

Electronic structure and electron phonon coupling in Sc doped MgB2 — •Vivien Petzold and Helge Rosner — MPI for Chemical Physics of Solids

Recently, Agrestini et al. reported a detailed study of the effects of Sc substitution in $Mg_{1-x}Sc_xB_2$ [1]. For the achievable Sc doping levels (x=0.12...0.27), the compound shows only a very small lattice expansion, allowing this way the separation of lattice and doping effects on the critical temperature $T_c(x)$ and on the frequency $\omega_{E_{2g}}$ of the E_{2g} phonon. To investigate the influence of the Sc concentration x on the electronic properties, we present band structure calculations using different levels of approximation: rigid band and virtual crystal approach as well as supercell calculations and coherent potential approximation. We show that the latter two lead to consistent results with respect to lattice expansion and electronic properties (density of states, Fermi surfaces). We demonstrate that the doping dependent changes in the electronic structure are strongly influenced by the sp^2(B)-d(Sc) hybridization. The dependence of the electronic topological transition proposed by Agrestini et al.[1] from the Sc concentration is discussed.
[1] Agrestini et al. Phys. Rev. B **70** 134514 (2004).

TT 23.32 Mo 14:00 Poster TU D

Observation of a second energy gap in Nb_3Sn — •M. Marz[1], R. Lortz[2], A. Junod[2], W. Goldacker[3], and G. Goll[1] — [1]Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany — [2]Department of Condensed Matter Physics, University of Geneva, CH-1211 Geneva 4, Switzerland — [3]Forschungszentrum Karlsruhe, Institut für Technische Physik, D-76021 Karlsruhe, Germany

Nb_3Sn is a well-known technically applied superconductor with critical temperature $T_c \approx 18\,\mathrm{K}$. Recently, a low-temperature anomaly in the specific-heat data on a particularly dense and homogeneous polycrystalline sample has been interpreted in terms of the presence of a second superconducting gap [1]. We performed point-contact spectroscopy on samples of the same batch using the break-junction technique. A small bar of Nb_3Sn has been broken at liquid-helium temperature in order to obtain a freshly cleaved surface. We measured the differential resistance as a function of applied voltage in the temperature range between 1.5 and 20 K. Several characteristic minima in the dV/dI vs V curves can be interpreted only under the assumption of two superconducting energy gaps in Nb_3Sn. From a comparison with calculated curves for superconductor-superconductor contacts we deduced a large gap $\Delta_L = 3.5 \pm 0.2\,\mathrm{meV}$ and a small gap of $\Delta_S = 0.8 \pm 0.2\,\mathrm{meV}$. This is the first spectroscopic confirmation of two-gap superconductivity in Nb_3Sn. We note that Δ_L is in line with previous tunnelling measurements and the result confirms the interpretation of the specific-heat data.
[1] V. Guritanu *et al.*, Phys. Rev. B (2004) in print.

TT 23.33 Mo 14:00 Poster TU D

Investigation of $CeCoIn_5$/Pt point contacts in the normal and superconducting states — •Stefan Kontermann[1], Gernot Goll[1], Todd Sayles[2], and M. Brian Maple[2] — [1]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe — [2]Institute for Pure and Applied Physical Sciences, University of California, San Diego, La Jolla, CA 92093, USA

The ternary rare-earth compound $CeCoIn_5$ becomes superconducting for temperatures $T \leq 2.3\,\mathrm{K}$, the highest transition temperature among the heavy-fermion superconductors. Power-law behavior of the specific heat and the thermal conductivity in the superconducting state give evidence that the superconductivity in this material is unconventional. We report on investigations of $CeCoIn_5$ by point-contact spectrocopy with Pt as the normal-metal counterelectrode. In the normal state a pronounced asymmetry of the differential resistance dV/dI as a function of applied bias V is observed which becomes more pronounced as the temperature is reduced. For a contact in the ballistic regime the asymmetry can be attributed to the emergence of the coherent heavy-fermion liquid. In the superconducting state Andreev reflection of quasiparticles at a normal metal/superconductor interface leads to characteristic minima in the dV/dI vs V spectra. We measured spectra which show either a reduced resistance for bias $|V| < \Delta/e$ or a single minimum of dI/dV for $V = 0$, i. e. a zero-bias anomaly. The observation of a zero-bias anomaly is expected only if the order parameter exhibits a sign change as a function of $\vec{k}$ which leads to an Andreev bound state at the surface.

TT 23.34 Mo 14:00 Poster TU D

Unusual electronic and magnetic properties of intermetallic antiperovskites — •Claire Loison, Andreas Leithe-Jasper, and Helge Rosner — Max Planck Institut für Chemische Physik fester Stoffe, Nöthnitzerstrasse 40, 01187 Dresden, Germany

In the last years, cubic perovskites XYT_3 (X=Mg,Cu,La..., Y=B,C,N... and T a transition metal) have received considerable attention because of many unusual physical properties caused by different competing interactions. Examples are the recently discovered superconductor $MgCNi_3$ or the non-collinear magnet $CuNMn_3$. Here, we present a systematic study of a series of antiperovskites (RB_xPd_3 where R is a rare-earth metal, and x varies between 0 and 1) using density functional theory (DFT) electronic structure calculations within the local spin density approximation (LSDA). To investigate the role of possible strong Coulomb repulsion we applied as well LSDA+U. We investigate the effects of pressure and doping on the electronic properties and magnetism. In order to interpret the discrepancies between the results on the lattice constants of LaB_xPd_3 as published by Dhar et al.[1] and our theoretical calculations, we examined this compound experimentally too. The insertion of boron in $LaPd_3$ (a=4.1862(1)Å) could not be detected, but the exposure to oxygen resulted in an increased lattice constant of a=4.2368(2)Å close to the value published in [1]. They report a lattice constant independent of x; according to our calculations, it should increase almost linearly and substantially with x. Thus, our results are inconsistent with the formation of LaB_xPd_3.
[1] Dhar et al. Mat. Res. Bull. **16** 1557 (1981).

TT 23.35 Mo 14:00 Poster TU D

Mirage phenomena in quantum corrals of s-wave superconductors — •Markus Schmid and Arno P. Kampf — Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg

We investigate the local density of states (LDOS) for an s-wave superconductor in an elliptic quantum corral. Using a T-matrix analysis we explore the spatial structure of the LDOS in the presence of one or two magnetic/non-magnetic impurities and observe a variety of quantum mirage phenomena. In particular, we discuss mirage effects for localized impurity bound states and analyze the interference patterns for the scattering processes from two magnetic impurities in the quantum corral.

TT 23.36 Mo 14:00 Poster TU D

Josephson current through a Pb/Cu/Pb nanobridge — •Jonas Hanisch[1], Alexander Cosceev[1], Christoph Sürgers[1], Hilbert v. Löhneysen[1,2], and Gernot Goll[1] — [1]Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany — [2]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe, Germany

The superconducting state is a macroscopic quantum state characterized by a macroscopic wave function with amplitude and phase. The