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Supplementary Information

Pure CO_2 electrolysis over an Ni/YSZ cathode in a solid oxide electrolysis cell

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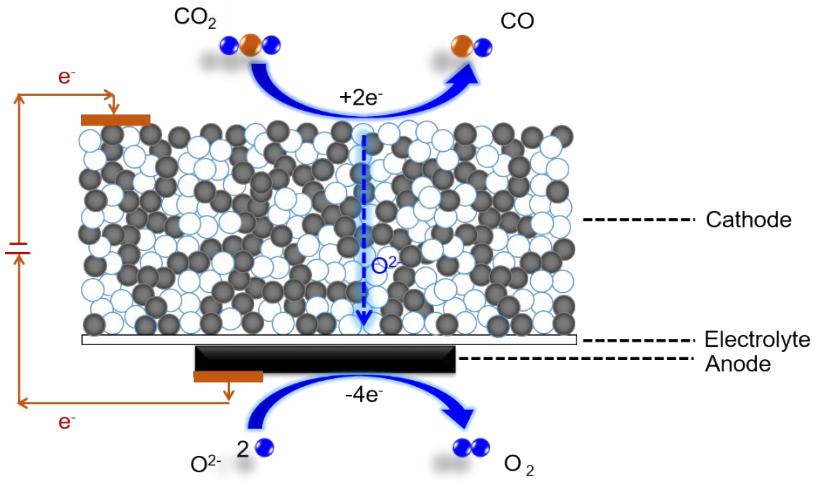

Figure S1. Schematic diagram of the SOEC for CO_2 electrolysis.

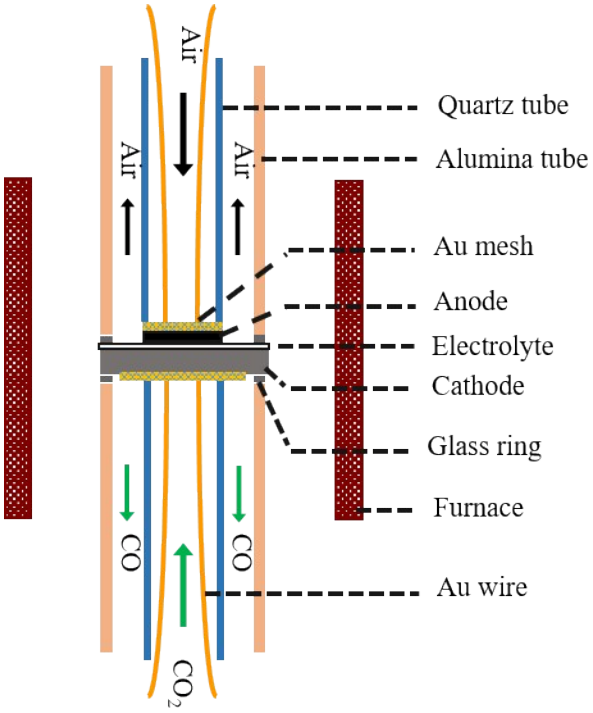

Figure S2. Schematic diagram of the SOEC test station.

Table S1. High-temperature CO_2 electrolysis over Ni/YSZ cathode.

