Supporting Information

Multi-doped ceria-based composite as a promising low-temperature electrolyte with enhanced ionic conductivity for steam electrolysis

Yuheng Liu[a], Ming Xu[b] , Yunlong Zhao[b], Bahman Amini Horri[*a]

a. School of Chemistry and Chemical Engineering, Faculty of Engineering & Physical Sciences, University of Surrey, GU2 7XH, Guildford, Surrey, United Kingdom
b. Advanced Technology Institute, Faculty of Engineering & Physical Sciences, University of Surrey, GU2 7XH, Guildford, Surrey, United Kingdom

Characterisation details

Physicochemical characterisation

The lattice parameters were calculated from the following Bragg's equation[1]:

$$\alpha = d\left(\sqrt{h^2 + k^2 + l^2}\right) \quad \text{Eq. S1}$$

where α is the cubic lattice parameter, d is the lattice spacing between the planes in the atomic lattice and h, k and l are the miller indices of the plane of diffraction. The Scherrer's equation was employed to estimate the size of crystallites[1]:

$$D = \frac{0.9\lambda}{\beta cos(\theta)} \quad \text{Eq. S2}$$

where D is the mean crystallite size (nm), λ is the X-ray wavelength (nm), β is the line broadening at half maximum intensity (FWHM) (rads) and θ is the Bragg angle (rads).
Theoretical densities (ρ) were calculated from the following crystallographic equation:

$$\rho = \frac{\sum_i v_i * Z_i * M_i}{a^3 * N_A} \quad \text{Eq. S3}$$

where v_i is the stoichiometric coefficient, Z_i is the number of atom i per unit cell (face-centred cubic for a ceria system), M_i is the molar mass of atom i in g·mol⁻¹, a is the lattice parameter from XRD patterns and N_A is Avogadro's number.

Electrochemical characterisation

The following equation was used to calculate the bulk conductivity (σ_{GI}), grain-boundary conductivity (σ_{GB}), and total conductivity (σ_t) of the GDC samples:

$$\sigma = L/RA \quad \text{Eq. S4}$$

Where σ is the electrical conductivity, L is the thickness of the prepared GDC pellet, A is the electrode surface area contacting with the ceramic pellet (the silver coating), and R (R_{GI}, R_{GB}, and R_t) are resistances calculated by modelling analogous circuits.
The electrical conductivity and activation energy were estimated by a temperature-dependent Arrhenius conductivity model as below:

$$\sigma_T = \sigma_0 e^{-Ea/kT} \quad \text{Eq. S5}$$

Where Ea is the activation energy, σ_T is the temperature-dependent electrical conductivity, T is the absolute temperature, K is the Boltzmann constant (1.36×10^{-23} J/K), and σ_0 is a pre-exponential factor representing the intrinsic conductivity of the electrolyte polycrystalline structure.

Results and discussion

Table S1 Lattice parameters and particle size of sintered pellets and GDC (reference card).

Sample	Lattice parameter (Å)	Particle size (nm)
5LB1C-1	5.423	37.54
5LB1C-2	5.431	33.62
5LB1C-3	5.430	29.09
5LB-1	5.419	35.87
5LB-2	5.426	32.31
5LB-3	5.425	29.04
GDC (reference card)	5.423	-

The measurement average error: ＜±0.1%.

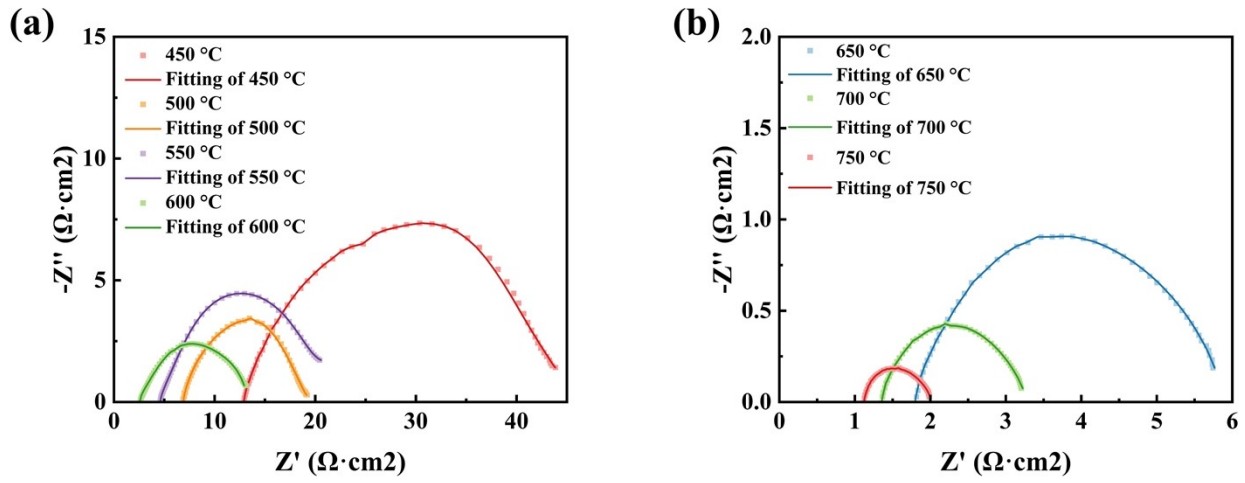

Figure S1 (a)Nyquist plots and fitting curves of 5LB1C-1 at 450, 500, 550, 600 °C, (b) Nyquist plots and fitting curves of 5LB1C-1 at 650, 700, 750 °C,

Notes and references

1. I. Unal, S. Meisuria, M. Choolaei, T. R. Reina and B. A. Horri, *Ceramics International*, 2018, **44**, 6851-6860.

