Supporting information

High temperature structural stability, electrical properties and chemical reactivity of $NdBaCo_{2-x}Mn_xO_{5+\delta}$ ($0 \leq x < 2$) perovskites for use as cathode in Solid Oxide Fuel Cells.

Thibault Broux[1], Mona Bahout[1*], James M. Hanlon[1], Olivier Hernandez[1], Serge Paofai[1], Andrey Berenov[2] and Stephen J. Skinner[2*]

[1]Institut des Sciences Chimiques de Rennes, Equipe « Chimie du Solide et Matériaux », UMR CNRS 6226, Université de Rennes 1, 263 Avenue du Général Leclerc, 35042 Rennes, France
[2] Department of Materials, Imperial College London, Exhibition Road, London SW7 2AZ, United Kingdom

Results and discussion

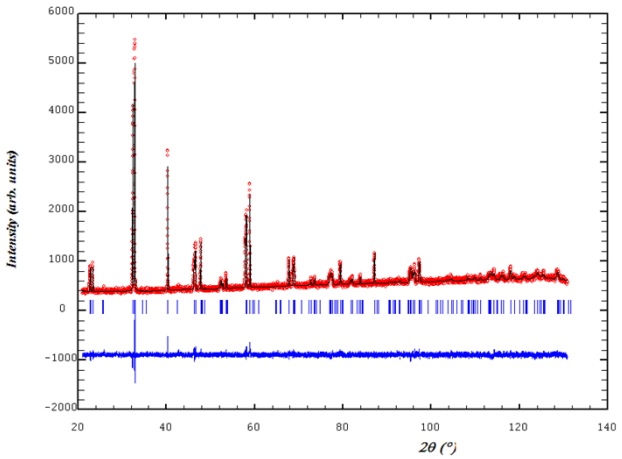

Figure S1. Measured, calculated and difference XRD patterns for $NdBaCo_2O_{5+\delta}$.

Table S1. Refined structural parameters for $NdBaCo_2O_{5+\delta}$ from XRD data.

Atoms	*Site*	*x*	*y*	*z*	*Occupancy*
Nd	1*c*	0	0	0.5	1.00#
Ba	1*a*	0	0	0	1.00#
Co	2*t*	0.5	0.5	0.250(2)	1.00#
O1	1*f*	0.5	0.5	0	1.00#
O2	2*t*	0.5	0.5	0.278(1)	1.00#
O3	2*s*	0.5	0	0.278(1)	1.00#
O4	1*h*	0.5	0.5	0.5	0.76(1)

Space group *Pmmm:* # fixed, a = 3.94560(3) Å, b = 3.95208(3) Å, c = 7.57080(5) Å, $B_{overall}$ = 0.5(3) Å², R_{wp} = 4,8%, R_p = 4.8%, R_{Bragg} = 7.0 %, χ^2 = 1.36. The z-positions for O2 and O3 were constrained to be equal.

