

TT 2 Correlated Electrons - Metal Insulator Transition

Zeit: Freitag 10:15–13:00

Raum: TU H2053

TT 2.1 Fr 10:15 TU H2053

The orbital degree of freedom in single- and bilayered manganites — ●M. MERZ¹, P. REUTLER², B. BÜCHNER², A. REVCOLEVSCHII³, Y. IDZERDA⁴, S. TOKUMITSU⁵, and S. SCHUPPLER⁵ — ¹Inst. für Kristallographie, RWTH-Aachen — ²IFW Dresden — ³Uni. Paris-Sud — ⁴NRL, Washington — ⁵Forschungszentrum Karlsruhe, IFP

Transition metal oxides like the manganites are fascinating materials since their physical properties are intimately connected with an unusual interrelation between spin, charge, and orbital degrees of freedom. Yet, only little is known about the nature of the experimentally observed ordered phases and the principal factors determining the ordering scheme. To better understand the phenomena of charge/orbital ordering (CO/OO) and to isolate the fundamental properties which serve as a driving force for CO/OO we have investigated layered manganites with x-ray diffraction and near-edge x-ray absorption spectroscopy. The current data demonstrate that the energy difference between $d_{3z^2-r^2}$, $d_{3y^2-r^2}$, and $d_{3x^2-r^2}$ orbitals is very small for single- and bilayered systems and indicate that the orbital degree of freedom is determined not only by crystal field effects but also by orbital coupling.

TT 2.2 Fr 10:30 TU H2053

Local Green's operator and its applications to manganites — ●HORACIO ALIAGA — Theo. III, Uni-Augsburg, D-86135 Augsburg, Germany

An algorithm is presented to calculate the electronic local Green's operator for manganites-related hamiltonians. This algorithm is proved to scale linearly with the number of states in the Hilbert-space, is able of parallel implementation, and outperforms computationally the Exact Diagonalization (ED) method for clusters larger than 400 sites. This method together with the Monte Carlo (MC) technique is used to derive new results for the manganites phase diagram for the spatial dimension $D=3$ and half-filling.

TT 2.3 Fr 10:45 TU H2053

Role of lattice distortion and orbital splitting in Mott-Hubbard transitions — ●K. HELD, A. YAMASAKI, R. ARITA, M. FELDBACHER, and O.K. ANDERSEN — MPI for solid state research, Stuttgart

Lattice distortions lift the degeneracy orbitals have e.g. in a cubic phase. By means of a two band model study, we show that even a small splitting of the orbitals can have a dramatic effect, if a system is close to a Mott-Hubbard transition. Then, electronic correlations grossly enhance the splitting. There can be one or two transition in which the two split bands become insulating. We also report on realistic LDA+DMFT (local density approximation + dynamical mean field theory) calculations for the pressure-induced Mott-Hubbard transition in LaMnO_3 at room temperature. Our conclusion is that the Jahn-Teller and GdFeO_3 distortion and its change are essential for the Mott-Hubbard transition.

TT 2.4 Fr 11:00 TU H2053

Electronic gap closure and structural changes in YTiO_3 and LaTiO_3 at high pressures — ●INGO LOA¹, X. WANG¹, K. SYASSEN¹, M. HANFLAND², T. LORENZ³, H. ROTH³, and Y.-L. MATHIS⁴ — ¹Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart — ²European Synchrotron Radiation Facility, F-38043 Grenoble — ³II. Physikalisches Institut, Universität zu Köln, D-50937 Köln — ⁴Forschungszentrum Karlsruhe, ISS/ANKA, D-76021 Karlsruhe

