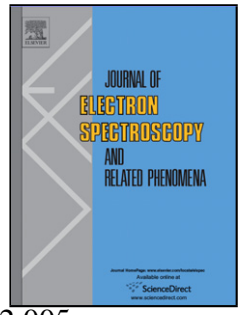

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Electronic structure of 5*d* transition-metal compounds

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Abstract

In this contribution, we describe fundamental electronic structures and spin-charge-orbital orderings of 5*d* transition-metal compounds. By reviewing photoemission spectroscopy studies on $CuIr_2S_4$, $IrTe_2$, $Cs_2Au_2Br_6$, and $AuTe_2$, we discuss the difference between the t_{2g} and e_g systems with respect to the spin-orbit splitting *versus* the Jahn-Teller splitting. In contrast to the Ir oxides with Mott-Hubbard character, the smallness of the charge-transfer energy plays essential roles in the exotic spin-charge-orbital orderings of the Ir and Au chalcogenides and halides. In particular, the Te 5*p* hole provides an interesting interplay between the charge-orbital order and the spin-orbit interaction in $IrTe_2$.

Key words: 5*d* transition-metal compounds, spin-orbit interaction, spin-charge-orbital order, photoemission spectroscopy

1. Introduction

The transition-metal compounds exhibit extremely rich physical properties, and their fundamental electronic structures have been targets of various spectroscopic and theoretical studies [1, 2, 3]. Among them, 5*d* transition-metal compounds tend to have complicated multi-orbital band structures that would be entangled by the large spin-orbit interaction of the 5*d* subshell and the strong hybridization with the ligand orbitals. For example, angle-resolved photoemission spectroscopy (ARPES) revealed the drastic band-structure reconstruction due to charge density wave in 1T-$TaSe_2$ [4], the polaron formation and remnant Fermi surfaces in Na_xWO_3 [5], and the excitonic insulator transition in Ta_2NiSe_5 [6]. Various Ir compounds have been attracting great interest due to exotic metal-insulator transitions and magnetic behaviors such as the orbitally-induced Peierls transition in $CuIr_2S_4$ [7], the spin-orbit induced metal-insulator transition in Sr_2IrO_4 [8], and the frustrated (and topological) magnetic state in Na_2IrO_3 [9, 10, 11]. These 5*d* transition-metal compounds are basically t_{2g} systems in which the spin-orbit interaction would be relevant.

In the atomic limit, the five 5*d* orbitals with spin up and spin down are split into the low-lying $j_{3/2}$ and the high-lying $j_{5/2}$ levels due to the spin-orbit interaction $\lambda \vec{l} \cdot \vec{s}$ ($\lambda > 0$). When the 5*d* transition-metal ions are octahedrally coordinated by ligand anions, the five 5*d* orbitals are split into the triply degenerate t_{2g} and the doubly degenerate e_g orbitals due to the ligand field. The ligand field splitting between the t_{2g} and e_g levels tends to be larger in the 5*d* systems than that

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