

agonalization (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 — ²Laboaratoire 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 ($x \approx 0.05, 0.04 \leq \delta \leq 0.1$).

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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 ap-

proximation. 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)

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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,