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Spin-resolved momentum densities: probing orbitals in magnetic oxides

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Studies of spin-resolved electron momentum densities involve the measurement of the so-called magnetic Compton profile. This is a one-dimensional projection of the electron momentum distribution of only those electrons that contribute to the spin moment of a sample. The technique is applicable to ferri- and ferromagnetic materials. Since electrons originating from different atomic orbitals have specific momentum densities, it is often possible to determine the origin of the magnetism present. Typically, interpretation requires the use of electronic structure calculations using molecular orbital and band structure approaches. The profile is obtained experimentally via the inelastic "Compton" scattering of high energy X-rays. For the experiments discussed here, the high energy beamlines at the ESRF and SPring-8 synchrotron X-ray sources were used, where we have a cryomagnet which can provide a sample environment with applied magnetic fields up to 9 Tesla, at temperatures from 1.3K to 600K. In this talk, we discuss our combined experimental and theoretical study of the spin density of the low-dimensional frustrated metamagnet $Ca_3Co_2O_6$. The spin moment, measured using magnetic Compton scattering, confirms the existence of a large unquenched Co orbital moment (1.3 ± 0.1 μB). With regards to the orbital occupation, we have performed molecular orbital calculations on the active trigonal CoO_6 cluster in order to determine which Co 3d orbitals are responsible for the observed electronic and magnetic behaviour and the observed orbital moment, and revealing the existence a oxygen spin moment of approximately 0.9 μB. Electronic structure calculations with a Hubbard U energy term give Compton profiles which are in good agreement with our experimental data. The magnetic Compton profile exhibits oscillations, which are well described, and their frequency in momentum space corresponds to the real-space inter-cobalt site bond length.

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