

Abstract Submitted
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Orbital Hierarchy Inversion and Magnetic Transition in Mn Doped $\text{Sr}_3\text{Ru}_2\text{O}_7$ ¹ MUHAMMED HOSSAIN, University of British Columbia, M.W. HAVERKORT, Z.H. HU, T. BURNUS, C.F. CHANG, S. KLEIN, J.D. DENLINGER, H.-J. LIN, C.T. CHEN, R. MATHIEU, Y. KANEKO, Y. TOKURA, S. SATOW, Y. YOSHIDA, H. TAKAGI, A. TANAKA, I.S. ELFIMOV, G.A. SAWATZKY, L.H. TJENG, A. DAMASCELLI — Ruthenium oxides are a very important class of compounds that are extremely sensitive to impurities. Here we present a study of the Mn doped $\text{Sr}_3\text{Ru}_2\text{O}_7$ by X-ray Absorption Spectroscopy (XAS) and a combination of density functional theory (LSDA) and cluster calculations. We find that delocalized RuO matrix forces the Mn impurities to behave as a negative charge transfer system and donate a hole. As a result Mn impurities behave as Mn³⁺ acceptors. Our XAS data clearly shows that the occupied e_g orbitals have an in-plane alignment: a very surprising result in a tetragonally distorted system elongated along the c -axis. LSDA calculations reveal very strong anisotropy in oxygen bandwidth leading to a reversal of the e_g crystal field hierarchy. This work further establishes that the Mn atoms are sitting in a bath of a uniaxial exchange field that gradually goes out-of-plane to in-plane as the Mn doping level is increased. Overall, the behavior has some similarities with Mn doped GaAs and may be relevant to the physics of dilute magnetic semiconductors.

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