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Impurity-controlled valence, spin, and orbital state in Sr3Ru2O7.

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Impurity doping is one of the most effective means of tuning the properties of materials. We have discovered a possible way for orbital hierarchy inversion, valence control, and magneto-crystalline anisotropy rotation in complex oxides, by embedding 'localized' impurity orbitals in a 'delocalized' host matrix. Here we present a comprehensive analysis of experimental and theoretical results on Sr3(Ru1 xMnx)2O7 by a combination of angle-resolved photoemission (ARPES), x-ray absorption spectroscopy (XAS), density functional theory (LSDA), and cluster multiplet calculations. We find that Mn impurities do not exhibit the same 4+ valence of Ru ions, but behave as Mn3+ acceptors. The extra electron occupies in-plane eg orbitals instead of the out-of-plane $3z^2 - r^2 orbital predicted by crystal field theory, a counter intuitive result which might be termed as inverse Jahn - Teller effect. This behavior has profound implications for the spin and orbital ordering of the system as a whole, and might indicate new pathways toward the design of novel orbit$
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