

SUPPORTING INFORMATION

Eu₂SrCo_{1.5}Fe_{0.5}O₇ a new promising Ruddlesden–Popper member as cathode component for intermediate temperature solid oxide fuel cells

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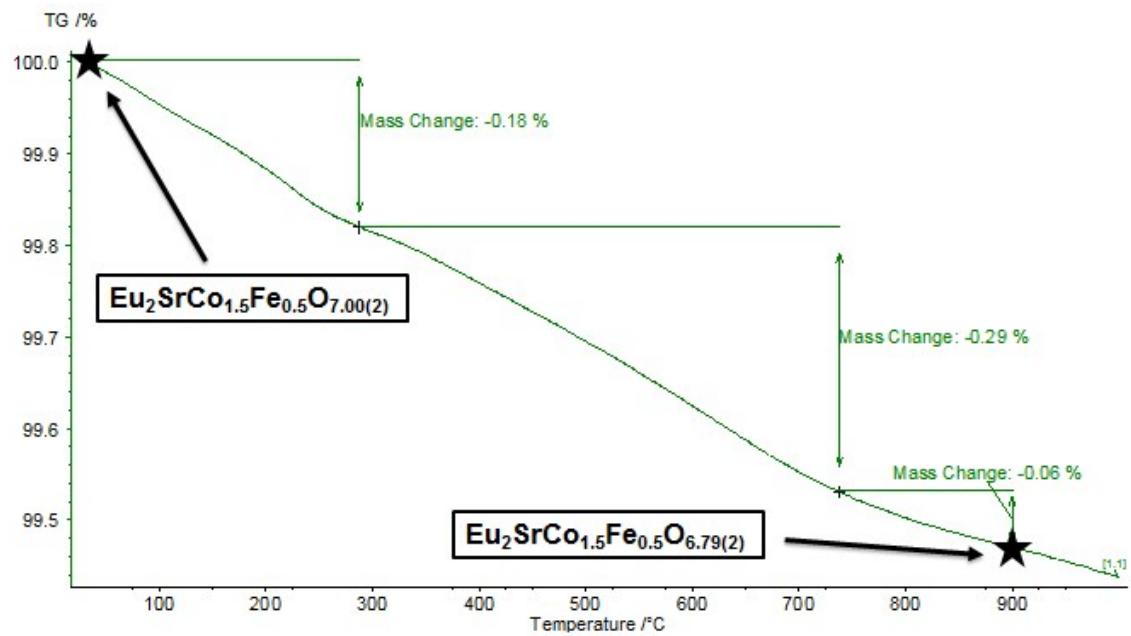


Figure SI 1. TGA analysis of $\text{Eu}_2\text{SrCo}_{1.5}\text{Fe}_{0.5}\text{O}_7$ under air.