The structure of SOEC	Reactant gas to cathode	Temperature	Ref.
Ni-YSZ|YSZ|YSZ-LSM|LSM	CO_2 + CO	700°C - 800°C	1
Ni-YSZ|YSZ|YSZ-LSM	CO_2 + CO	800°C	2
Ni-GDC|YSZ|GDC|LSM-YSZ	CO_2 + CO	800°C	3
Ni-YSZ| YSZ|LSM-YSZ	CO_2 + CO CO_2 + H_2	700°C - 1000°C	4
Ni-YSZ|YSZ|YDC|LSFC	CO_2 + H_2	700°C	5
Ni-YSZ|YSZ|GDC|PBC-GDC	CO_2 + CO	700°C	6
Ni-YSZ|YSZ|LSM-YSZ	CO_2 + H_2O + H_2	850°C	7
Ni-YSZ|YSZ|LSM-YSZ	CO_2 + CO	850°C	8
Ni-YSZ|YSZ|LSM-YSZ	CO_2 + H_2O + H_2	800°C 850°C	9
Ni-YSZ|YSZ|LSM-YSZ	CO_2 + H_2O + H_2	~875°C	10
Ni-YSZ|YSZ|LSM-YSZ	CO_2 + CO	850°C	11
Ni-YSZ|YSZ|LSM-YSZ	CO_2 + H_2O + H_2	800°C	12
Ni-YSZ|YSZ|LSM-YSZ	CO_2 + CO	850°C	13
Ni-YSZ|YSZ|LSCF-GDC Ni-YSZ|YSZ|LSM-YSZ	CO_2 + H_2O + H_2	800°C	14
Ni-YSZ|YSZ|LSCF-GDC	CO_2 + H_2	800°C	15
Ni-YSZ|YSZ|LSM-ESB	CO_2 + H_2	800°C	16
Ni-YSZ|YSZ|GDC|LSCF Ni-GDC|YSZ|GDC|LSCF Ni-YSZ|YSZ|LSM-YSZ	CO_2 + H_2 + N_2	1000°C	17
Ni-YSZ|YSZ|GDC|LSCF|LSM	CO_2 + CO	650°C 700°C 750°C	18
Ni-YSZ|YSZ|LSM-YSZ	CO_2 + CO CO_2 + H_2	1000°C	19
Ni-YSZ|YSZ|LSM-YSZ Ni-SDC|YSZ|LSM-YSZ	CO_2 + H_2 + N_2	1000°C	20

Table S2. Theoretical OCV of Ni/YSZ-supported SOEC with 95% CO_2 + 5% N_2 at cathode and air at anode.

	700 °C	750 °C	800 °C
K_1	3.001×10^{-3}	3.987×10^{-3}	5.160×10^{-3}
K_2	2.380×10^{-11}	1.312×10^{-10}	6.163×10^{-10}
$[O_2]$	0.6290×10^{-16}	0.1083×10^{-14}	0.1427×10^{-13}
$OCV_{theoretical}$	0.749 V	0.725 V	0.701 V

$CO_2(g) + Ni = NiO + CO(g)$; K_1

$CO_2(g) = CO(g) + 1/2O_2(g)$; K_2

$$K_1 = \frac{[CO]}{CO_2}$$

$$K_2 = \frac{[CO][O_2]^{1/2}}{CO_2}$$

$$[O_2]_{Cathode} = \left(\frac{K_2}{K_1}\right)^2$$

$$E_{Nernst} = \frac{RT}{4F}\ln\left(\frac{[O_2]Anode}{[O_2]Cathode}\right)$$ R = 8.314 J mol^{-1} K^{-1}, F = 96485 C mol^{-1}, $[O_2]_{Anode}$ = 0.21

Table S3. Theoretical OCV of SOEC with 95% CO_2 + 5% N_2 at cathode and air at anode.

	700 °C	750 °C	800 °C
K_2	2.380×10^{-11}	1.312×10^{-10}	6.163×10^{-10}
$[O_2]$	0.521×10^{-8}	0.163×10^{-7}	0.456×10^{-7}
$OCV_{theoretical}$	0.320 V	0.311 V	0.302 V

$CO_2(g) = CO(g) + 1/2O_2(g)$; K_2

$$K_2 = \frac{[CO][O_2]^{1/2}}{[CO_2]} = \frac{2[O_2]^{3/2}}{[CO_2]} \longrightarrow [O_2]_{Cathode} = \left(\frac{K_2[CO_2]}{2}\right)^{2/3}$$

$$E_{Nernst} = \frac{RT}{4F}\ln\left(\frac{[O_2]Anode}{[O_2]Cathode}\right)$$ R = 8.314 J mol^{-1} K^{-1}, F = 96485 C mol^{-1}, $[O_2]_{Anode}$ = 0.21

