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Theoretical Study on Angular Dependence of X-ray Natural Circular Dichroism HIROSHI KATSUMOTO, ISIR, Osaka Univ., HITOSHI FUJII, NIMS, MI2I, TAMIO OGUCHI, ISIR, Osaka Univ., NIMS, MI2I — Natural circular dichroism (NCD) can be detected as a difference in the photo-absorption between right- and left-circularly polarized lights in a non-centrosymmetric crystal. It originates in an interference term of electric dipole (E1) and magnetic dipole (M1) transitions in optical ranges, while in that of E1 and electric quadruple (E2) transition in x-ray ranges. In the latter case, the electronic transitions occur from particular inner core states to empty conduction bands depending on the x-ray energy and polarization, being called selection rules. To cause such an interference, the final states should be parity violated because of the selection rules for the E1 and E2 transitions. In this study, we calculate x-ray NCD (XNCD) spectra by using density-functional-theory electronic structure calculation method and Fermi's golden rule for $LiIO_3$ (space group P63) and TeO_2 (P212121). The dependence of the incident angle in the XNCD spectra is calculated and discussed in detail by comparing with its analytic expression.

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