Novel Insulating Phase in Moderately Spin-orbit Coupled $Sr_{2-x}La_xRhO_4$ Triggered by Lifshitz Transition

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ABSTRACT

$Sr_{2-x}La_xRhO_4$ undergoes a metal-insulator transition (MIT) at a non-integer number of x = 0.4 that is clearly distinguished from conventional Mott transitions. We performed systematic doping dependent electronic structure studies to investigate the origin of the exotic MIT. A gap opening in the spectral function is found to occur at x = 0.4, as expected from resistivity data. Moreover, we discovered that the α-band goes through a Lifshitz transition at x = 0.4. Based on these observations, we propose a new MIT mechanism for the moderately spin-orbit coupled $Sr_{2-x}La_xRhO_4$.

INTRODUCTION

Mott insulators are one of the most studied topics in condensed matter physics. Many 3d transition metal oxides (TMOs) are known to have a Mott insulating phase due to their large electron-electron correlation. However, the discovery of the relativistic Mott insulating phase in Sr_2IrO_4 triggered a new field of study in Mott insulators [1]. Spin-orbit coupling (SOC) is a key parameter in the description of the relativistic Mott insulating phase in 5d TMO systems. The SOC leads to a well-separated band with J_{eff} = 1/2 character, which results in reduced hopping and thus increased effective correlation.

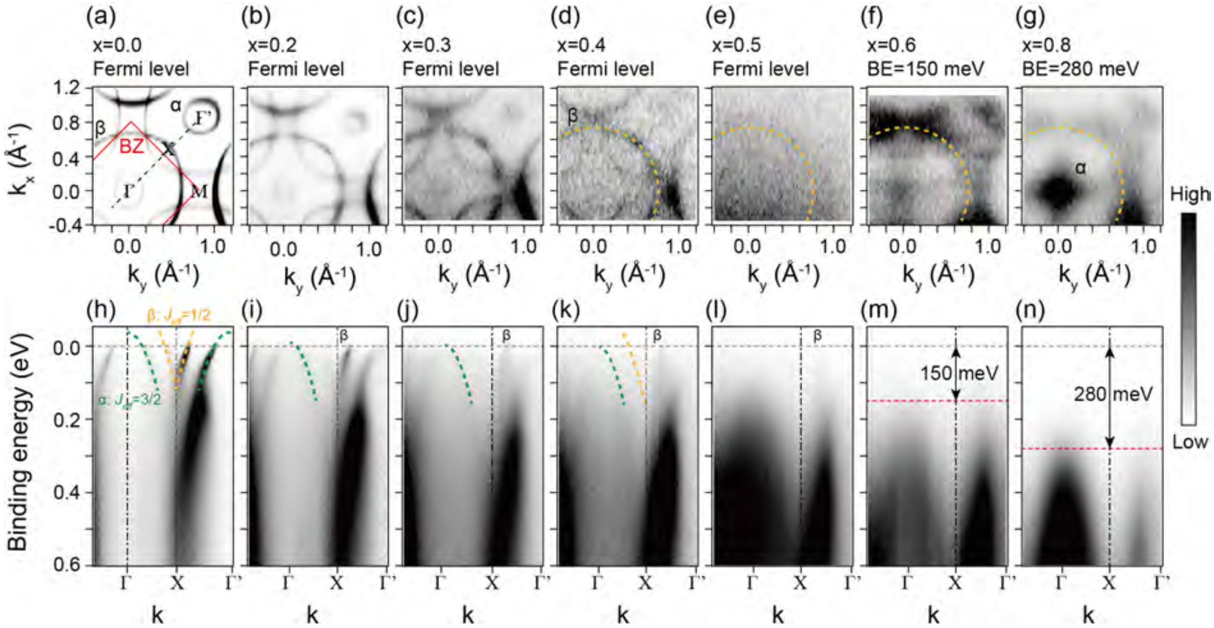

Fig. 1: Experimentally obtained doping dependent electronic structure. Panels (a-g) show doping dependent constant energy surfaces while (h-n) show doping dependent E-k distribution along the Γ-X direction. Adopted from Ref. [4].

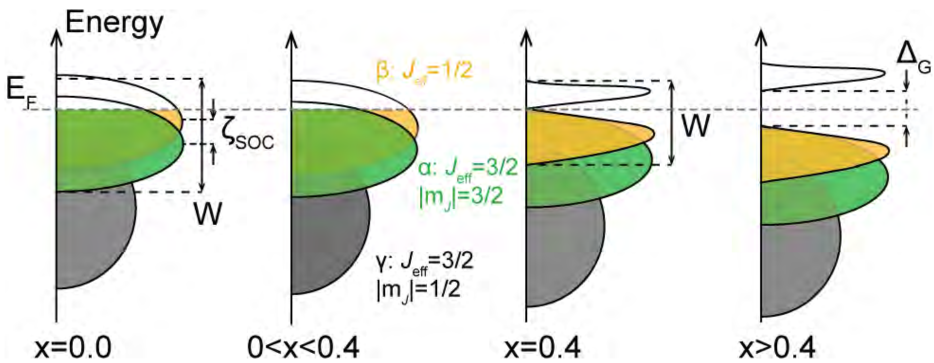

Fig. 2: Schematic illustrating the MIT mechanism in $Sr_{2-x}La_xRhO_4$. Adopted from Ref. [4].

