Electronic Supplementary Material (ESI) for Dalton Transactions.

Ordering effects in the crystal structure and electrochemical properties of the $Gd_{0.5}Ba_{0.5}Mn_{0.5}Fe_{0.5}O_{3-\delta}$ perovskite

Daniel Muñoz-Gil,[a] David Ávila-Brande,[a] Esteban Urones-Garrote [b] and Susana García-Martín [a] *

[a] Departamento de Química Inorgánica, Facultad de C.C. Químicas, Universidad Complutense, 28040-Madrid, Spain.

[b] Centro Nacional de Microscopía Electrónica, Universidad Complutense, E-28040, Madrid, Spain

Figure Captions of Supporting Information

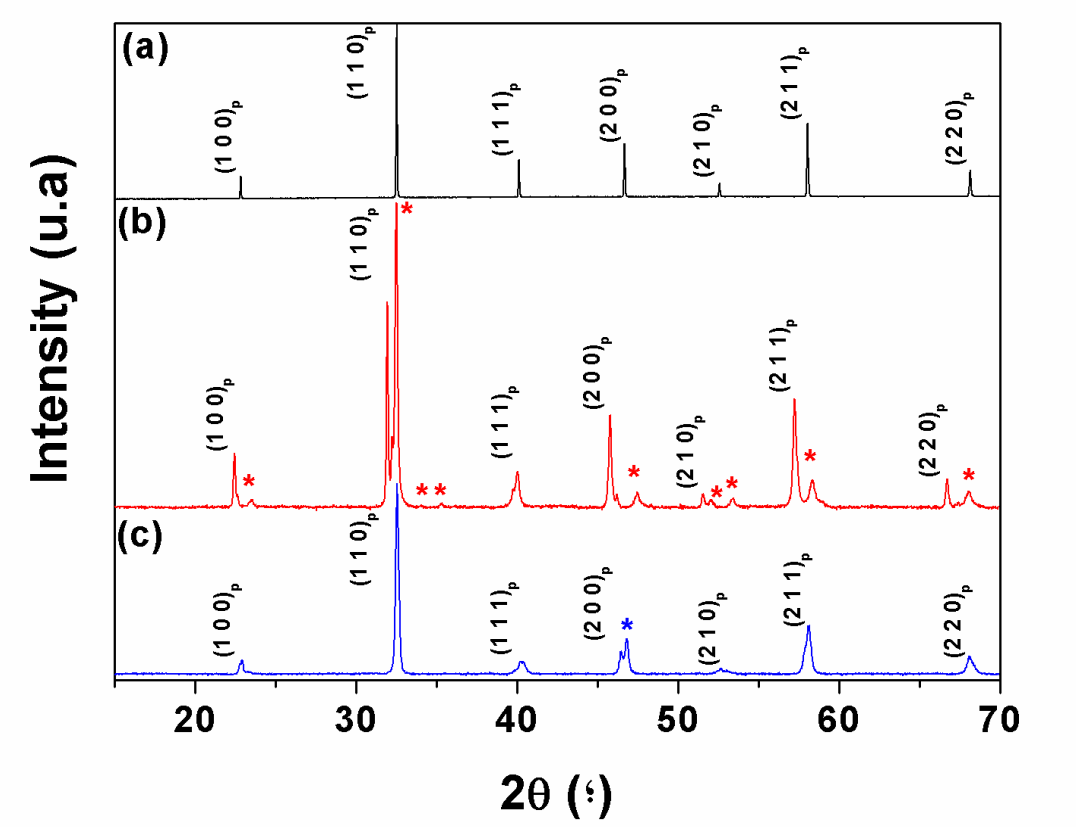

Fig. 1 SI: PXRD patterns of a sample prepared in air a); a sample prepared in H_2/N_2 b) and a sample prepared in H_2/N_2 and afterwards oxidized. Splitting of reflections and extra reflections are indicated with asterisks. Reflections of cubic perovskite structure are indicated by the corresponding Miller Indices.

