Interaction-induced quantum anomalous Hall phase in bilayers of 3d transition-metal oxide

YILIN WANG, ZHONG FANG, XI DAI, Institute of Physics, The Chinese Academy of Sciences; Beijing National Laboratory for Condensed Matter Physics — In the present paper, we have studied the electronic structure of 3d transition-metal oxide LaCoO$_3$ thin film grown on the [111] surface of SrTiO$_3$. By using first-principles calculation under local density approximation implemented with Gutzwiller variational method (LDA+G), we have studied the bilayer systems of LaCoO$_3$ thin films grown along the [111] direction on SrTiO$_3$. The LDA results show that two nearly flat bands locate at the top and bottom of eg bands of Co atoms, and the Fermi level crosses the lower one, which is almost half-filled. After including both the spin-orbit coupling and the rotational invariant Coulomb interaction in the LDA+G method, we found that the Coulomb interaction will enhance the effective spin-orbit coupling, and a ferromagnetic insulator phase with a gap as large as 0.15 eV will be stabilized. Further calculations indicate that such a ferromagnetic insulator phase will have non zero Chern number one leading to quantum anomalous Hall effect. Increasing Hund’s rule coupling in this system will generate a low spin to high spin transition and destroy the quantum anomalous Hall phase.