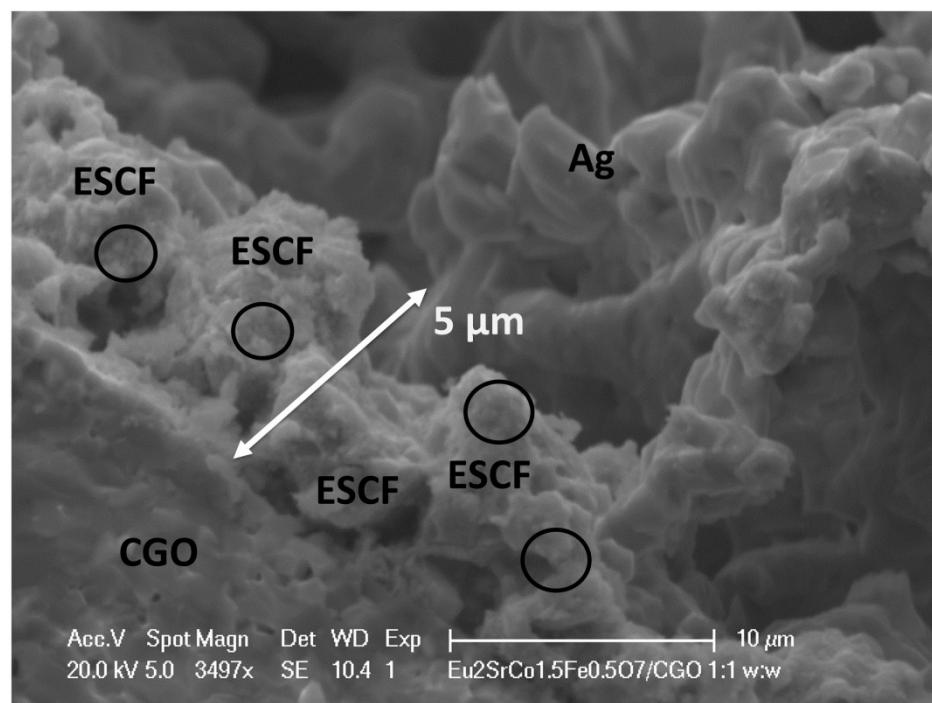
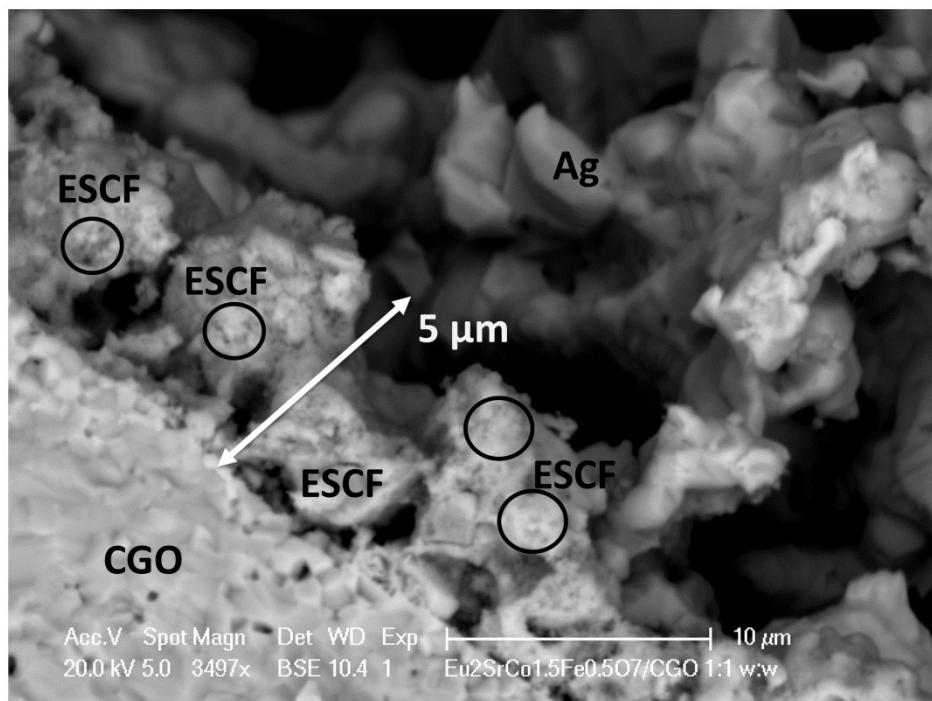


Figure SI 2. SEM images (BSE upper panel, SE lower panel) of one cathode of composition Eu₂SrCo_{1.5}Fe_{0.5}O₇/CGO 70%:30% (w:w), after electrochemical measurements, deposited on a dense CGO pellet. The cathode is ca. 5μm thick and consists of micron-sized particles of ESCF1550 covered by submicron (or nano) sized particles of commercial CGO. The adherence between the electrolyte and the cathode is good but its porosity and tortuosity could be improved.

Table SI 1: Structural parameters for Eu₂SrCo_{1.5}Fe_{0.5}O₇ obtained from XRD data.

a (Å)	5.3925(1)		
c (Å)	19.5552(6)		
Eu position 8j		O(1) position 8h	
x	0.2349(5)	z	0.397(2)
z	0.1814(1)	Occ.	1.00(2)
Occ.	1.00	U*100 (Å²)	0.39(4)
U*100 (Å²)	0.68(5)	O(2) position 8j	
Sr position 4f		x	0.289(2)
x	0.2470(7)	z	0.296(1)
Occ.	1.00	Occ.	1.00(2)
U*100 (Å²)	0.21(2)	U*100 (Å²)	0.39(4)
Co/Fe position 8j		O(3) position 4e	
x	0.2453(7)	z	0.080(4)
z	0.4029(2)	Occ.	1.00(3)
Occ. Co/Fe	0.75/0.25	U*100 (Å²)	0.39(4)
U*100 (Å²)	0.14(4)	O(4) position 4e	
		z	0.390(4)
		Occ.	1.00(3)
		U*100 (Å²)	0.39(4)
		O(5) position 4g	
		x	0.296(2)
		Occ.	1.00(2)
		U*100 (Å²)	0.39(4)

