Ground States and Excitations in Half-Doped Manganites: Hard and Soft X-ray Scattering Studies

Hill, J.P.¹

¹Department of Physics, Brookhaven National Laboratory, Upton, NY 11973, USA, email: hill@bnl.gov

A complete understanding of the electronic properties of a given system requires an understanding of both the ground states and the excitations of that system. Here, we apply resonant x-ray scattering techniques to both aspects of this problem, focusing on the halfdoped manganites. K-edge elastic scattering studies were performed on Pr_{0.6}Ca_{0.4}MnO₃ [1]. This system has been previously argued to exhibit the checkerboard charge and orbitally ordered phase with a CE-type magnetic structure. K-edge studies are sensitive to the environment of the Mn ion and a detailed analysis of the resonant scattering reveals a partial d-occupancy on all Mn sites with $3x^2 - r^2/3y^2 - r^2$ type orbital order on the 'Mn^{3+'} sites and $x^2 - y^2$ occupancy on the 'Mn⁴⁺' sites. No evidence for a 1s core level shift was observed, suggesting that the charge disproportionation is small. To investigate this further, studies were also performed at the Mn L-edge [2]. Here, resonant scattering probes the 3d orbitals directly. Large enhancements were observed at the magnetic and orbital wavevectors. The magnetic correlation length was found to be significantly larger than the orbital correlation length. In addition, a large (3eV) shift in the spectral weight was observed between the magnetic and orbital resonant lineshapes. A relaxed charge order model is proposed to explain these results. Finally, inelastic x-ray scattering experiments were performed at the Mn K-edge on this and related manganites [3]. Significant changes were observed as a function of temperature, up to energies of several eV – well above thermal energies, demonstrating the extreme sensitivity of the electronic structure to weak perturbations in these materials. The changes are correlated with the magnetic transitions.

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References

- [1] S. Grenier, et al. cond-mat/0305216
- [2] K.J. Thomas et al., cond-mat/0311553
- [3] S. Grenier et al., unpublished work