

Collective excitations probed by L-edge RIXS in Iridium compounds

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The physics of 5d-based iridates has recently attracted much attention, since the competition between the large spin-orbit interaction and the Coulomb interaction makes their physical properties quite different from those of the 3d transition metal compounds. I report the recent theoretical study of our group on the L-edge RIXS from Iridium compounds, Sr_2IrO_4 and Na_2IrO_3 .

First we discuss the RIXS spectra in the antiferromagnetic insulator, Sr_2IrO_4 [1]. We analyse the spectra within the weak coupling theory in the itinerant electron picture. Introducing a multi-orbital tight-binding model, we employ the Hartree-Fock approximation (HFA) and the random phase approximation (RPA) to calculate the RIXS spectra. The magnetic excitations in the low energy region emerge as the bound states in the density-density correlation function, which are found to split into two modes. The excitonic excitations with high energies emerge as quasi-bound states. Both excitations thus obtained agree with the RIXS experiment [2].

Next we discuss the RIXS spectra in Na_2IrO_3 , a zigzag antiferromagnet on the honeycomb lattice [3]. Employing a multi-orbital tight-binding model, we calculate one-electron energy as well as the ground state energy within the HFA. Under the assumption the electron transfer between the Ir 5d states is allowed via oxygen 2p states, we obtain nearly flat energy bands due to the formation of quasi-molecular orbitals, and the ground states exhibits the zigzag spin order. The collective excitations emerge as bound states in the density-density correlation function within the RPA, in agreement with the RIXS experiment [5]. The inclusion of the direct d-d transfer is unfavorable in order to explain the observed aspects of Na_2IrO_3 such as the ordering pattern of the ground state and the excitation spectrum. These findings may indicate that the direct d-d transfer is suppressed by the structural distortions in the view of excitation spectroscopy, as having been pointed out in the ab initio calculation [6].

References

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