# $\mathbf{J_{eff} = \frac{1}{2}}$ insulating state in Ruddlesden-Popper iridates: An LDA+DMFT study

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The competition between strong spin-orbit coupling (SOC) and electron correlations in $5d$ compounds gives rise to many interesting phenomena. One particularly interesting case is the $J_{\rm eff} = \frac{1}{2}$ insulating phase found in $Sr_2IrO_4$ [1], which can be regarded as the $n$=1 member of the Ruddlesden-Popper series $Sr_{n+1}Ir_nO_{3n+1}$ with parent perovskite ($n$=$\infty$) $SrIrO_3$. We investigated the electronic structures of three members of this series with $n$=1, 2, and $\infty$. Our calculations were carried out using the dynamical mean field theory (DMFT) method [2], where both spin-orbit coupling and electron-electron correlations are considered consistently at the first principles level. We demonstrated that $Sr_2IrO_4$ and $Sr_3Ir_2O_7$ are in the $J_{\rm eff} = \frac{1}{2}$ insulating phase, with gaps of 400 and 250 meV respectively. $SrIrO_3$ is shown to be a correlated metal, with strongly renormalized bands of effective mass about $6{\sim}8\,m_e$ around the Fermi energy. The electronic structures we obtained are in good agreement with recent ARPES measurements [3-5]. Moreover, for $Sr_2IrO_4$, a detailed analysis of the electronic structures reveals that it is difficult to get the correct spin and orbital moments by performing LDA+U+SOC calculations, while our DMFT calculations give a total magnetic moment of 0.43 $\mu_B$ per Ir ion, with the ratio between spin and orbital moments being close to 1:2. Finally, we calculated the optical conductivity of all three compounds, and found good agreement with experimental results [6].

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