LaTiO_3 and YTiO_3 are two Mott-Hubbard-type insulators that are characterized by a single $3d$ electron occupying t_{2g} orbitals. Both compounds adopt a distorted perovskite-type structure at ambient pressure. We have investigated the pressure-induced changes in the electronic excitation gaps of LaTiO_3 and YTiO_3 by infrared reflection and absorption spectroscopy. These experiments evidence a pressure-induced insulator-to-metal transition in LaTiO_3 near 11 GPa ($T = 300$ K) while YTiO_3 remains insulating to at least 20 GPa. For YTiO_3 we observe a continuous down-shift of the absorption edge from 0.7 eV at ambient conditions to 0.4 eV at 17 GPa. Like in the case of LaTiO_3 this indicates an evolution towards a metallic state at high pressures. The associated structural changes were determined by synchrotron x-ray powder diffraction. We will present detailed information on the equations of state as well as the variations of bond lengths and bond angles as a function of pressure. For YTiO_3 we observe hardly any variation in bond angles with pressure,

which makes it attractive as a model system for theoretical investigations.

TT 2.5 Fr 11:15 TU H2053

Relevance Of Structural Distortions To The Metal Insulator Transition Of Doped LaTiO_3 — ●H. ROTH¹, K. KORDONIS¹, A. KOMAREK¹, M. CWIK¹, N. SCHITTNER¹, J. BAIER¹, M. KRIENER¹, T. LORENZ¹, N. JOHANNSEN¹, T. ZABEL¹, A. EL FILALI¹, G. ANDRÉ², M. BRADEN¹, and A. FREIMUTH¹ — ¹II. Physikalisches Institut, Universität zu Köln — ²Labaroatire Léon Brillouin, Saclay

LaTiO_3 is an antiferromagnetic insulator. Hole-doping suppresses T_N and induces a metal-insulator transition (MIT). We present a systematic study of magnetization, specific heat and resistivity of $\text{La}_{1-x}\text{Sr}_x\text{TiO}_3$ and $\text{LaTiO}_{3+\delta}$. While $\text{La}_{1-x}\text{Sr}_x\text{TiO}_3$ shows a MIT at a hole concentration $n = x \approx 4\%$, the oxygen-doped $\text{LaTiO}_{3+\delta}$ stays insulating up to a much higher charge-carrier concentration $n = 2\delta \approx 8\%$. Thus, the MIT of doped LaTiO_3 cannot be described by band filling alone. X-ray and neutron diffraction show that the orthorhombic splitting ϵ decreases upon doping, too. Both, the magnetic and the metal insulator transition scale with the size of ϵ , indicating that the orbital splitting is crucial for the magnetic and transport behaviour. Another aspect of the MIT in the studied systems is the coexistence of antiferromagnetic order and metallic behaviour in the intermediate doping range ($x \approx 0.05, 0.04 \leq \delta \leq 0.1$).

Supported by the DFG through SFB 608

TT 2.6 Fr 11:30 TU H2053

Charge order, orbital order, and electron localization in the Magnéli phase Ti_4O_7 — ●V. EYERT, U. SCHWINGENSCHLÖGL, and U. ECKERN — Institut für Physik, Universität Augsburg

The metal-insulator transition of the Magnéli phase Ti_4O_7 is studied by means of augmented spherical wave (ASW) electronic structure calculations as based on density functional theory and the local density approximation. The results show that the metal-insulator transition arises from a complex interplay of charge order, orbital order, and singlet formation of those Ti $3d$ states which mediate metal-metal bonding inside the four-atom chains characteristic of the material. Ti_4O_7 thus combines important aspects of Fe_3O_4 and VO_2 . While the charge ordering closely resembles that observed at the Verwey transition, the orbital order and singlet formation appear to be identical to the mechanisms driving the metal-insulator transition of vanadium dioxide.