Space Group P4₂/mnm (#136): 4e (0 0 z), 4f (x x 0), 4g (x -x 0), 8h (0 ½ z), 8j (x x z)
 $\chi^2 = 2.04$, R_{wp}= 1.94%, R_{exp}= 1.35%, R_B= 5.53%

Table SI 2: Selected structural information for $\text{Eu}_2\text{SrCo}_{1.5}\text{Fe}_{0.5}\text{O}_7$ obtained from XRD data. Angles are given in degrees and distances in Å, distortion Δ of the BO_n polyhedra is given as $\Delta = 1/n \sum_{j=1,n} \{(d_n - \langle d(\text{B-O}) \rangle) / \langle d(\text{B-O}) \rangle\}^2$ and $t = \langle r(\text{A}) \rangle + r(\text{O}) / \sqrt{2} \langle r(\text{B}) \rangle + r(\text{O})$.

Eu	O(1)	2.44(2) x 2
	O(2)	2.28(2)
	O(2)	2.444(9) x 2
	O(3)	2.679(8)
	O(4)	2.46(4)
average Eu-O distortion $\text{EuO}_7 \times 10^{-4}$		2.456(9) 19.356
Sr	O(1)	2.79(3) x 4
	O(3)	2.45(2) x 2
	O(5)	2.476(9) x 2
average Sr-O distortion $\text{SrO}_8 \times 10^{-4}$		2.722(8) 49.803
Co/Fe	O(1)	1.912(5) x 2
	O(2)	2.11(1)
	O(3)	1.972(8)
	O(4)	1.887(9)
	O(5)	1.926(8)
average Co/Fe-O distortion $(\text{Co/Fe})\text{O}_6 \times 10^{-4}$		1.953(8) 14.741
tilt angle^a		18.6(2)

^a along [110] pseudocubic axis in a given two-layer perovskite block and along [-110] direction in adjacent blocks.

Table SI 3 Final refined parameters used in the fitting of impedance spectra, capacitance, relaxation frequency and ASR values for Eu₂SrCo_{1.5}Fe_{0.5}O₇ at different temperatures.

Parameters	Temperature (°C)			
	550	600	650	700
R _{HF} (Ωcm ²)	1.49	0.36	0.23	0.15
Q _{HF} ((Fs) ¹⁻ⁿ cm ⁻²)	1.02 10 ⁻⁵	5.17 10 ⁻⁵	1.1 10 ⁻⁴	2.4 10 ⁻⁴
n _{HF}	0.34	0.50	0.48	0.46
C _{HF} (Fcm ⁻²)	3.8 10 ⁻¹⁵	1.08 10 ⁻⁹	1.18 10 ⁻⁹	1.42 10 ⁻⁹
f _{HF} (Hz)	2.7 10 ¹³	4.07 10 ⁸	5.85 10 ⁸	7.32 10 ⁸
E _a (eV)	0.95			
R _{IF} (Ωcm ²)	0.74	0.37	0.15	0.07
Q _{IF} ((Fs) ¹⁻ⁿ cm ⁻²)	5.1 10 ⁻³	4.68 10 ⁻³	5.9 10 ⁻³	1.02 10 ⁻²
n _{IF}	0.62	0.63	0.69	0.71
C _{IF} (Fcm ⁻²)	1.5 10 ⁻⁴	1.14 10 ⁻⁴	2.7 10 ⁻⁴	5.5 10 ⁻⁴
F _{IF} (Hz)	1376	4304	3843	4054
E _a (eV)	1.01			
R _{LF} (Ω.cm ²)	0.64	0.32	0.098	0.04
Q _{LF} ((Fs) ¹⁻ⁿ cm ⁻²)	9.2 10 ⁻²	4.8 10 ⁻²	6.05 10 ⁻²	8.90 10 ⁻²
n _{LF}	0.95	0.88	0.90	0.90
C _{LF} (Fcm ⁻²)	9.2 10 ⁻²	2.7 10 ⁻²	3.5 10 ⁻²	4.7 10 ⁻²
f _{LF} (Hz)	2.65	17.7	45.9	89.15
E _a (eV)	1.25			
χ ² (x 10 ⁵)	2.04	1.54	1.48	3.10
ASR (Ω.cm ²)	2.87	1.05	0.48	0.26