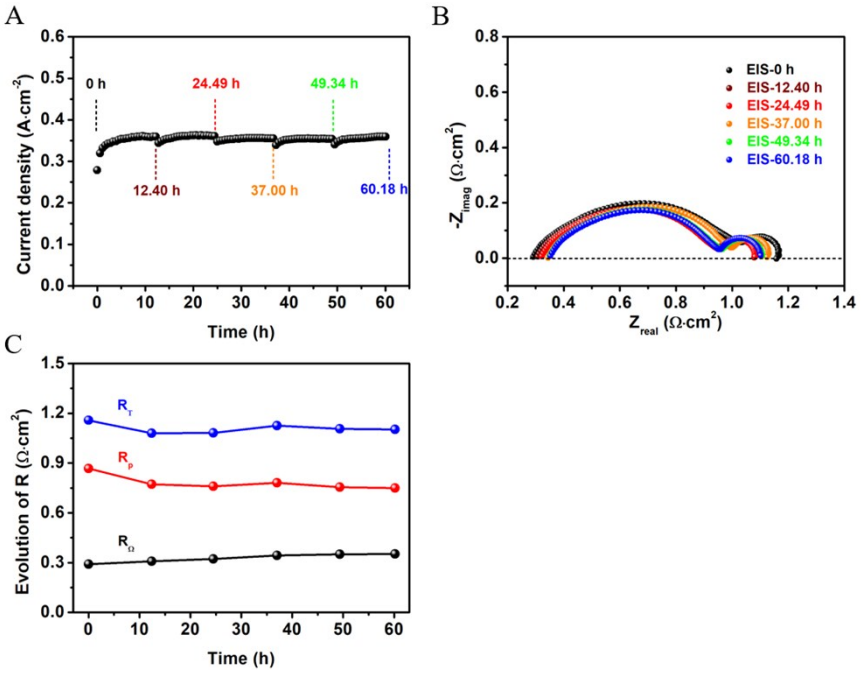

Figure S3. (A) Stability test of pure CO_2 electrolysis at the voltage of 1.5 V at 700 °C, (B) EIS of the cell at 1.5 V and 700 °C with pure CO_2 to the cathode and air to the anode and (C) The evolution of resistance.

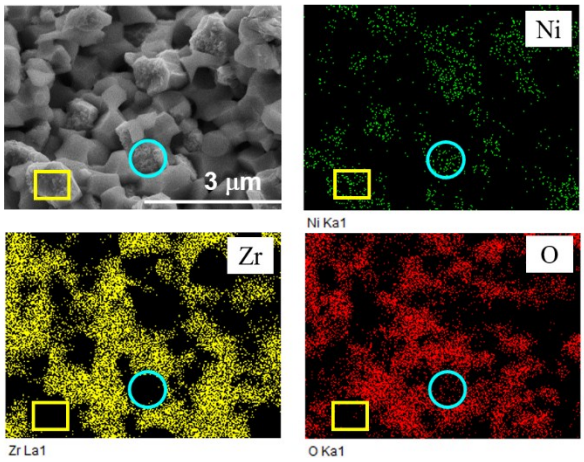

Figure S4. EDS mappings of the Ni/YSZ cathode after the stability test.

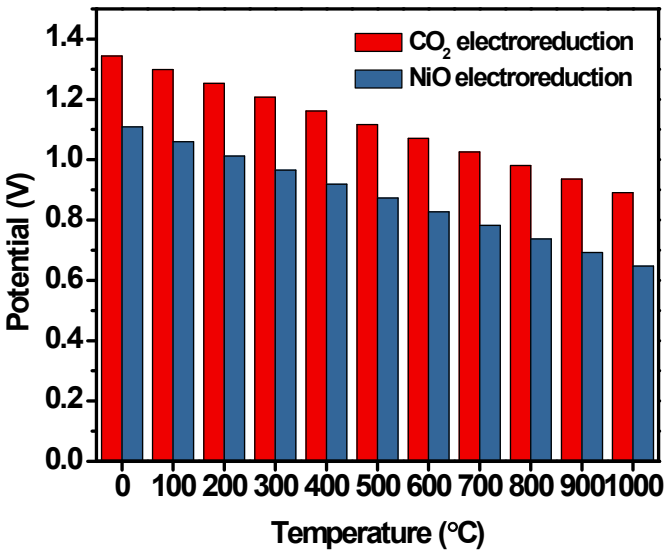

Figure R5. Bar chart for thermodynamic equilibrium voltage of CO_2 and NiO electrolysis at different temperatures.

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