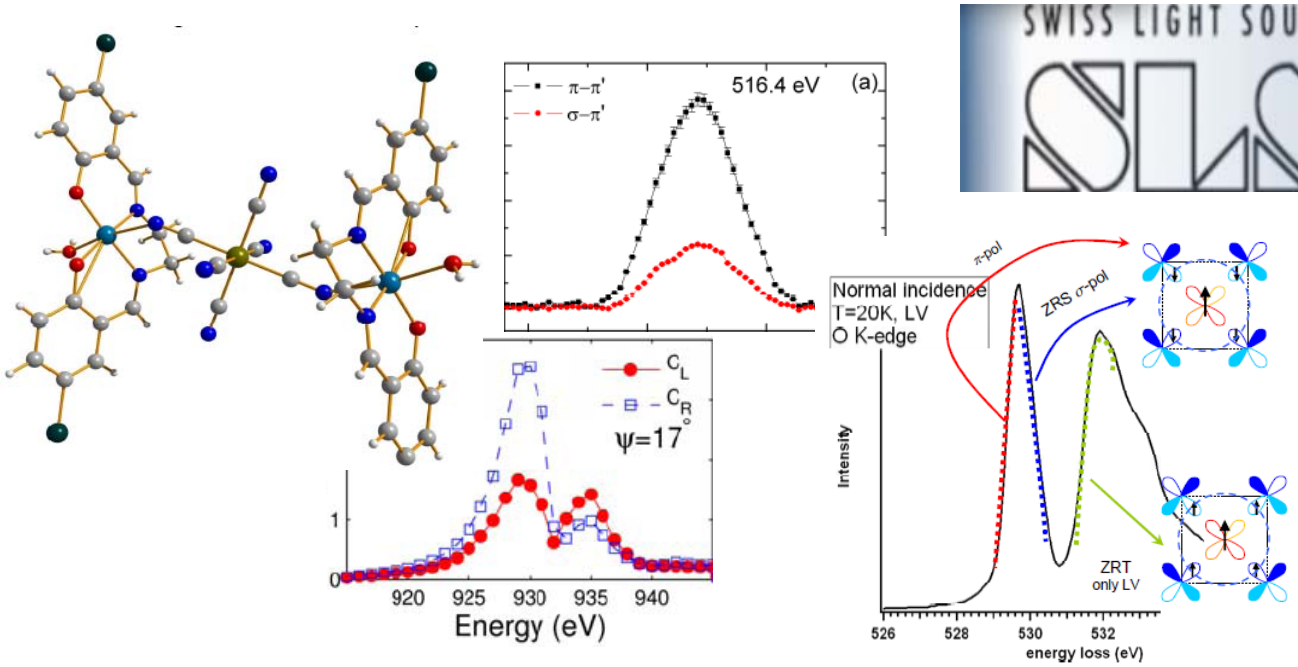

SLS Symposium on

Magnetism and X-Ray Scattering

Tuesday, November 9, 2010

10:00 to 12:15, WBGB/019

10:00 New light on molecular nanomagnets
Jan Dreiser, C. Piamonteze, F. Nolting, S. Rusponi, H. Brune, Kasper S. Pedersen, A. Schnegg, K. Holldack, M. Schau-Magnussen, J. Nehrkorn, O. Waldmann, H. Mutka, P. Tregenna-Piggott, H. Weihe, and J. Bendix

10:30 Resonant Inelastic X-ray Scattering on a prototype edge sharing chain cuprate
Claude Monney, V. Bisogni, K. J. Zhou, R. Kraus, V. N. Strocov, J. Geck, and T. Schmitt

11:00 Coffee

11:15 Cupric Oxide: a model system to explain high-Tc superconductivity?
Valerio Scagnoli, U. Staub, R. de Souza, Y. Bodenthin, M. Garganourakis, A. T. Boothroyd, D. Prabhakaran, and S.W. Lovesey

11:45 Addressing the origin of the low temperature phase transition TX in 1-dimensional $BaVS_3$
Raquel A. de Souza, U. Staub, M. Garganourakis,V. Scagnoli, Y. Bodenthin and H. Berger

New light on molecular nanomagnets

J. Dreiser,[1] C. Piamonteze,[1] F. Nolting,[1] S. Rusponi,[2] H. Brune,[2] Kasper S. Pedersen,[3] A. Schnegg,[4] K. Holldack,[5] M. Schau-Magnussen,[3] J. Nehrkorn,[6] O. Waldmann[6], H. Mutka,[7] P. Tregenna-Piggott,[8] H. Weihe,[3] and J. Bendix[3]

