Resonant Magnetic X-Ray Scattering from Transition-Metal Compounds and Actinide Compounds

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The *4p* states of transition metals are delocalized in solids. In usual situations, they attract only minor interest because they are not the states of constituting magnetic or orbital orders. Recently, understanding *4p* states becomes important, since x-ray spectroscopy using *K* edges of transition metals has become popular, in which core electrons are excited to 4p states through the dipole transition. Delocalized nature of *4p* states leads to sensitivilty to electronic structures at neighboring sites. This would make it difficult to analyze the spectra using a simple model. On the other hand, the band structure calculation is expected to work well for describing *4p* states, because electron correlations are small.

In this context, we report ab initio calculations of *K* edge magnetic resonant x-ray scattering (MRXS) spectra in transition-metal and actinide compounds, by taking account of the spin-orbit interaction (SOI) in the LDA scheme. First, we show the result of the MRXS spectra in $KCuF_3$[1] and NiO[2]. These studies demonstrate that the orbital polarization in the *4p* states is induced by their spin polarization through the SOI. Next, we present the calculation of the MRXS spectra in UGa_3, demonstrating that the orbital polarization in the Ga *4p* states is induced by the *5f* orbital moment at neighboring uranium sites through the *p-f* mixing. The study naturally explains the large MRXS intensity found in the experiment[3].

References

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