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Circular dichroism in crystalline coordination complexes using hard X-rays

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Natural Circular Dichroism (NCD), the differential absorption of right- and left-circularly polarized light, is a workhorse technique for the stereochemical characterization of molecules and macromolecules. While this technique is most often applied in the UV-visible energy range, core-level optical activity using X-rays demonstrates some unique features such as element specificity and orbital selectivity, but is limited to single crystal measurements.¹ The majority of X-ray Natural Circular Dichroism (XNCD) studies have been performed using synchrotron sources, especially the ESRF ID12 at the K-edge of light transition metals² or at the L_{2,3}-edge of heavier atoms, such as lanthanides.³

Our work is devoted to extending X-ray optical activity to new techniques and molecular crystals, especially those based on coordination complexes. To this end, we have recently observed the first example of Resonant Inelastic X-ray Scattering – NCD (RIXS-NCD) at the GALAXIES beamline at the SOLEIL synchrotron. We have also recently investigated at the ID12 optically active but non-chiral systems and fully characterized the polar and azimuthal dependence of a tetragonal crystal system, thus supporting theoretical predictions.⁴

These new results will be presented in conjunction with a presentation of our approach to the conception and synthesis of model systems

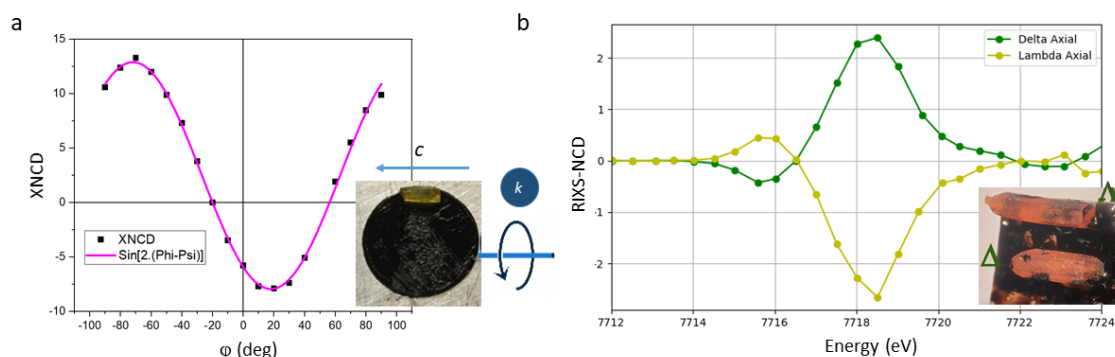


Figure a) Angular (azimuthal) dependence of the XNCD intensity of an achiral iron coordination complex; b) RIXS-NCD of enantiomers of a chiral cobalt complex.

- 1 J. Goulon, A. Rogalev and C. Brouder, *in* Comprehensive Chiroptical Spectroscopy (John Wiley & Sons, Ltd.), pp. 457–491 (2011).
- 2 A. Srinivasan, M. Cortijo, V. Bulicanu, A. Naim, R. Clerac, P. Saintavit, A. Rogalev, F. Wilhelm, P. Rosa and E. A. Hillard, *Chem. Sci.* 9, 1136–1143 (2018).
- 3 D. Mitcov, M. Platunov, C. D. Buch, A. Reinholdt, A. R. Døssing, F. Wilhelm, A. Rogalev and S. Piligkos, *Chem. Sci.* 11, 8306–8311 (2020).
- 4 C. R. Natoli, C. Brouder, Ph. Saintavit, J. Goulon, C. Goulon-Ginet and A. Rogalev, *Eur. Phys. J. B* 4, 1–11 (1998).