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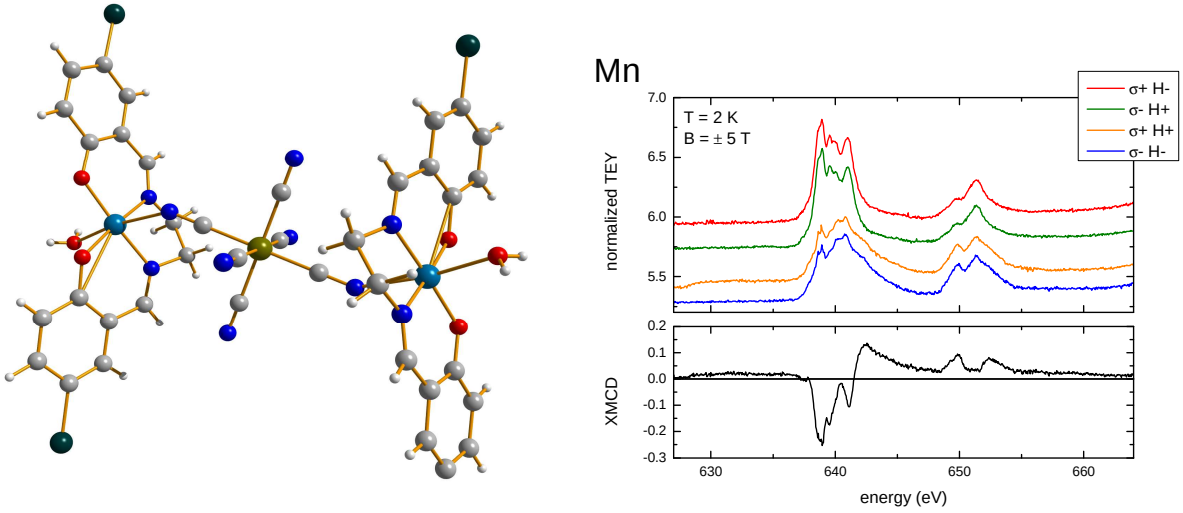
Molecular nanomagnets are exchange-coupled spin clusters which are mostly made of 3d metal ions, but also 4f and higher elements are employed. The so-called single-molecule magnets (SMMs) are part of this intriguing class of materials. SMMs, which became famous because many of them show quantum tunneling of magnetization, exhibit a high-spin ground state and slow relaxation of magnetization. Due to these properties, SMMs are attractive for potential device applications. In recent years, it has been shown that X-ray magnetic circular dichroism (XMCD) is a powerful tool for the investigation of molecular nanomagnets/SMMs because of its element specificity and its ultrahigh sensitivity reaching down to monolayers.

In this contribution we will show some first results obtained at the X-Treme beamline that is currently in the commissioning phase: We have performed XMCD on a powder sample of the trimeric SMM $(NEt_4)[Mn_2(5\text{-Brsalen})_2(MeOH)_2Cr(CN)_6$, in short MnCrMn. By measuring the magnetization of the Mn(III) ions and the Cr(III) ion separately we could directly confirm that in the ground state of the trimer the magnetic moments of Mn(III) and Cr(III) are aligned in an antiparallel fashion. This strongly supports spectroscopic data from inelastic neutron scattering and THz-EPR experiments.



Left: Molecular structure of the $[Mn_2(5\text{-Brsalen})_2(MeOH)_2Cr(CN)_6]^-$ anion. Right: Example XAS and XMCD spectra taken on the MnCrMn SMM at the Mn $L_{2,3}$ edges.

