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Interstitial oxygen as a source of p-type conductivity in $RMnO_3$ hexagonal manganites SANDRA HELEN SKJRV, ESPEN T. WEFRING, SILJE K. NESDAL, NIKOLAI H. GAUKS, GERHARD H. OLSEN, JULIA GLAUM, THOMAS TYBELL, SVERRE M. SELBACH, Norwegian Univ Tech (NTNU), DEPARTMENT OF ELECTRONICS AND TELECOMMUNICATIONS COLLABORATION, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING TEAM — We use a combination of experiments and first principles electronic structure calculations to elucidate the effect of interstitial oxygen anions, O_i, on the electrical and structural properties of h-$YMnO_3$. Hexagonal manganites, h-RMnO$_3$ (R = Sc, Y, Ho-Lu) have been intensively studied for their multiferroic properties, magnetoelectric coupling, topological defects and electrically conducting domain walls. Although point defects strongly affect the conductivity of transition metal oxides, the defect chemistry of h-RMnO$_3$ has received little attention. Enthalpy stabilized interstitial oxygen anions are shown to be the main source of p-type electronic conductivity, without reducing the spontaneous ferroelectric polarization. A low energy barrier interstitialcy mechanism is inferred from Density Functional Theory calculations to be the microscopic migration path of O_i. Since the O_i content governs the concentration of charge carrier holes, controlling the thermal and atmospheric history provides a simple and fully reversible way of tuning the electrical properties of h-RMnO$_3$.

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