Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

YBaCuO-type perovskites as potential air electrodes for SOFCs. The case of $YSr_2Cu_2FeO_{7+\delta}$

Sara A. López-Paz,[a] Rafael Marín-Gamero,[a] Xabier Martínez de Irujo-Labalde,[a] Jorge Sánchez-Marcos,[b] Domingo Perez-Coll,[c] Miguel Ángel Alario y Franco[a], Susana García-Martín[a*]

[a] Departamento de Química Inorgánica, Facultad de Ciencias Químicas, Universidad Complutense, 28040 Madrid, Spain

[b] Departamento de Química Física Aplicada, Universidad Autónoma de Madrid, 28049 Madrid, Spain

[c] Instituto de Cerámica y Vidrio, CSIS, Cantoblanco, 28049 Madrid, Spain

e-mail: sgmartin@ucm.es

Figure 1 SI. Rietveld refinement of the room temperature PXRD pattern of the $YSr_2Cu_2FeO_{7.56}$ oxide prepared at air within the P4/mmm space group. Oxygen content and cation location are determined from the experiments indicated in the article. **Table 1SI** collects the refined atomic parameters and agreement factors.

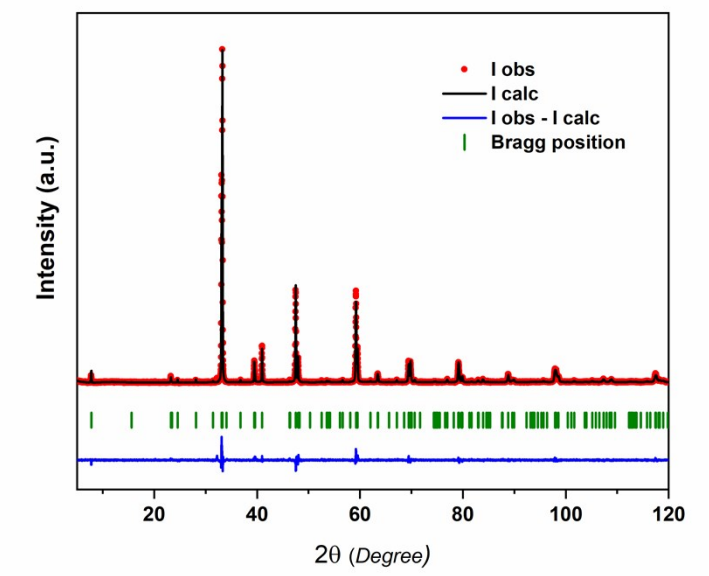

Table 1 SI. Refined cell and atomic parameters as obtained from Rietveld refinement of the room temperature PXRD pattern of the $YSr_2Cu_2FeO_{7.56}$ oxide prepared at air within the P4/mmm space group.

Atom	Site	*x/a*	*y/b*	*z/c*	B_{iso} (Å^2)	*Occupancy*
Fe1/Cu1	1*a*	0	0	0	1.3(1)	0.66/0.34[a]
Cu2/Fe2	2g	0	0	0.3482(3)	0.14(7)	0.83/0.17[a]
Sr	2*h*	0.5	0.5	0.1816(2)	0.91(7)	1
Y	*1d*	0.5	0.5	0.5	0.37(9)	1
O1	2g	0	0	0.148(1)	1.5(6)	1
O2	4i	0	0.5	0.3700(6)	0.64(7)	1
O3	4*n*	0.086(1)	0.5	0	1.8(6)	0.392[b]

Space group *P*4/*mmm* (No. 123); *a* = 3.82412 (5) Å, *c* = 11.3716 (2) Å, *V* = 166.297 (4) Å^3.

R_p = 3.92 %; R_{wp} = 5.30 %; χ^2 = 2.44; R_{Bragg} = 4.45 %

[a] **Occupancy fixed to the values obtained from Mössbauer spectroscopy**

[b] **Occupancy fixed to the value obtained from TGA**

Figure 2 SI. Normalized Fe K-edge XAS spectra for the $YSr_2Cu_2FeO_{7+\delta}$ oxide prepared at air (in blue), together with $Sr_2Fe^{3+}{}_2O_5$ (in black) and $SrFe^{4+}O_3$ (in red) oxides measured as a reference.