On the other hand, 4d TMOs have a smaller SOC than 5d systems and thus are generally believed not to have novel SOC features. However, there is a recent theoretical report that Sr_2RhO_4 has a band structure similar to that of Sr_2IrO_4, which can be understood within the J_{eff} scheme [2]. Hence, the discovery of the metal-insulator transition (MIT) in polycrystalline $Sr_{2-x}La_xRhO_4$ [3] may suggest the significant role of SOC in the MIT. In order to investigate the role of SOC in the MIT, we performed angle-resolved photoemission spectroscopy (ARPES) studies on single crystals of $Sr_{2-x}La_xRhO_4$. The experimental spectral functions show that an MIT occurs at x = 0.4 as expected from the transport data [4]. Based on the result of systematic electronic structure studies, we propose a new type of insulating phase triggered by a Lifshitz transition and moderate SOC.

EXOTIC METAL-INSULATOR TRANSITION - EXPERIMENTAL OBSERVATION

ARPES performed on single crystals can provide the band structure needed to study the MIT mechanism. Figure 1 shows the experimental band structure. Plotted in panel (a) is the Fermi surface of non-doped system for which there are three bands (and their replicas). Theoretical studies show that the two bands, α (green dashed line) and β (yellow dashed line), correspond to J_{eff} = 3/2 and J_{eff} = 1/2 bands, respectively. Due to the extra electrons that La substitution provides, the α band shows a rigid-band-like shift and sinks below the Fermi level at x = 0.4, resulting in a Lifshitz transition as shown in Figs. 1(h-k). The β band, on the other hand, shows a sudden loss of spectral weight at the Fermi level starting from x = 0.4, which is very indicative of a correlation gap. The gap keeps increasing with the doping as shown in Figs. 1(l-n). The electronic structure study thus suggests that α and β bands have different MITs (rigid band shift and Mott-like, respectively) but they have MITs at the same doping of x = 0.4.

PROPOSAL FOR A NEW MIT IN SYSTEMS WITH MODERATE SPIN-ORBIT COUPLING

It is not easy to understand the MIT mechanism of $Sr_{2-x}La_xRhO_4$ intuitively. Unlike other systems, the critical electron number of the MIT is a non-integer (n_e = 5.4), where the remaining β band has only 1.4 electrons. In addition, it is known that the system has neither electronic nor magnetic order. Hence, the MIT mechanism in $Sr_{2-x}La_xRhO_4$ cannot be purely electronic.

Figure 2 shows a schematic for a possible mechanism. The undoped system has two bands crossing the Fermi level as Fig. 1(a) shows. The two bands are split by the SOC, which is indicated with the ζ_{SOC} in the schematic in Fig. 2. Both bands contribute to the electron hopping in the undoped system and the bandwidth *W* is thus defined by the two bands, as shown in the schematic. This is the critical difference between Sr_2RhO_4 and Sr_2IrO_4; while only one band crosses the Fermi level for Sr_2IrO_4, two bands cross the Fermi level for Sr_2RhO_4, which inhibits the Mott transition.

What happens when we electron dope Sr_2RhO_4, so that only one band crosses the Fermi level? La can donate additional electrons and raise the chemical potential. As a result, the α band, being located at a lower energy compared to the β band, can be fully filled before the β band. After such a Lifshitz transition of the α band, only the β band contributes to the electron hopping. The bandwidth of the conduction band is redefined only by the width of the β band, which is smaller than the undoped case. Such a bandwidth transition at the critical doping of x = 0.4 is the essential factor that increases the U/W and opens a correlation gap in the β band.

The role of SOC and moderateness of the SOC is critical in the MIT. If there is no SOC, the splitting between the α and β bands vanishes, and the Lifshitz transition of the α band that triggers the bandwidth transition cannot occur. On the other hand, when the SOC is too large, the α band is well separated from the β band. Then, the α band is fully filled for x = 0, essentially becoming the Sr_2IrO_4 case. Only a moderately spin-orbit coupled system can provide multiple bands for the Lifshitz transition that triggers the bandwidth transition.

SUMMARY

Our study suggests that the MIT in $Sr_{2-x}La_xRhO_4$ is a new type that can occur only in materials with moderate SOC such as 4d TMO systems. The electronic structure study shows that the Lifshitz transition upon electron doping triggers the MIT. The study suggests that the moderately spin-orbit coupled band structure is crucial to provide the Lifshitz transition and such a Lifshitz transition triggers bandwidth reduction and creates a correlation driven gap. The discovery of the MIT in $Sr_{2-x}La_xRhO_4$ is a new milestone in the study of the role of SOC in 4d TMO compounds. Starting from this $Sr_{2-x}La_xRhO_4$ study, a moderate SOC regime should be a new field to discover novel physical phenomena.

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References

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