Resonant Inelastic X-ray Scattering on a prototype edge-sharing chain cuprate

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The quasi-one-dimensional cuprate Li_2CuO_2 is a prototype edge-sharing chain compound [1]. The Cu^{2+} ions in this strongly correlated material give rise to one spin ½ per CuO_4 plaquette with a nearest neighbor Cu-O-Cu bond angle close to 90° implying weak superexchange coupling between Cu spins and indicating that other exchange paths are important for this material. As a result, spins order antiferromagnetically between the chains below T_N~9K, but ferromagnetically in the chains.
We have performed Resonant Inelastic X-ray Scattering (RIXS) at Cu L_3 and O K-resonances at the ADRESS beamline on this compound. Our momentum resolved RIXS measurements at the Cu L_3-edge allow analyzing orbital and charge transfer excitations with high sensitivity. At the O K-edge, the RIXS spectra display a complicated interplay of low-energy excitations from charge, orbital and lattice degrees of freedom.
In particular, we discuss charge transfer related spectral components in the scenario of exotic Zhang-Rice singlet and triplet excitations which can be reached in the final state with O K-edge RIXS [2,3]. Our recent temperature dependent measurements evidence clear opposite temperature behaviors for these two features, in good agreement with optical conductivity calculations [4]. This suggests RIXS as an excellent probe for investigating local magnetic order.

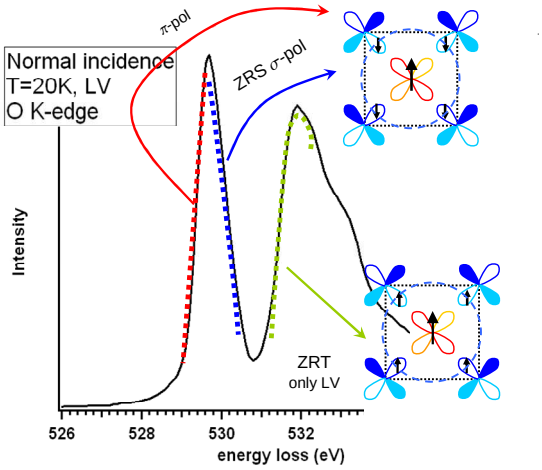

Figure: when probing the pre-edge (dashed red) of the O K-edge x-ray absorption with π-polarization, a Zhang-Rice singlet excitation is observed in the RIXS spectra, while it appears post-edge (dashed blue) for σ-polarization
In contrast, the Zhang-Rice triplet excitation is observed in RIXS when the O K-edge is probed at higher energy (dashed green).

References:

[1] – R. Neudert *et al.*, Phys. Rev. B **60**, 13413, (1999).
[2] – T. Learmonth *et al.*, Euro. Phys. Lett. **79**, 47012, (2007).
[3] – K. Okada and A. Kotani, Phys. Rev. B **63**, 45103, (2001).
[4] – J. Malek *et al.*, Phys. Rev. B **78**, 060508(R) (2008).

Cupric Oxide: a model system to explain high-T_c superconductivity?

V. Scagnoli[1], U. Staub[1], R. de Souza[1], Y. Bodenthin[1], M. Garganourakis[1], A. T. Boothroyd[2], D. Prabhakaran[2], and S.W. Lovesey[3]

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Cupric oxide (CuO) has recently attracted much interest as a magnetically driven multiferroic with the highest Tc (~230K). In this material a non-collinear spiral magnetic order (215K<T<230K) breaks crystal inversion symmetry, inducing ferroelectricity. We use resonant x-ray diffraction at the Cu L edges to probe the subtle changes in the Cu electronic structure occurring at the appearance of multiferroicity and test the magnetic ground-state, proposed by neutron diffraction, to be a collinear antiferromagnet. In both phases we have found a strong dependence of the diffracted intensity on the polarization of the incident light. Such dependence is totally unexpected in a simple collinear antiferromagnetic phase. In this model the Cu magnetic moment are aligned (antiferromagnetically) along the b-axis. The observed polarization dependence could reflect and be a direct measurement of the presence of orbital currents surrounding the Cu ions. Such observations are long sought proofs for theoretical model explaining the behavior of the normal state of high-T_c superconductors. Understanding such state is the key to unravel the true origin of the superconducting phase transition in cuprates materials.

