

# Evaluating the effect of B-site cation doping on the properties of $\text{Pr}_{0.4}\text{Sr}_{0.5}\text{Fe}_{0.9}\text{Mo}_{0.1}\text{O}_3$ for reversible single-component cell

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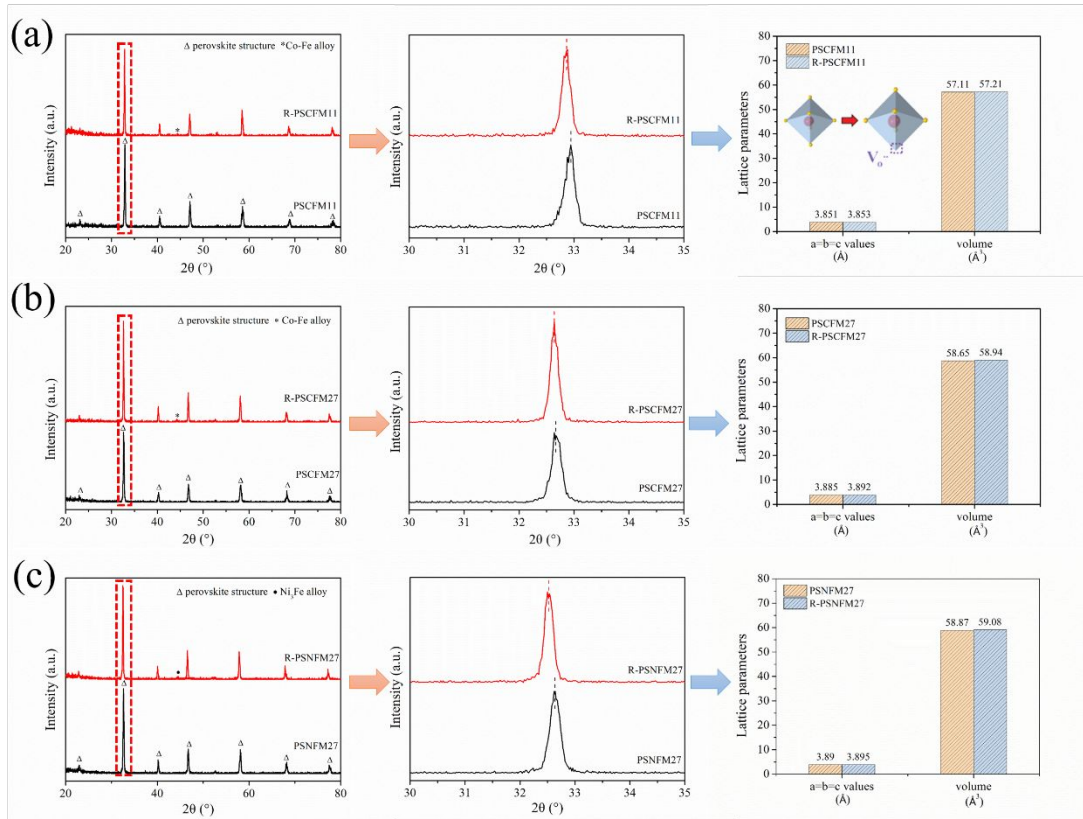
