Abstract

In this thesis, we study the ground-state properties of the multi-band Hubbard model with electron-phonon couplings to obtain the comprehensive understanding of the various phase competitions in the series of compounds $A\mathrm{NiO}_2$. These compounds have geometrically-frustrated triangular lattice structure, and in addition, the charge, spin, and orbital degrees of freedom are all active. By the mean-field calculations, we find that the phase diagram includes the charge ordered (CO) metallic phase and the orbital-ferro (OF) spin-ferro (SF) insulating phase which are candidates for the low-temperature states in AgNiO_2 and NaNiO_2, respectively. We find that the electron-phonon couplings and the cooperative phonon terms play an important role to stabilize these phases. The CO metallic phase appears in a rather weak correlation region in our results. This phase appears in a subtle balance between the repulsive Coulomb interaction and the effectively attractive interaction coming from the breathing type electron-phonon coupling. On the other hand, the OF SF insulating phase appears in a strong correlation region. The Jahn-Teller type electron-phonon coupling plays an important role in stabilizing this phase. The difference in U between OF SF and the CO phases might be ascribed to the screening effect from Na and Ag bands.