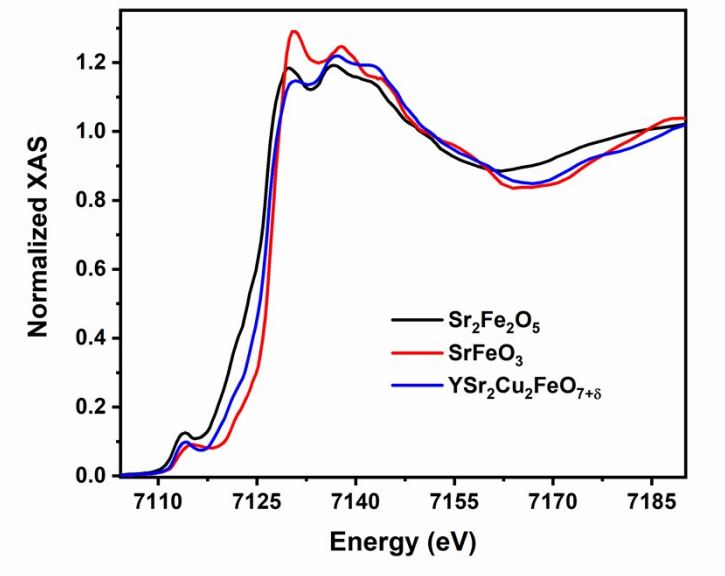

Figure 3 SI. Crystal structure of the (a) $YSr_2Cu_2FeO_{7.08}$ (29) and $YSr_2Cu_2FeO_{7.85}$ (25) compounds synthesized in N_2 and O_3 atmosphere, respectively. The Fe-coordination environment at the charge reservoir layers changes from tetrahedral $[Fe^{3+}O_4]$ to octahedral $[Fe^{4+}O_6]$ with increasing the oxygen content.

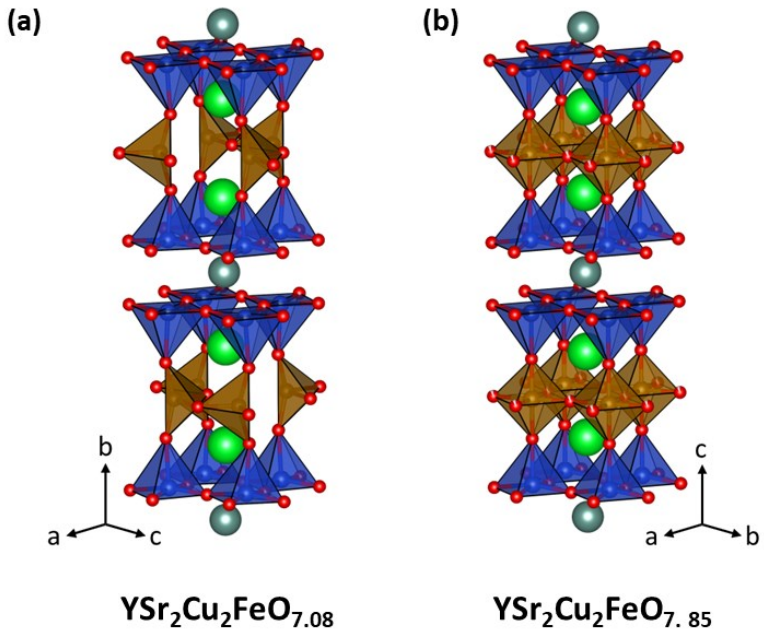

Fig. 4 SI. Thermogravimetric analysis (TGA) at air of the $YSr_2Cu_2FeO_{7.56}$ oxide.