TT 2.7 Fr 11:45 TU H2053

Local Structure of V_2O_3 in the vicinity of the metal-insulator transition — ●P. PFALZER¹, M. KLEMM¹, M. L. DENBOER² und S. HORN¹ — ¹Universität Augsburg, Lehrstuhl für Experimentalphysik II, Universitätsstr. 1, 86135 Augsburg — ²Queens College of CUNY, 65-30 Kissena Blvd., Flushing, New York 11367, USA

We have measured the temperature dependence of the local structure of V_2O_3 close to the metal-insulator transition (MIT). Polarization dependent EXAFS-measurements give evidence that the emergence of the insulating state is directly connected to the trigonal distortion of the O coordination octahedra, which is determined by the distance of the V atoms along the hexagonal c-axis. While this V-V pair-distance shows a sharp jump exactly at the temperature of the MIT, the properties of the Vanadium bonds in the a-b (basal-)plane are smeared out and no abrupt changes are detected at the MIT. Even in the metallic phase the full trigonal symmetry is not recovered, but a local monoclinic distortion — although significantly reduced in size — persists up to room temperature. This suggests that the driving forces for the MIT are due to interactions between V ions in the basal plane, leading to the insulating state e.g. via changes in hybridization.

TT 2.8 Fr 12:00 TU H2053

Thermal Conductivity, Thermopower, and Figure of Merit of $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ — ●M. KRIENER, K. BERGGOLD, I. KLASSEN, T. LORENZ, C. ZOBEL, and A. FREIMUTH — II. Physikalisches Institut, Universität zu Köln, 50937 Köln

Cobaltates attract strong interest because Co ions have the possibility to occur in different spin states. Especially, LaCoO_3 shows a temperature-induced spin-state transition whose microscopic origin is still discussed controversially. Recently, the layered cobaltate $\text{Na}_x\text{CoO}_2 \cdot y\text{H}_2\text{O}$ attracted

much interest due to its superconductivity and the water-free compound Na_xCoO_2 due to its possible relevance for thermoelectric cooling. Na_xCoO_2 has a low electrical resistivity ρ , a low thermal conductivity κ , and a large thermopower S , leading to a rather large thermoelectric figure of merit $ZT = S^2T / \kappa\rho$ which should approach unity for an effective thermoelectric cooling. In this talk we present a systematic study of the figure of merit on a series of single crystals of $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$. Substituting La^{3+} in LaCoO_3 by Sr^{2+} drives the compound from a nonmagnetic insulator through a spin-glass phase ($x \geq 0.04$) to a ferromagnetic metal for $x \geq 0.18$ [1]. The entire series of $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ has rather low κ values, whereas S strongly decreases with increasing x . For intermediate Sr concentrations in the spin-glass region we find notably large values of Z indicating that Co-based materials could be promising candidates for thermoelectric cooling.

[1] M. Kriener *et al.*, Phys. Rev. B **69**, 094417 (2004)

Supported by the DFG through SFB 608.

TT 2.9 Fr 12:15 TU H2053

Modelling the magnetic susceptibility of LaCoO_3 — •THOMAS MÖLLER^{1,2} and ERWIN MÜLLER-HARTMANN¹ — ¹Institut für Theoretische Physik, — ²II. Physikalisches Institut, Universität zu Köln

LaCoO_3 is a non-magnetic insulator, which develops a Curie susceptibility above ~ 100 K. According to the Hund's rules the 5D -quintet with $S = 2$ (high spin) should form the ground state for the $3d^6$ electron configuration of Co^{3+} . A sufficiently large cubic crystal field breaks Hund's first rule, and the ground state becomes non-magnetic ($S = 0$, low spin). However, this high-spin / low-spin scenario is not in agreement with the experimental results [1]. Radwański and Ropka [2] suggested another model for LaCoO_3 . Here, the ground state is the high spin state, but this multiplet is split by spin orbit coupling and a trigonal Jahn-Teller distortion in such a way that a non-magnetic ground state develops. We calculated the magnetic susceptibility in this model and find a strong anisotropy where the Curie susceptibility disappears in the plane perpendicular to the Jahn-Teller distortion and only a large van-Vleck term remains. For a D_{4h} distortion, this can be explained by pure symmetry. A vanishing Curie susceptibility is found also in case of a D_{3d} distortion, but here the reason is still unclear. Due to its strong anisotropy the T-dependence of the averaged susceptibility $\bar{\chi} = \frac{1}{3}\chi_{\parallel} + \frac{2}{3}\chi_{\perp}$ differs from that observed in LaCoO_3 .

