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Microscopic Mechanism of Giant Non-reciprocal Directional Dichroism in CuB_2O_4 SHINGO TOYODA, NOBUYUKI ABE, Department of Advanced Materials Science, University of Tokyo, SHOJIRO KIMURA, Institute for Materials Research, Tohoku University, TAKA-HISA ARIMA, Department of Advanced Materials Science, University of Tokyo — CuB_2O_4 shows giant Non-reciprocal Directional Dichroism (NDD) at 1.405 eV, which corresponds to the intratomic $d_{x^2-y^2}$-d_{xy} transition of Cu^{2+} hole. To clarify the origin of NDD, we performed measurements of the optical absorption in high magnetic fields up to 15 T. The g-factor estimated from the Zeeman splitting was as large as 2.8. This result suggests that orbital angular momentum contributes to the magnetic moments. To make sure of this estimation, we conducted an exact-diagonalization calculation considering crystal field, spin-orbit coupling, and Zeeman energy. The calculation reveals that d_{xy} hybridizes with d_{yz}, d_{zx} to form a spin-orbital coupled state. The calculated g-factor of this state is 2.6, which is comparable with the observed g-factor. We further calculated the oscillator strength of the transition from $d_{x^2-y^2}$ to the spin-orbital coupled state. The resulting oscillator strength successfully explains the experimental results of the magnetic field direction dependence of NDD.

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