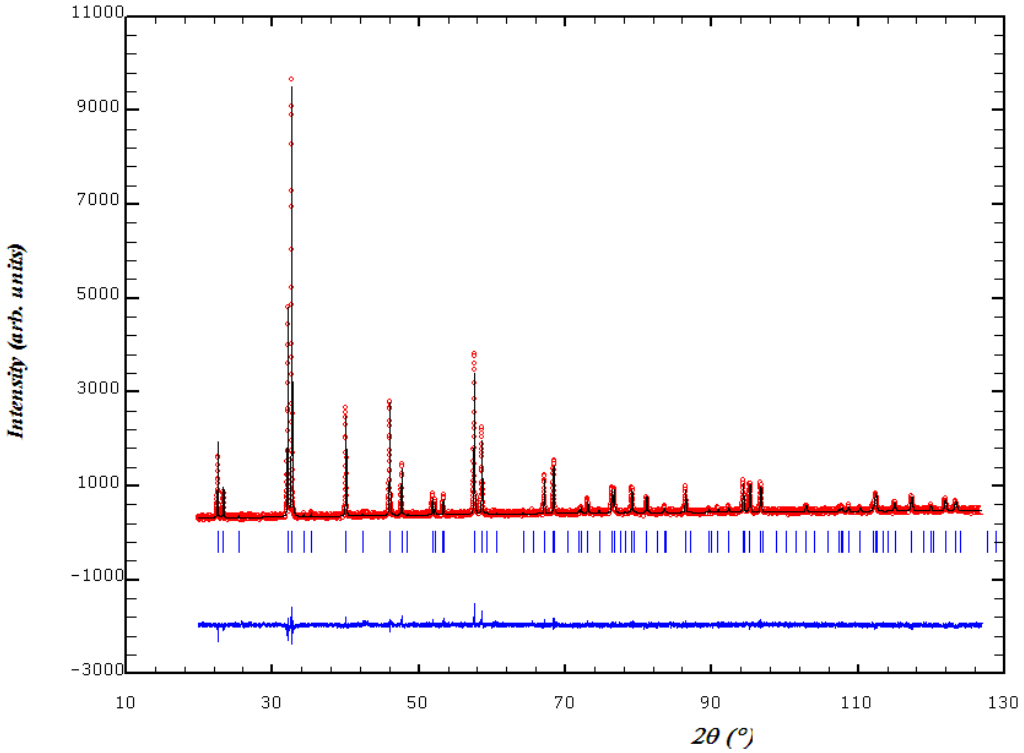

Figure S2. Measured, calculated and difference XRD patterns for $NdBaCo_{1.5}Mn_{0.5}O_{5+\delta}$.

Table 2. Refined structural parameters for $NdBaCo_{1.5}Mn_{0.5}O_{5+\delta}$ from XRD data.

Atoms	*Site*	*x*	*y*	*z*	*Occupancy*
Nd	1*a*	0	0	0.5	1.00#
Ba	1*b*	0	0	0	1.00#
Co/Mn	2*h*	0.5	0.5	0.256(3)	0.75/0.25#
O1	4*i*	0.5	0	0.299(1)	1.00#
O2	1*c*	0.5	0.5	0	1.00#
O3	1*d*	0.5	0.5	0.5	0.60(2)

Space group *P4/mmm:* # fixed, a = 3.94016(4) Å, c = 7.62584(6) Å, $B_{overall}$ = 0.4(2) Å², R_{wp} = 5.55%, R_p = 4.35%, R_{Bragg} = 10.2%, χ^2 = 1.52.

