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Ferroelectricity driven by Y d^0-ness with re-hybridization in $YMnO_3$ J.-H. PARK, POSTECH, D.-Y. CHO, SNU, J.-Y. KIM, PAL, B.-G. PARK, K.-J. RHO, POSTECH, H.-J. NOH, B.-J. KIM, S.-J. OH, SNU, H.-M. PARK, KRIST, J.-S. AHN, H. ISHIBASHI, S-W. CHEONG, Rutgers University, J. H. LEE, P. MURUGAVEL, T. W. NOH, SNU, A. TANAKA, T. JO, Hiroshima University — Recently multiferroicity, in which magnetism and ferroelectricity co-exist, takes much attention due to its exotic magnetoelecric (ME) phenomena. Hexagonal $R\mathrm{MnO}_3$ (R = Ho, Er, Tm, Yb, Lu, Y, Sc) exhibits multiferroicity with high ferroelectric and low antiferromagnetic transition temperature ($T_E > 600$K, $T_M \sim 90$K). The hexagonal structure ($P6_3cm$) brings out soft mode phonons required for ferroelectricity, but its driving force has been puzzled. We investigated electronic structure of hexagonal multiferroic YMnO_3 using the polarization dependent x-ray absorption spectroscopy (PXAS) at O K- and Mn $L_{2,3}$-edges. PXAS exhibits strong polarization dependence at both edges, reflecting anisotropic Mn $3d$ orbital occupation. Moreover, the O K-edge spectra show that Y $4d$ states are strongly hybridized with O $2p$ ones, resulting in large anomalies in Born effective charges on off-centering Y- and O-ions. These results manifest that the Y d^0-ness with re-hybridization is the driving force for the ferroelectricity, and suggest a new approach to understand the multiferroicity in the hexagonal manganites.

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