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Crystal-Field Level Inversion in Lightly Mn-Doped $Sr_3Ru_2O_7$[1]
MUHAMMED HOSSAIN, University of British Columbia (UBC), Z. HU, M.W. HAVERKORT, T. BURNUS, C.F. CHANG, S. KLEIN, Universität zu Köln, J.D. DENLINGER, Advanced Light Source, LBNL, H.-J. LIN, C.T. CHEN, NSRRC, Taiwan, R. MATHIEU, Y. KANEKO, Y. TOKURA, S. SATOW, H. TAKAGI, University of Tokyo, Y. YOSHIDA, National Institute of Advanced Industrial Science and Technology (AIST), A. TANAKA, Hiroshima University, I.S. ELFIMOV, G.A. SAWATZKY, UBC, L.H. TJENG, Universität zu Köln, A. DAMASCELLI, UBC —
$Sr_3(Ru_{1-x}Mn_x)_2O_7$, in which $4d$-Ru is substituted by the more localized $3d$-Mn, is studied by x-ray dichroism and spin-resolved density functional theory. We find that Mn impurities do not exhibit the same 4+ valence of Ru, but act as 3+ acceptors; the extra e_g electron occupies the in-plane $3d_{x^2-y^2}$ orbital instead of the expected out-of-plane $3d_{3z^2-r^2}$. We propose that the $3d$-$4d$ interplay, via the ligand oxygen orbitals, is responsible for this crystal-field level inversion and the material's transition to an antiferromagnetic, possibly orbitally ordered, low-temperature state. Published: Phys. Rev. Lett. 101, 016404 (2008).

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Muhammed Hossain
University of British Columbia

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