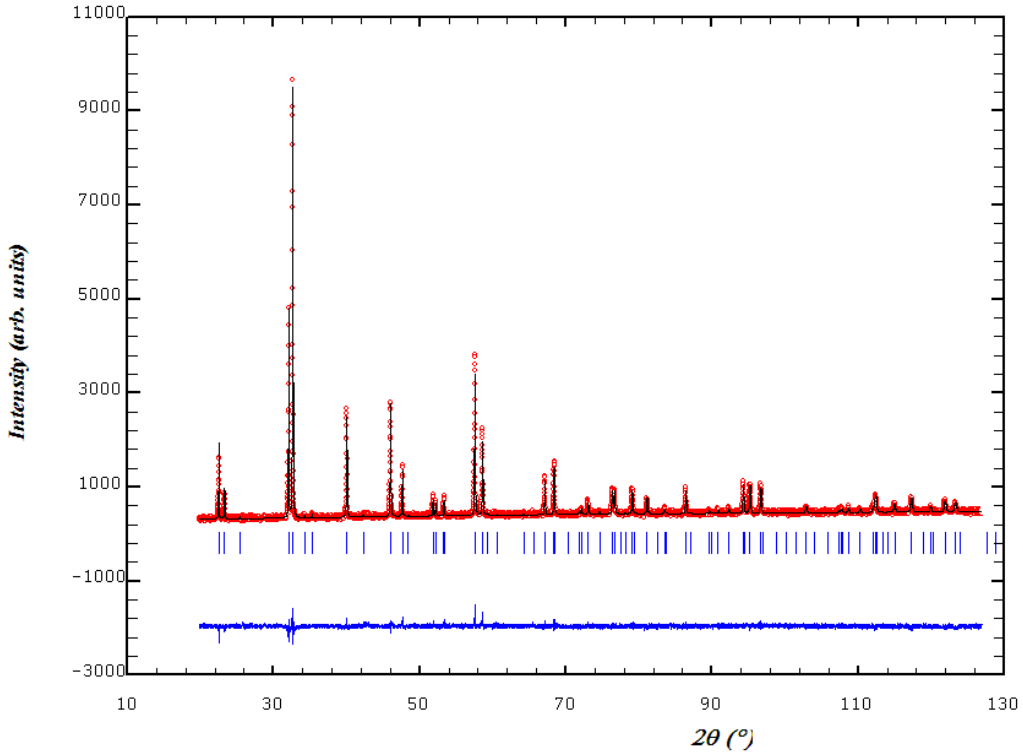

Figure S3. Measured, calculated and difference XRD patterns for $NdBaCoMnO_{5+\delta}$.

Table 3. Refined structural parameters for $NdBaCoMnO_{5+\delta}$ from XRD data.

Atoms	*Site*	*x*	*y*	*z*	*Occupancy*
Nd	1*b*	0	0	0.5	1.00#
Ba	1*a*	0	0	0	1.00#
Co/Mn	2*h*	0.5	0.5	0.254(1)	0.5/0.5#
O1	4*i*	0.5	0	0.295(1)	1.00#
O2	1*c*	0.5	0.5	0	1.00#
O3	1d	0.5	0.5	0.5	0.62(2)

Space group *P4/mmm*: # fixed, a = 3.92757(3) Å, c = 7.67617(6) Å, $B_{overall}$ = 0.4(2) Å², R_{wp} = 7.01%, R_p = 5.41%, R_{Bragg} = 14.4%, χ^2 = 1.74.

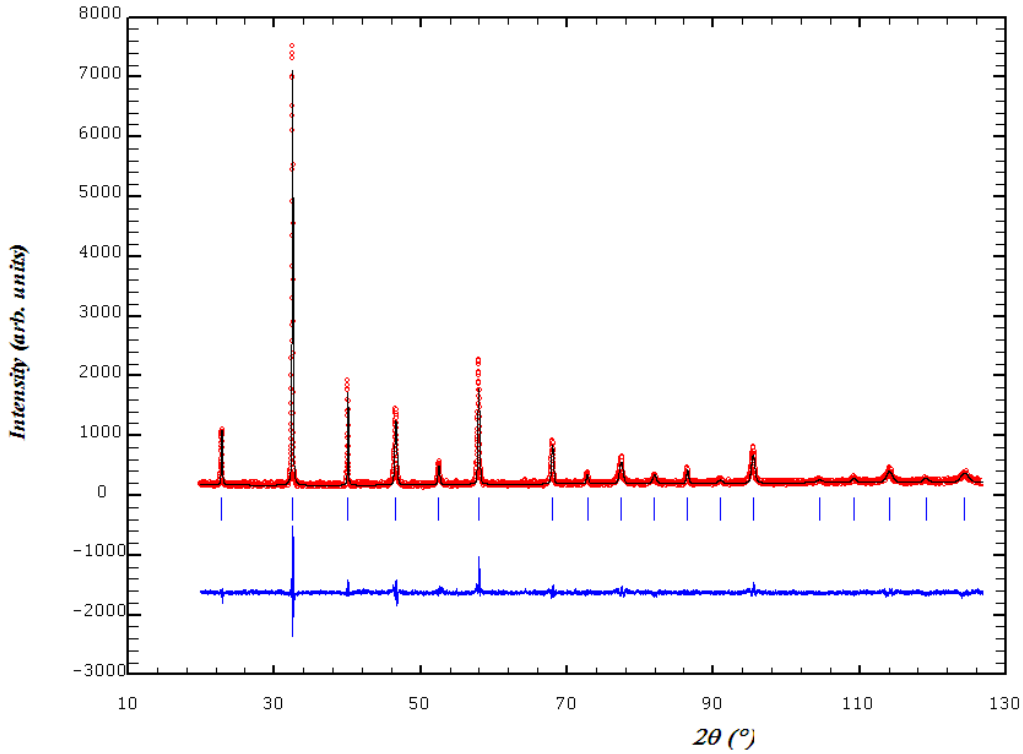

Figure S4. Measured, calculated and difference XRD patterns for $NdBaCoMn_{1.5}O_{5+\delta}$.

