Compton profile calculation using the FLAPW-code BANDS01

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abstract

Within the impulse approximation the spin dependent directional Compton profile is given by

$$J^{\sigma}_{\hat{\boldsymbol{q}}}(p_q) = \int_{-\infty}^{\infty} d^3\boldsymbol{p}\ \gamma^{\sigma}(\boldsymbol{p})\delta(\boldsymbol{p}\bullet\hat{\boldsymbol{q}} - p_q) \qquad \sigma = \uparrow, \downarrow$$

where $\boldsymbol{q}$ is the scattering vector and $\gamma^{\sigma}(\boldsymbol{p})$ is the electron momentum density with spin σ. Using a lattice harmonics expansion of the electron momentum density[1], one obtains

$$J^{\sigma}_{\hat{\boldsymbol{q}}}(p_q) = 2\pi \sum_{\ell=0}^{\ell_{end}} \sum_{\mu=1}^{\mu_{end}(\ell)} \int_{|p_q|}^{p_{max}} p dp\ \gamma^{\sigma}_{\ell\mu}(p) P_{\ell}(\frac{p_q}{p}) F_{\ell\mu}(\theta_q, \phi_q)$$

where $\gamma^{\sigma}_{\ell\mu}(p)$ is the expansion coefficients, P_{ℓ} is the Legendre polynomial of order ℓ, $F_{\ell\mu}$ is the lattice harmonics, ℓ_{end} is the cutoff angular momentum and p_{max} is the cutoff momentum.

We shall show the magnetic Compton profiles(MCP) of Fe and $La_{2-2x}Sr_{1+2x}Mn_2O_7$. First of all, in order to check the dependence of parameters and the accuracy of our approximation, we calculate the MCP of iron and compare with the experiment[2] and other theoretical calculation[3]. A good agreement between our calculation and the experiment[2] is found in the MCP's along many directions. Next, we calculate the directional MCP's of $La_{2-2x}Sr_{1+2x}Mn_2O_7$ at x=0.35 and 0.42 along the [100], [110] and [001] directions using a virtual crystal approximation. Our LSDA+U calculations show an excellent agreement with experimental data[4].

References

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