

Abstract Submitted
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Direct crystallographic evidence of charge ordering in the novel double perovskite mixed-valence (NaMn₃)Mn₄O₁₂ A. PRODI, IMEM-CNR, B. SCHMITT, F. GOZZO, SLS-PSI, Q. HUANG, J.W. LYNN, NIST, F. BOLZONI, E. GILIOLI, F. LICCI, IMEM-CNR, M. MAREZIO, CRETA-CNRS, A. GAUZZI, IMEM-CNR — By means of high-resolution synchrotron X-ray powder diffraction measurements, we studied in detail the temperature-dependent crystal structure of the mixed-valence manganese oxide, (NaMn₃)Mn₄O₁₂. At 176 K, we observed a static ordering of the Jahn-Teller distortion of the Mn³⁺O₆ octahedra that drives a cubic-monoclinic structural transition concomitant to the Mn³⁺-Mn⁴⁺ charge ordering of the octahedral B-sites of the double-perovskite structure AA'₃B₄O₁₂. This transition is followed by a CE-type magnetic ordering of these sites at 125K and by an independent antiferromagnetic ordering of the Mn A' sites at 90 K. Remarkably, both neutron [1] and X-ray data show that the charge ordering is intrinsic to the low symmetry phase, resulting in the setting up of two distinct MnO₆ octahedra with very different average Mn-O distances. A bond valence sum analysis shows that these two Mn sites exactly correspond to 3+ and 4+ formal valence states. This direct evidence of charge disproportionation has never been reported in half-doped manganites, where charge order has been believed to occur only from controversial analysis of structural modulations. Ref: [1] A. Prodi *et al.*, *Nature Materials* **3**, 48 (2004).

Andrea Prodi
IMEM-CNR

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