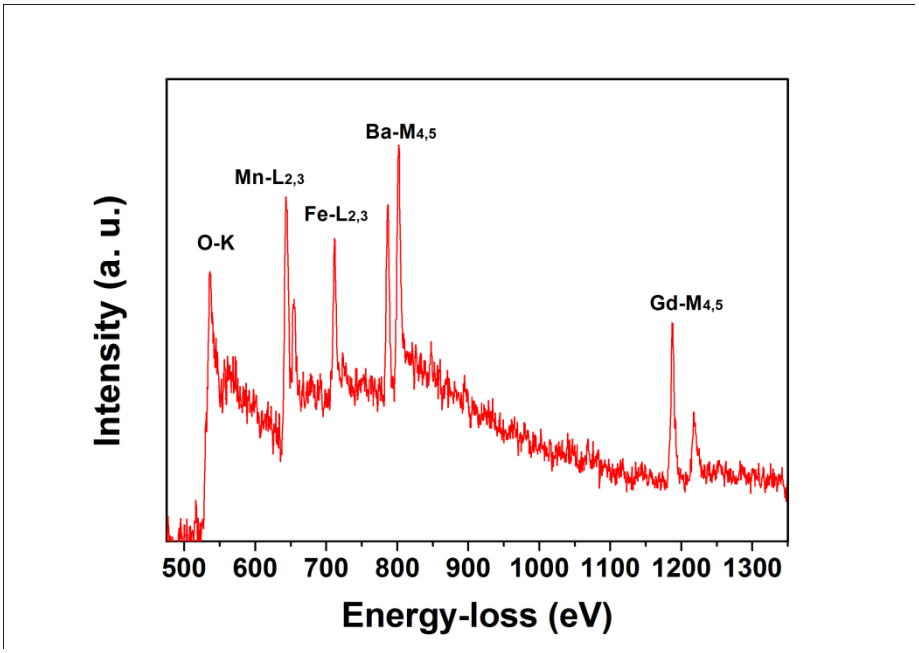

Fig. 2 SI: EELS spectrum of $GdBaMnFeO_{6-\delta}$ showing the O-K, Mn-$L_{2,3}$, Fe-$L_{2,3}$, Ba-$M_{4,5}$ and Gd-$M_{4,5}$ ionization edges.

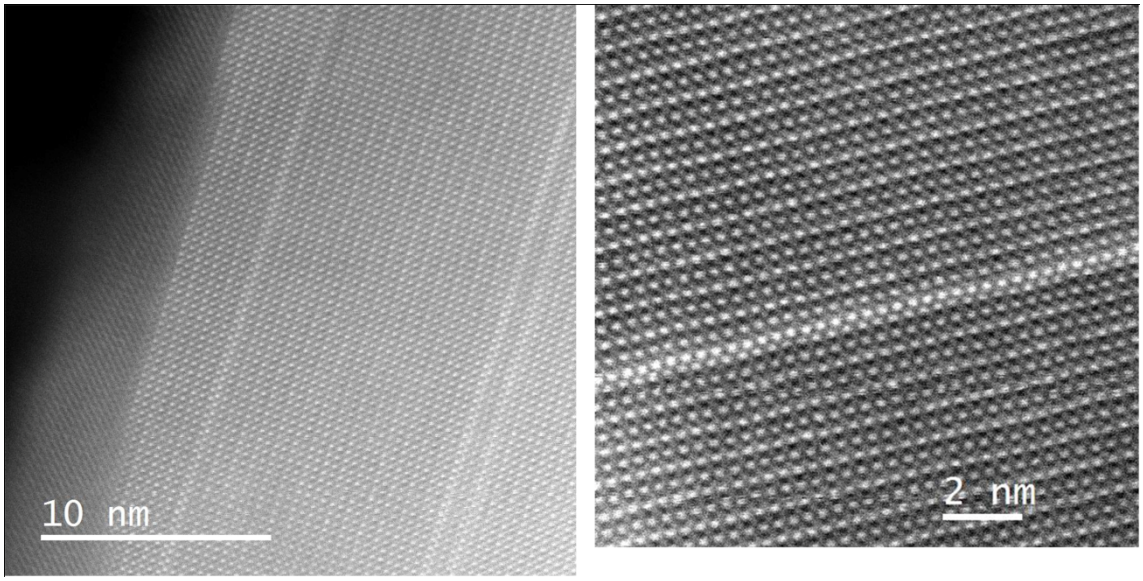

Fig. 3 SI: HAADF-STEM images of a $GdBaMnFeO_{6-\delta}$ crystal along the $[010]_p$ zone axis taken at different magnification.

