

## ELECTRONIC SUPPLEMENTARY INFORMATION FOR

### **From theory to experiment: $\text{BaFe}_{0.125}\text{Co}_{0.125}\text{Zr}_{0.75}\text{O}_{3-\delta}$ , a highly promising cathode for intermediate temperature SOFCs**

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**SI1 – Synchrotron X-ray diffraction**

**SI2 – Neutron diffraction**

**SI3 – X-ray thermodiffraction and Thermal Expansion Coefficient (TEC)**

**SI4 – Impedance Spectroscopy of the cells (Heating and cooling)**

## SI1 – Synchrotron X-ray diffraction

Table SI1.1. Refined structural parameters obtained from synchrotron X-ray diffraction for  $\text{BaFe}_{0.125}\text{Co}_{0.125}\text{Zr}_{0.75}\text{O}_{3-6}$  (BFCZO) at room temperature in the space group  $Pm\bar{3}m$ . Occupancy values for the BFCZO phase are fixed to the result obtained by neutron diffraction data. Information about the secondary phase,  $\text{BaZrO}_3$  (BZO) is also added.

Phases	BFCZO	BZO
Lattice parameter, $a / \text{Å}$	4.1863(1)	4.1798(1)
Occ. Ba	0.3333	0.3333
Occ. Fe	0.042	0
Occ. Co	0.044	0
Occ. Zr	0.248	0.3333
Occ. O (1)	0.966	1
$R_p$ (%)	3.77	
$R_{wp}$ (%)	5.09	
$R_{exp}$ (%)	1.49	
Bragg $R$ -factor	3.33	1.2

## SI2 – Neutron diffraction

Rietveld refinement  
(anisotropic oxygen)

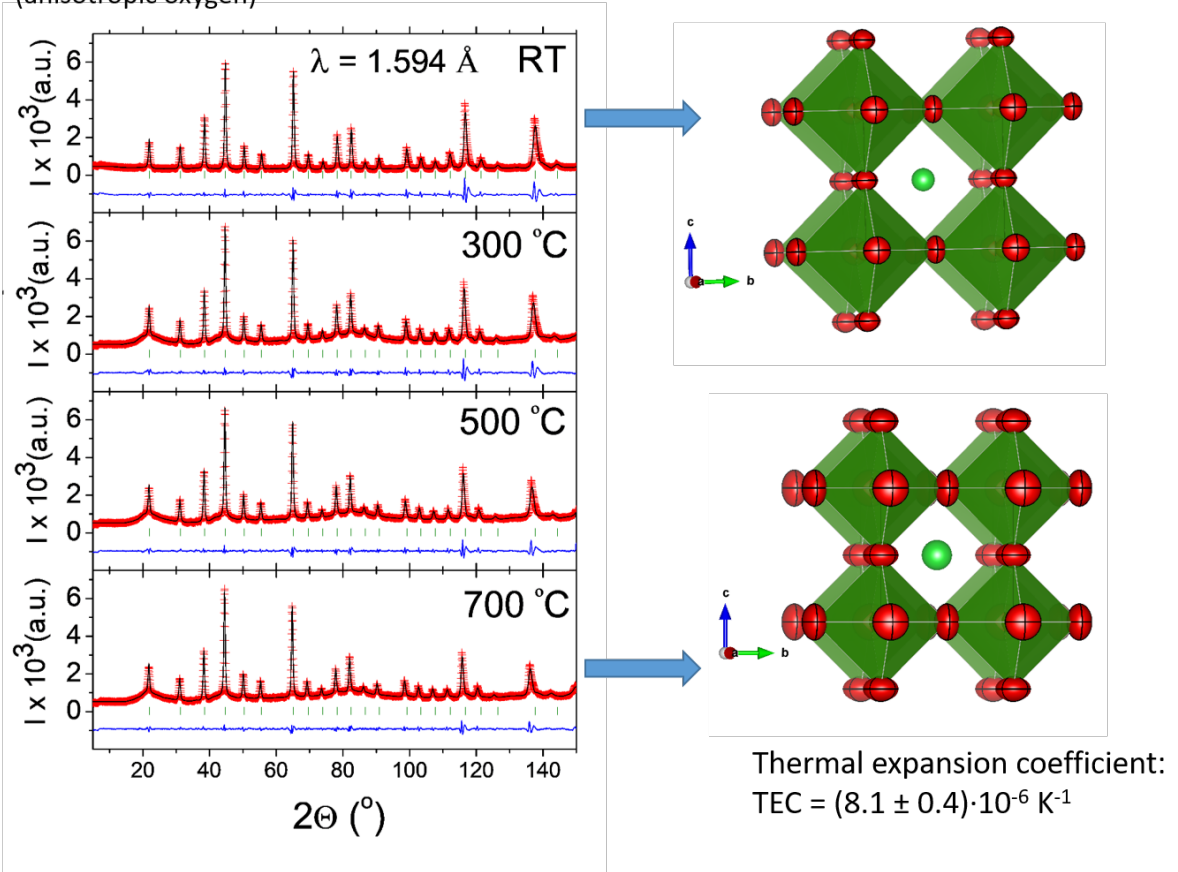
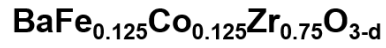


