Abstract

Noncentrosymmetric systems with broken spatial inversion symmetry exhibit intriguing phenomena through the entanglement of spin and orbital degrees of freedom in electrons, such as spin splitting of the electronic band structures and nonreciprocal transport. Of particular interest are the cases with spontaneous parity breaking, where fluctuations associated with the phase transitions might cause gigantic effects in the spin-orbital coupled phenomena. A pyrochlore oxide $Cd_2Re_2O_7$ is an archetypal compound showing such spontaneous parity breaking. While this compound shows a variety of noncentrosymmetric phases depending on temperature and pressure, the origin of the phase transitions remains elusive. In addition, unconventional magnetocurrent effects and nonreciprocal responses were proposed by a group theoretical analysis of the elevant multipoles, but the quantitative estimates have been lacked despite the relevance to the experimental observation. In this thesis, we theoretically investigate the electronic and transport properties in $Cd_2Re_2O_7$, focusing on three phases at ambient pressure including two parity-breaking phases. We analyze the electronic band structures for the three phases by the first-principles calculations with structural optimization. Based on the results, we construct the multiorbital tight-binding model by the maximally-localized Wannier function analysis. From these analyses, we obtain the systematic changes of the band structures and the Fermi surfaces. We clarify the spin and orbital angular momentum on the Fermi surfaces in the parity-breaking phases. From these results, we discuss the form of the ASOC and compare it with the group theoretical prediction. We also calculate the electrical conductivity and the magnetocurrent coefficients based on the multiorbital tight-binding model. Our estimates of the conductivity are semiquantitatively consistent with the experimental values. In addition, we obtain nonzero magnetocurrent coefficients in the parity-breaking phases. Our results are consisitent with the electric toroidal quadraopole orders recently proposed by the group theoretical analysis. From the quantitative estimates, we find the contribution from the orbital angular momentum is substantial. In addition, we discuss the effect of the electron-electron cor-

relations within the random phase approximation to clarify the origin of the parity-breaking phase transition. Our findings will help understanding of the microscopic mechanisms of the parity-breaking phase transitions in $Cd_2Re_2O_7$ and stimulate further experiments to clarify the unconventional phenomena related with the spontaneously-induced ASOC.