[1] Zobel *et al.*, Phys. Rev. B **66**, 020402(R) (2002)

[2] Radwański and Ropka, Solid State. Comm. **112**, 621 (1999)

TT 2.10 Fr 12:30 TU H2053

Unconventional temperature-dependence of charge order in $\text{La}_{1.8}\text{Sr}_{0.2}\text{NiO}_4$ — •J. SCHLAPPA¹, C. SCHÜSSLER-LANGEHEINE¹, C.-F. CHANG¹, Z. HU¹, M. BENOMAR¹, E. SCHIERLE², H. OTT^{1,2}, E. WESCHKE², G. KAINDL², A. TANAKA³, M. BRADEN¹, and L. H. TJENG¹ — ¹II. Physikalisches Institut, Universität zu Köln — ²Institut für Experimentalphysik, Freie Universität Berlin — ³ADSM, Hiroshima University, Japan

We report on a detailed study of charge order in Sr-doped La_2NiO_4 , using the new technique of resonant soft x-ray diffraction at the Ni $L_{2,3}$ and La $M_{4,5}$ resonances. For $\text{La}_{2-x}\text{Sr}_x\text{NiO}_4$ we observe a decrease of the coherence length of charge order, as determined from the width of the corresponding superstructure peak, not only when the system is heated up, but also when it is cooled below ≈ 65 K. While the superstructure-peak height decreases towards higher temperatures in a way resembling usual 2nd-order phase transitions, the change in the integrated intensity is much smaller, thus showing a behavior that is significantly different from that of the order parameter of other phase transitions. This means that upon heating the charge order breaks into smaller and smaller domains, while inside these domains the character of the order, as given by its period length and the energy dependence of the superstructure peak across the resonance, is conserved. A similar behavior is found upon cooling. A possible reason for this loss of coherence at low-temperatures is the influence of the disorder potential formed by the dopant atoms; a frustration caused by a competing magnetic order appears unlikely considering the observed temperature dependence.

TT 2.11 Fr 12:45 TU H2053

Effect of pressure on the electric transport properties of RNiO_3 — •R. LENGSDORF¹, J.A. ALONSO², D.I. KHOMSKII¹, H. MICKLITZ¹, and M.M. ABD-ELMEGUID¹ — ¹II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — ²Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, E-28049 Madrid, Spain

The temperature-induced metal-insulator (MI) transition in the RNiO_3 series has been ascribed to an opening of a small charge transfer gap at $T < T_{MI}$ which is intimately connected with either a slight but abrupt expansion of the unit cell volume or an orthorhombic ($Pbnm$) to monoclinic ($P2_1/n$) structural transition for large ($R=\text{Pr}, \dots, \text{Eu}$) and small ($R=\text{Dy}, \dots, \text{Lu}$) R^{3+} ions, respectively. The monoclinic symmetry in the insulating state implies two independent Ni-sites and the presence of charge ordering. Experimental evidence for such a charge ordered state in larger R^{3+} nickelates has recently been reported (e.g. EuNiO_3 and NdNiO_3 thin films), supporting the importance of charge ordering for the occurrence of the temperature-induced MI transition. For a deeper understanding of the mechanism of the MI transition in the RNiO_3 series, we have studied the effect of pressure on the transport properties of some selected RNiO_3 ($R=\text{Sm}, \text{Eu}, \text{Y}$ and Lu) oxides. While the monoclinic structure of YNiO_3 ($T_{MI}=582$ K and $T_N=138$ K) and LuNiO_3 ($T_{MI}=599$ K and $T_N=125$ K) remains stable up to 14 GPa and 16 GPa, respectively, the pressure-temperature dependence of the electrical resistance clearly indicates a transition to a metallic state already at $p \geq 5$ GPa. Possible mechanisms responsible for the pressure-induced insulator-metal transition in RNiO_3 series will be discussed.