Fig SI2.1. Anisotropic atomic displacement analysis of oxygen atoms from Neutron powder diffraction data: Illustration of the perovskite crystal structure including 95% probability displacement ellipsoids for room temperature and 700 °C data.

### SI3 –X-ray thermodiffraction and Thermal Expansion Coefficient (TEC)

X-ray thermodiffraction was performed from room temperature to 1100 °C on a PANalytical modelo X'Pert PRO diffractometer using Cu radiation.

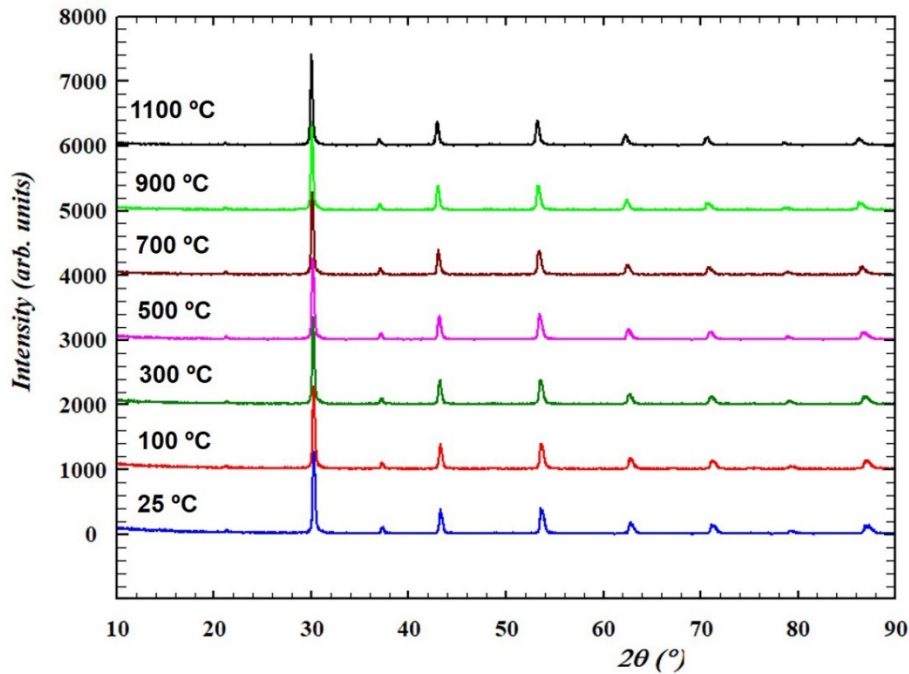


Figure SI3.1. X-ray thermodiffraction of BaFe<sub>0.125</sub>Co<sub>0.125</sub>Zr<sub>0.75</sub>O<sub>3-6</sub>

Table SI3.1. Temperature dependence of the cell parameters obtained from Le Bail analysis.

