Abstract

The interplay between charge, spin, and orbital degrees of freedom of electrons has provided a fertile ground in condensed matter physics. In particular, the relativistic spin-orbit coupling (SOC) has gained a great attention as it leads to intriguing phenomena, e.g., topological insulators and multiferroics. Such SOC depends on the crystalline electric field, in which electrons move, and thus takes a different form depending on the spatial symmetry of the systems. For instance, in the systems without spatial inversion symmetry, the crystalline electric field acquires an odd-parity component, which leads to the so-called antisymmetric spin-orbit coupling (ASOC). The ASOC has been intensively discussed as the origin of unconventional superconductivities and magnetoelectric effects. On the other hand, in the centrosymmetric systems where the inversion centers are not located at lattice sites, which we call the centrosymmetric systems with local asymmetry, there exists a hidden ASOC in a site-dependent form. In this case, interestingly, the spontaneous parity breaking by electronic ordering can activate the hidden ASOC and leads to intriguing properties, e.g., asymmetric modulation of the band structure with respect to the wave number, spin and valley splitting, magnetoelectric effects, and anomalous Hall effects. This provides a new way of controlling the SOC physics through the electronic degrees of freedom.

In this thesis, we theoretically explore the emergent SOC physics by the spontaneous parity breaking. So far, most of the previous works have been done for effective single-band models in the centrosymmetric systems with local asymmetry, such as a zigzag chain and honeycomb lattice. Therefore, in order to deepen the fundamental understanding and explore the new aspects of the spontaneous parity breaking, we here consider two directions.

One is to elucidate the role of orbital degree of freedom in the spontaneous parity breaking. The explicit consideration of the orbital degree of freedom possibly gives rise to the emergence of novel phenomena, for instance, a pure multipole order that does not accompany magnetic moments and peculiar responses via the orbital channel. In order to pursue such possibilities, we derive an effective *d*-*p* model on a zigzag chain. Using the mean-field approximation, we study the ground state of the model at half-filling while changing the intra and interorbital Coulomb interactions. We find that an excitonic insulator with an antiferroic spin-orbital order appears between the band insulator with the *d*-*p* hybridization gap and the antiferromagnetic insulator caused by the strong intraorbital Coulomb interaction. Remarkably, the antiferroic spin-orbital order breaks both spatial inversion and time reversal symmetry, but has no local magnetic moments. Thus, this antiferroic spin-

orbital order can be regarded as the multipole order with odd parity. We also clarify two peculiar properties associated with the antiferroic spin-orbital insulator. One is the asymmetric modulation of the band structure in an applied magnetic field. The other is the spin-orbital response for an alternating electric field. These are the consequences of novel emergent SOC physics due to the spontaneous parity breaking by the multipole order.

The other direction is to pursue the emergent SOC physics in the centrosymmetric system without local asymmetry. In the centrosymmetric systems without local asymmetry, e.g., a triangular lattice system, one can expect two stages of spontaneous symmetry breaking for the emergent SOC physics; the first one is the electronic order that brings about local asymmetry in the system and the second stage is the spontaneous parity breaking. In order to examine such two-stage physics, we investigate an extended two-orbital Hubbard model on a triangular lattice with SOC. In particular, we focus on spontaneous charge ordering. Using the mean-field approximation, we obtain the ground-state phase diagram that contains charge ordered phases, where the charge disproportionations form a honeycomb or kagome network. We find that these charge ordered phases can be topological insulators by electron correlations since the charge ordering with local asymmetry activates the SOC. In addition, we clarify that, when introducing the bond distortion lacking parity symmetry, the system shows spin splitting in the band structure, in a similar way observed in monolayers of transition metal dichalcogenides.