

Analysis of Resonant Soft X-ray Scattering Experiments and the Orbital and Magnetic Order in Manganites *

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Resonant soft X-ray scattering at the *Mn* L-edges is expected to be a sensitive probe of the *3d*-electrons in manganites [1], and can be used to elucidate the properties and the interplay of different electronic order parameters, such as the orbital, charge and magnetic long-range order. The only important constraint is that the wavelength of the photon λ restricts the applicability of the method to systems with sufficiently long periods d , $2d > \lambda$. Recent experiments [2-6] at the $L_{2,3}$ edges show a rich structure in the dependence of the scattering intensity on the energy of the incoming photon, and strong polarization and azimuthal angle dependent effects. In order to extract meaningful information from these results, simulations of the scattering intensity for Mn ions in a crystal field were performed by atomic multiplet calculations. Results will be presented for $La_{0.5}Sr_{1.5}MnO_4$, and the bilayer manganite $LaSr_2Mn_2O_7$. Unlike scattering at the K-edge, where the intensity is mostly determined by the lattice distortion related to the Jahn-Teller effect [7], at the L edges features mostly related either to the lattice distortion or to purely electronic features, such as orbital order, can be identified. We are therefore able to identify the presence of orbital order in the bilayer system, where Jahn-Teller distortions are very small. Perspectives and limitations of these calculations will be addressed, with regard to topics such as the temperature dependence of the spectra, the orientation of the magnetic moments, and the charge state of the *Mn* ions.

* Work performed in collaboration with N. Binggeli and N. Stojic, *Abdus Salam ICTP, Trieste, Italy*

- [1] C.W.M. Castleton and M. Altarelli, *Phys. Rev. B* **62**, 1003 (2000)
- [2] S.B. Wilkins *et al.*, *Phys. Rev. Lett.* **90**, 187201 (2003)
- [3] S.B. Wilkins *et al.*, *Phys. Rev. Lett.* **91**, 167205 (2003)
- [4] S.S. Dhesi *et al.*, *Phys. Rev. Lett.* **92**, 056403 (2004)
- [5] K.J. Thomas *et al.*, *Phys. Rev. Lett.* **92**, 237204 (2004)
- [6] U. Staub *et al.*, *Phys. Rev. B.*, in press (2005)
- [7] H. Ohsumi *et al.*, *J. Phys. Soc. Jpn.* **72**, 1006 (2003)