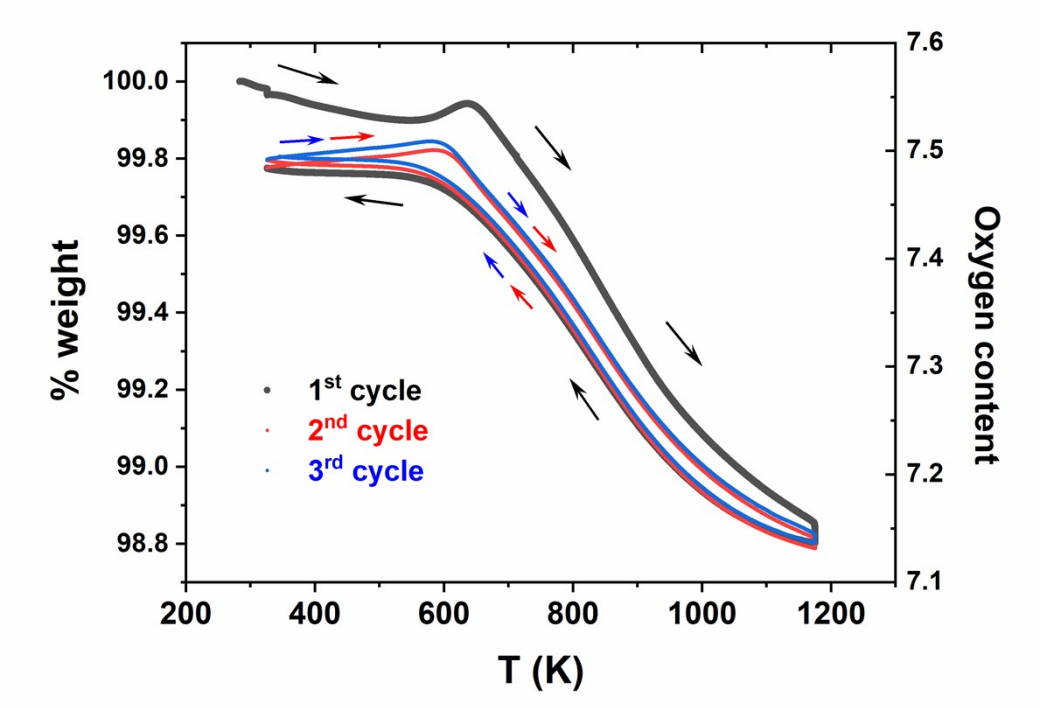

Fig. 5 SI. LeBail fitting of the PXRD pattern for the $YSr_2Cu_2FeO_{7.56}$ oxide (P4/mmm space group) before (upper panel; R_p =2.41, R_{wp} = 5.11, R_{Bragg} = 2.88) and after (lower panel; R_p =2.47, R_{wp} = 5.06, R_{Bragg} = 2.81) thermogravimetric analysis (TGA) at air.