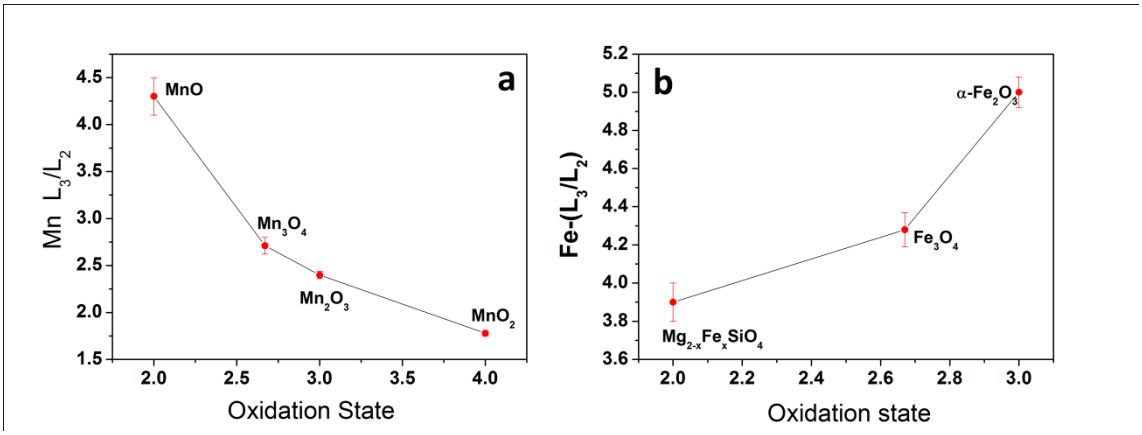

Fig. 4 SI: Graphic representations of L_3/L_2 intensity ratio versus a) Mn oxidation state in standard Mn oxides and b) Fe oxidation state in standard Fe oxides.

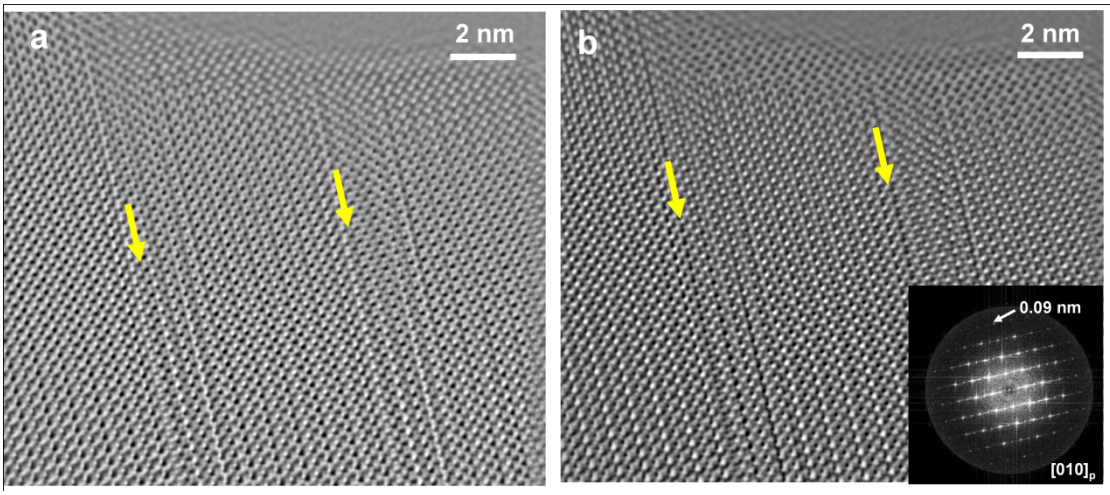

Fig. 5 SI: a) Amplitude and b) Phase image of the reconstructed exit plane wave of a $GdBaMnFeO_{6-\delta}$ crystal along the $[010]_p$ zone axis. The IFFT on the inset at the bottom shows the information limit reached after the exit wave reconstruction. Yellow arrows mark the isolated GdO defects.

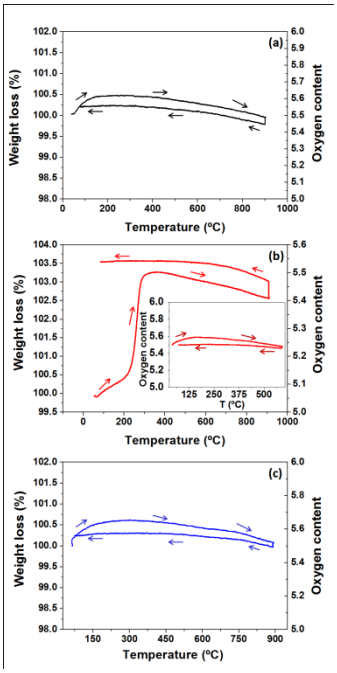

Fig. 6 SI: Thermogravimetric curves in ambient air for (a) a sample prepared in air, (b) a sample prepared in air+H_2/N_2 and (c) a sample prepared in air + H_2/N_2 + O_2. Heating and cooling cycles are indicated by arrows. The inset corresponds to a second heating-cooling cycle.