Thesis Summary

First Principal Calculation and Angle-resolved Photoemission Spectroscopy Study of Ultrathin Cr_2O_3 and $CrTe_2$ Films
(第一原理計算と角度分解光電子分光によるCr_2O_3超薄膜および$CrTe_2$薄膜の研究)

Name HOU XUEYAO

The multiferroic materials have attract wide attention due to its controllable ferroic properties by additional parameters of non-conjugate external fields. Thereinto, Cr_2O_3 would be a great research target for its intrinsic multiferroic characteristic. In this work, we use first-principles density functional theory (DFT) calculations and angle-resolved photoemission spectroscopy (ARPES) to study the band structure of Cr_2O_3/Gr/Ni(111) heterostructure. Our calculations have shown that the electronic band structures are distinct between the O- and Cr-terminated interfaces of the Cr_2O_3/Gr/Ni(111) heterostructure. An interesting spin-polarized mid-gap states are predicted to exist in the O-terminated model, whose spin direction can be flipped by reversing the substrate magnetization direction. In the ARPES experiments, we have observed the existence of such mid-gap band at the energy of ~ -0.20 eV in interface of Cr_2O_3 and graphene. The mid-gap band was further confirmed to have a Cr nature by resonance photoemission spectroscopy. Our findings indicate that one can control the spin-polarized mid-gap states in the antiferromagnetic Cr_2O_3 as well as the bandgap of graphene by interface engineering, paving the way for spintronic applications.

The calculation for $CrTe_2$ slabs is performed to examine the electronic structures and corresponding physical properties that can be compared with experiments. The effect of thickness, magnetic configuration and graphene buffer layer are all considered during calculation. We find that the thickness is crucial for its properties, the $CrTe_2$ slabs recovers to its bulk properties as thickness increases. Besides, the 1unit cell(UC) and 2UC slabs show a stronger spin-oscillation than that of others. With the AFM magnetic configuration, there will be an unusual unoccupied state at 3.5 eV above the E_F, which is distributed by the in-plane states of Cr 3*d* and Te 5*p* orbitals. The graphene buffer layer will weaken the spin-oscillation of 1UC and 2UC films, and make it recovers to bulk properties.