T (°C)	a (Å)
25	4.1878(1)
100	4.1916(1)
300	4.1980(1)
500	4.2051(1)
700	4.2098(1)
900	4.2181(1)
1100	4.2245(1)

The thermal expansion coefficient was determined using the lattice parameters at different temperatures by the expression:

$$TEC = \frac{(a_{T_2} - a_{T_1}) / a_{T_1}}{\Delta T}$$

where  $a_{T_x}$  is the lattice parameter at a selected temperature and  $\Delta T$  corresponds to the difference of temperature. A TEC value of  $8.0 \times 10^{-6} \text{ K}^{-1}$  is found from room temperature to 1100 °C.

### SI4 – Impedance Spectroscopy of the cells (Heating and cooling)

Table SI4.1. Area specific polarization resistance (ASRp) and ohmic resistance (ASRs) for the symmetrical cells tested in stagnant air in a 2-electrode configuration (heating process).

T (°C)	500	550	600	650	700	750	800
<b>BFCZO Cell</b>							
ASRp ( $\Omega \cdot \text{cm}^2$ )	7.19	3.39	1.47	0.66	0.33	0.22	0.13
ASRs ( $\Omega \cdot \text{cm}^2$ )	7.21	4.85	3.37	2.50	1.97	1.48	1.18
<b>BFCZO-GDC cell</b>							
ASRp ( $\Omega \cdot \text{cm}^2$ )	5.89	2.13	0.83	0.33	0.13	0.08	0.05
ASRs ( $\Omega \cdot \text{cm}^2$ )	7.64	4.82	3.28	2.35	1.78	1.31	1.02

BFCZO cell:

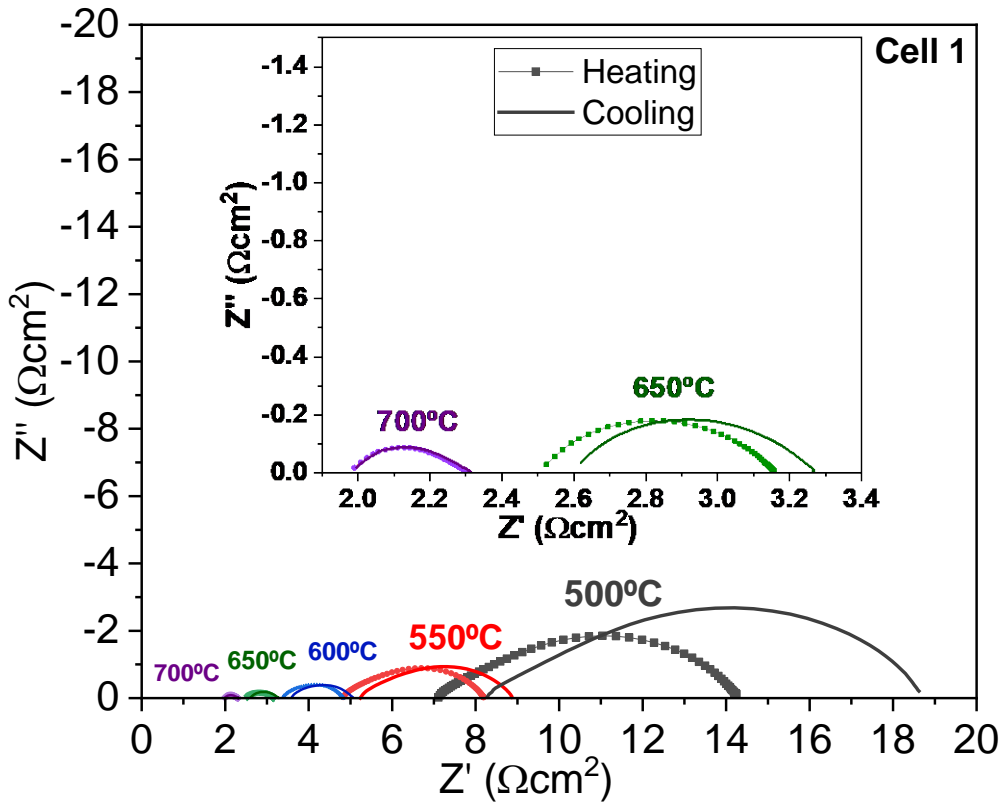


Fig SI4.1. Impedance spectroscopy data from a BFCZO symmetrical cell in a 2-electrode configuration from 500 °C to 700 °C during heating and cooling. Insets show the spectra at 650 °C and 700 °C zoomed in.