Table 4. Refined structural parameters for $NdBaCo_{0.5}Mn_{1.5}O_{5+\delta}$ from XRD data.

Atoms	*Site*	*x*	*y*	*z*	*Occupancy*
Nd/Ba	1*a*	0	0	0	0.5/0.5#
Co/Mn	1*b*	0.5	0.5	0.5	0.25/0.75#
O	3*c*	0.5	0.5	0	0.90(2)

Space group *Pm-3m*: # fixed, a = 3.89518(5) Å, $B_{overall}$ = 0.2(1) Å², R_{wp} = 9.43%, R_p = 7.33%, R_{Bragg} = 7.38%, χ^2 = 2.24.

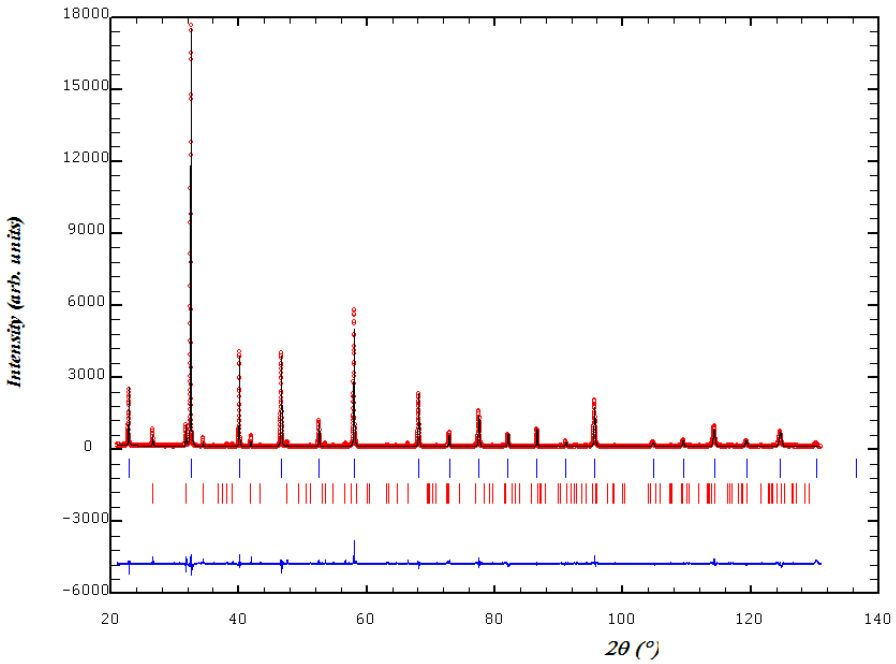

Figure S5. Measured, calculated and difference XRD patterns for $NdBaMn_2O_{5+\delta}$. The lower tick marks correspond to a hexagonal $BaMnO_3$ impurity.

Table 5. Refined structural parameters for $NdBaMn_2O_{5+\delta}$ (99.9(3) wt %) from XRD data.

Atoms	*Site*	*x/a*	*y/b*	*z/c*	*Occupancy*
Nd/Ba	1*a*	0	0	0	0.5/0.5#
Co/Mn	1*b*	0.5	0.5	0.5	0.25/0.75#
O	3*c*	0.5	0.5	0	0.90(2)

Space group *Pm-3m*: # fixed, a = 3.89675(3) Å, $B_{overall}$ = 0.3(1) Å², R_{wp} = 11.3%, R_p = 8.80%, $R_{Bragg}(NdBaMn_2O_6)$ = 7.97%, χ^2 = 2.62.