Computational Study of X-ray Absorption Spectroscopy in *g*-type Altermagnets with Distinct Relativistic Magnetic Symmetries

K. Sakurai[1*], J. Kuneš[2] and A. Hariki[1]

[1]*Department of Physics and Electronics, Osaka Metropolitan University, Osaka, Japan,*

[2]*Department of Condensed Matter Physics, Masaryk University, Czech Republic*

*sr25655k@omu.ac.jp

Altermagnetism is a new type of collinear magnetism that has no magnetization in the non-relativistic limit, yet exhibits spin polarized bands, giving rise to phenomena associated with time reversal symmetry breaking. To detect its realization, x-ray magnetic circular dichroism (XMCD) has been proposed and was successfully applied to α-MnTe, a canonical *g*-type altermagnet [1]. However, the presence of XMCD is restricted by relativistic magnetic symmetry, that is, it depends on the Néel-vector orientation relative to the crystallographic axes, which lies outside the non-relativistic classification of altermagnetism. Hence, XMCD can be forbidden even in altermagnet candidates belonging to the same *g*-type altermagnetic symmetry class as MnTe.

In this study, based on computational simulations combining density functional theory (DFT) and dynamical mean field theory (DMFT), we explore several complementary approaches to characterize *g*-type altermagnets using x-ray absorption spectroscopy (XAS) at the transition metal *L*-edge. In addition to x-ray polarizations, whose symmetry properties are well defined, we exploit the frequency dependence of the spectra, which reflects nontrivial many body interactions with the core hole in the XAS final states and can be experimentally selected by tuning the incident photon energy. Besides typical *g*-type altermagnets (α-MnTe, CrSb), we simulate α-Fe_2O_3, which exhibits the so-called Morin transition, where the Neel vector undergoes a reorientation while the underlying *g*-type altermagnetic structure remains essentially unchanged. We show how the altermagnetic phases with XMCD-allowed and -forbidden Néel-vector direction can be characterized using XAS based techniques. In particular, we demonstrate imaging of XMCD-forbidden altermagnetic phases by resolving domain walls using the polarization-averaged XAS profile.

References

[1] A. Hariki *et al*., Phys. Rev. Lett. **132**, 176701 (2024).