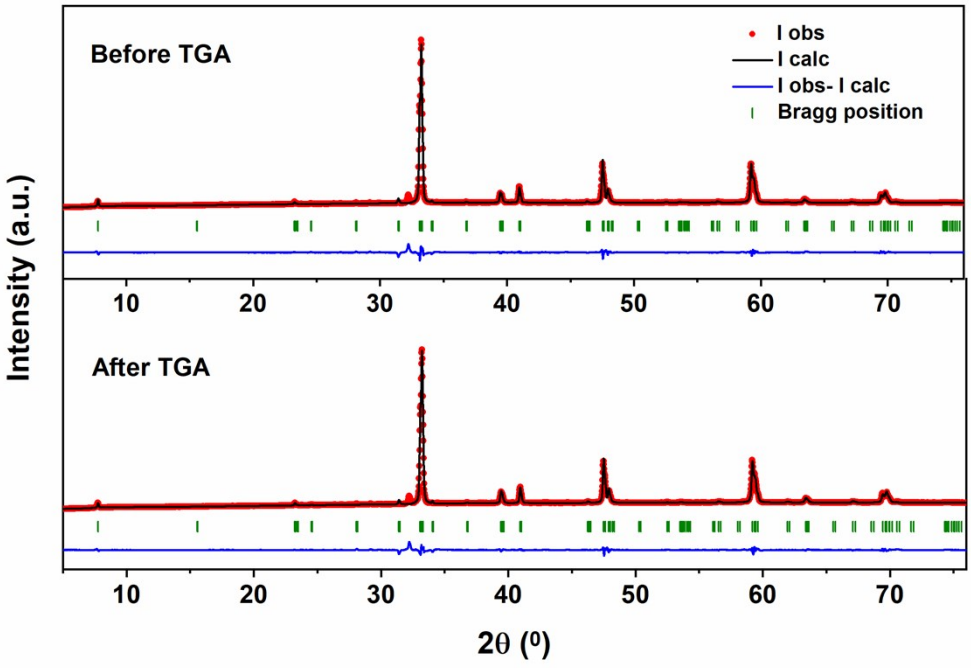

Fig. 6 SI. The PXRD pattern of the mixture of $YSr_2Cu_2FeO_{7.56}$ with CGO (70:30 wt%) heated in air at 1173 K for 48 hours. PXRD patterns of $YSr_2Cu_2FeO_{7.56}$ and CGO are also shown for reference.

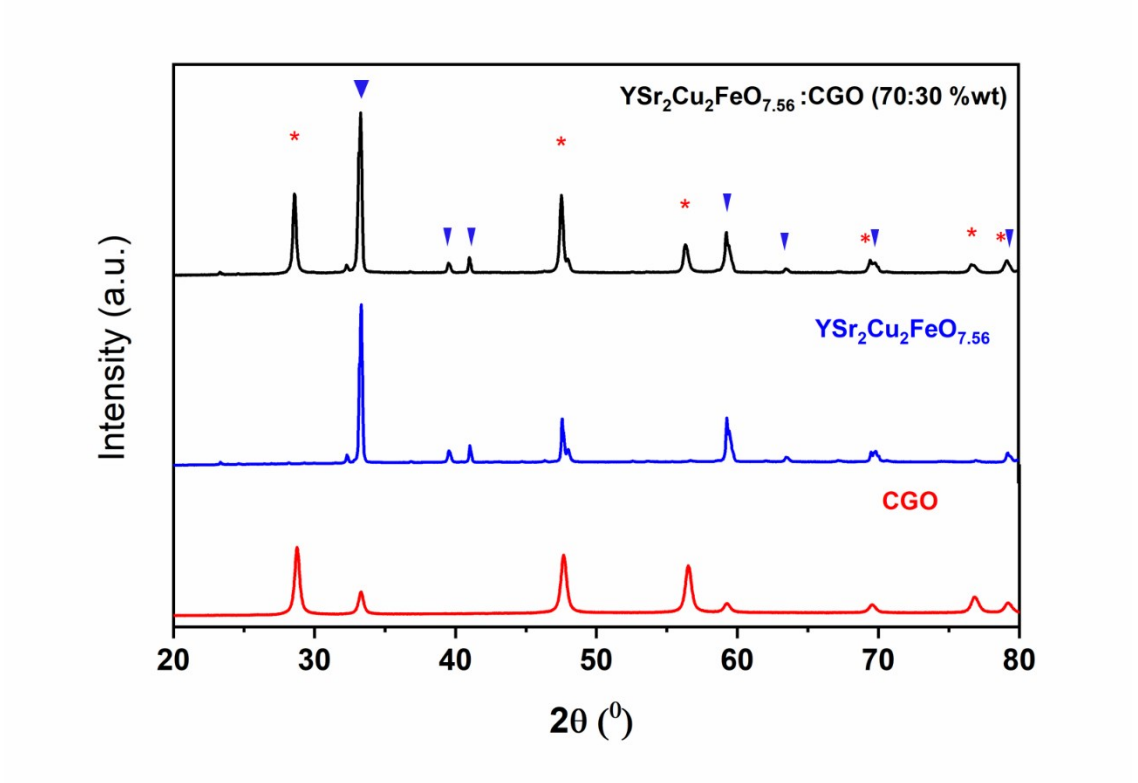

Fig. 7 SI. Unit cell volume values of $YSr_2Cu_2FeO_{7+\delta}$ at different temperatures. Thermal expansion coefficients are calculated using linear-fit parameters in two ranges, below and above 673 K.