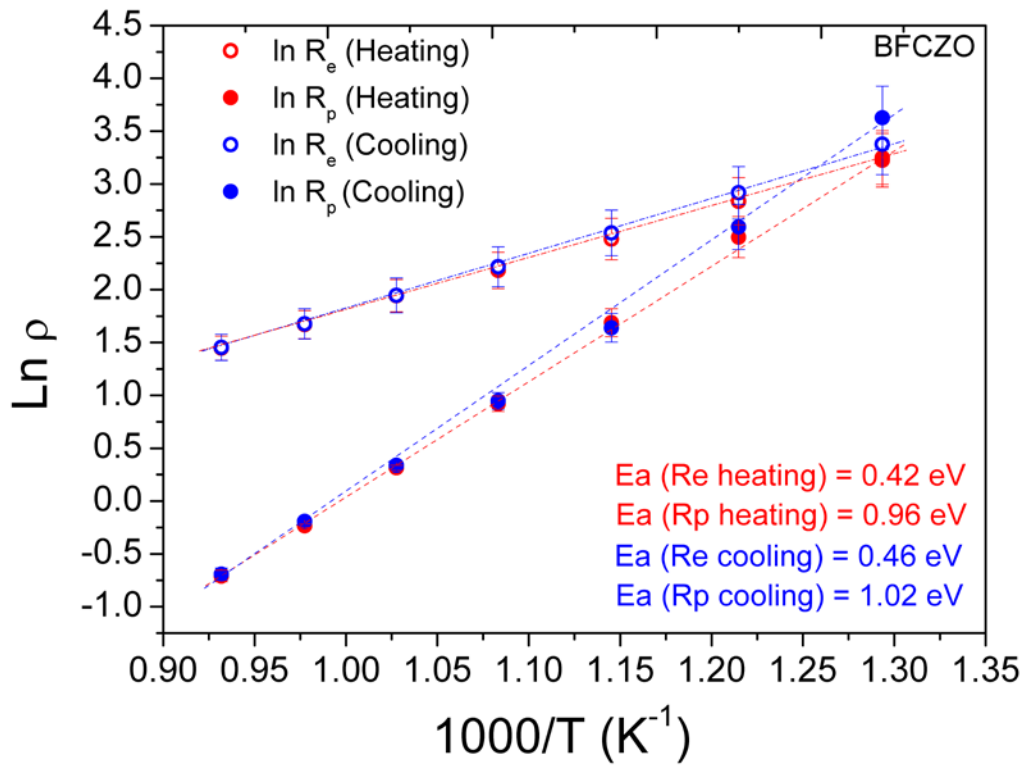


Figure S14.2. Temperature dependence of the resistivity for BFCZO cell during heating and cooling processes.

BFCZO-GDC cell:

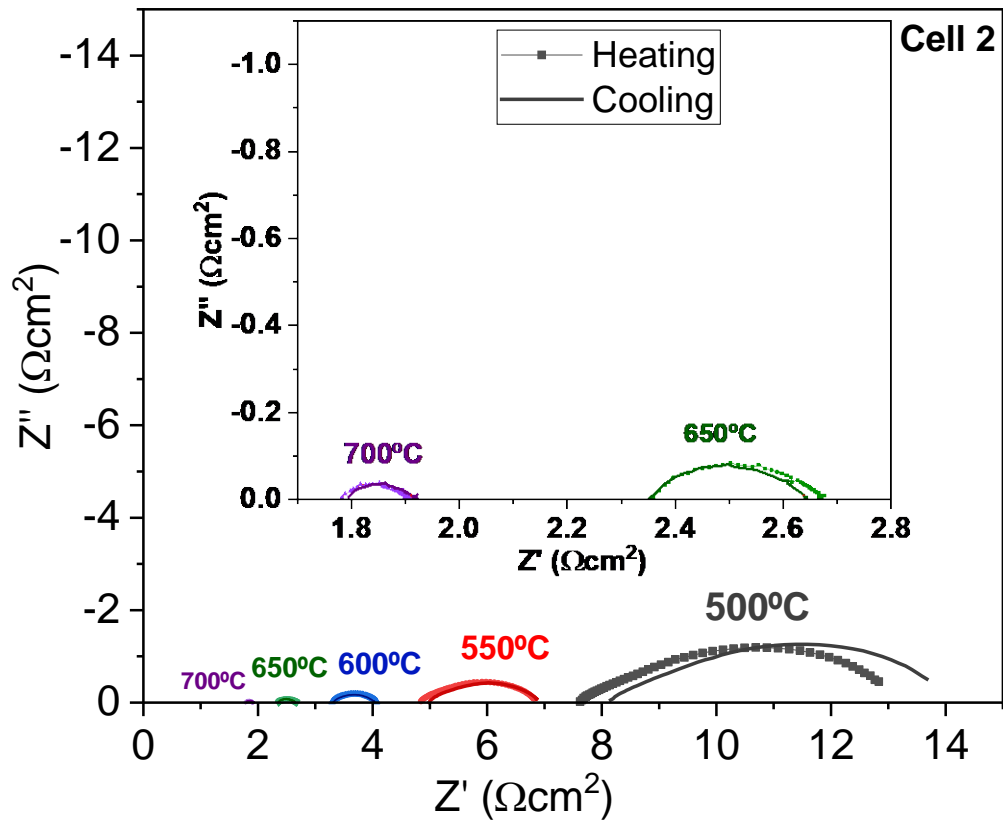


Fig SI4.3. Impedance spectroscopy data from a BFCZO-GDC symmetrical cell in a 2-electrode configuration from 500 °C to 700 °C during heating and cooling. Insets show the spectra at 650 °C and 700 °C zoomed in.

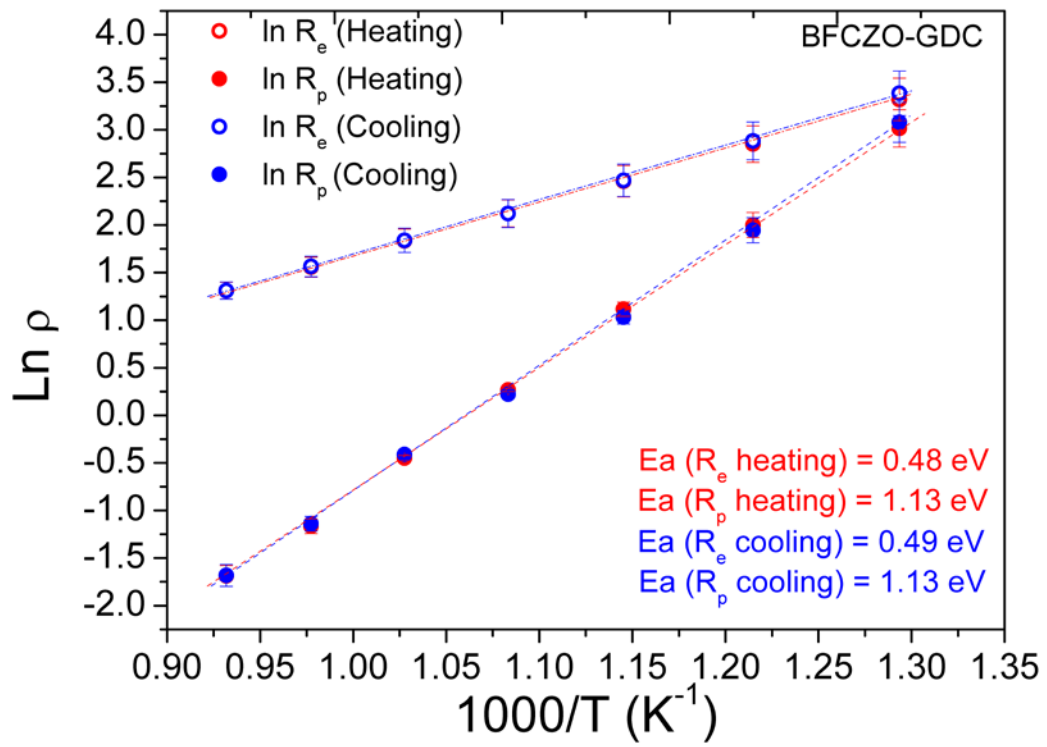


Figure SI4.4. Temperature dependence of the resistivity for BFCZO-GDC cell during heating and cooling processes.