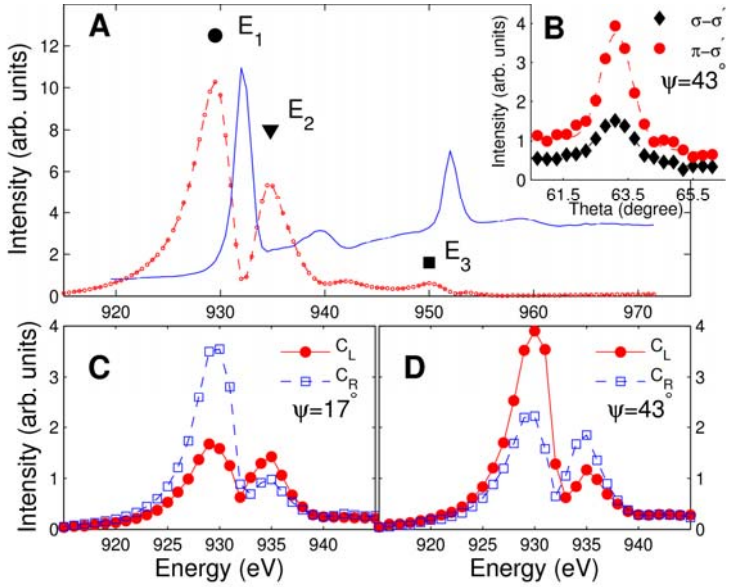

Figure 1: Resonant enhancement of the (1/2, 0, -1/2) superlattice reflection at the $L_{3,2}$ edges in CuO for different incident x-ray polarization. More details for the curious that will come!

Addressing the origin of the low temperature phase transition T_X in 1-dimensional $BaVS_3$

R.A. de Souza,[1] U. Staub[1], M. Garganourakis[1],V. Scagnoli[1], Y. Bodenthin[1] and H. Berger [2]

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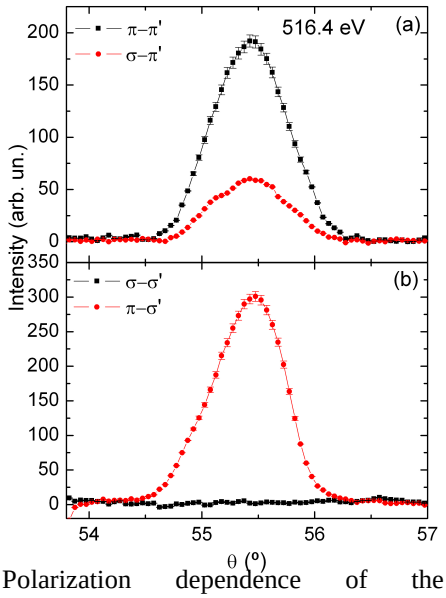
Transition metal oxides exhibiting low-dimensional strongly electron correlated systems presents phenomena like, metal-insulator (MI) transition, charge, spin and orbital ordering and superconductivity [1]. In contrast to oxides, sulfides are much less explored. They present reduced ionicity of the metal-sulphur bond, thereby increasing the effect of hybridization, which allows to study interesting electronic phenomena from a different base. The compound $BaVS_3$ crystallizes in a hexagonal structure, with the formation of VS_6 chains running along the c axis, what gives to this compound structural quasi-1D properties. This compound undergoes a MI transition at T_{MI} =70K [1], below which a charge density wave with superstructure corresponding to a doubling along the chain direction develops [3]. Another transition is observed at T_X=30K, whose origin is still a matter of controversy. At this temperature a maximum is observed at the magnetic susceptibility, although no long range magnetic order is observed. Neutron powder diffraction studies provided evidence for incommensurate reflection below this temperature [4]. Based on the assumption of no inter chain coupling, the modulation vector of (0.226 0.226 0), in the hexagonal structure, of the possible magnetic order was suggested. However, NMR studies [5] suggest the presence of orbital order to occur at this temperature. The exact nature of the transition at T_X is not yet clear, and the ground state of $BaVS_3$ is unknown.



Polarization dependence of the superlattice reflection taken at the L_3-edge.

Here we studied the origin of the mysterious electronic phase transition (T_X=30 K) caused by a single electron occupied t_{2g} orbital in quasi one-dimensional $BaVS_3$ is studied by means of resonant soft x-ray diffraction on the V $L_{2;3}$ absorption edges. This technique has been proved very powerful in the study of charge, orbital and magnetic order in many systems, since it probes directly the 3d electrons. The analysis of the scattered polarization indicates a pure magnetic origin of the observed reflection. These results are related to the different electronic models proposed.

References

[1] Iamada et. al, Metal-insulator transitions, Vol. 70, No. 4, 1039 (1998)
[2] Sayetat et. al, J. Phys. C: Solid State Phys.,15 1627 (1982)
[3] Fagot et al, Phys. Rev. Lett. 90, 196401 (2003)
[4] Nakamura et. al, J. Phys. Soc. of Japan, Vol 69, No.9, 2763 (2000)
[5] Nakamura et. al, Possible, Phys. Rev. Lett. 79, 3779 (1997)