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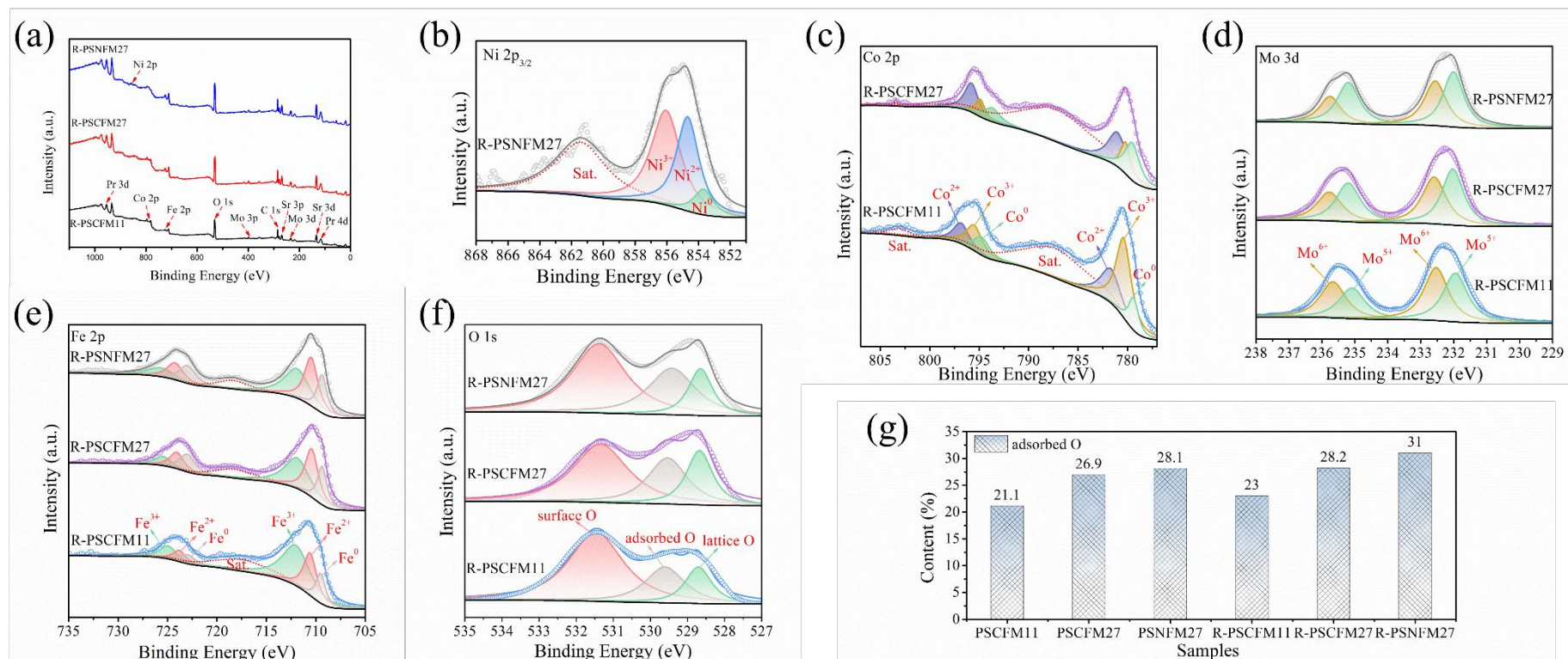
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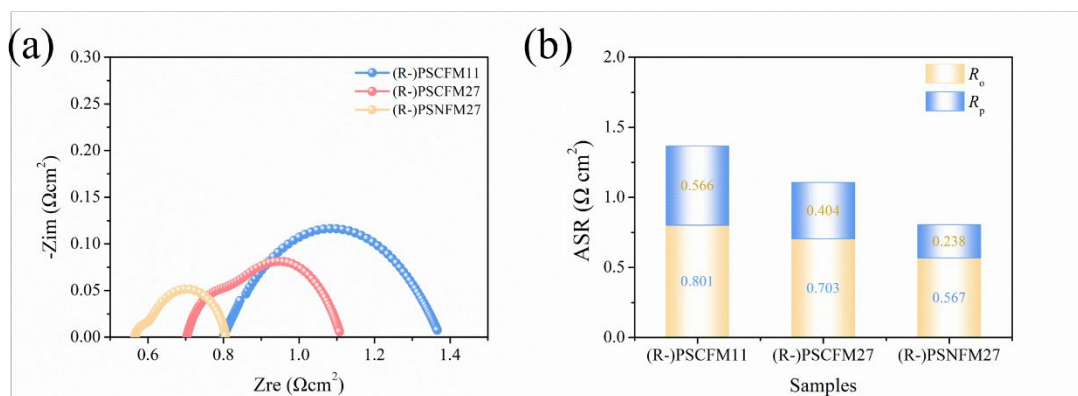
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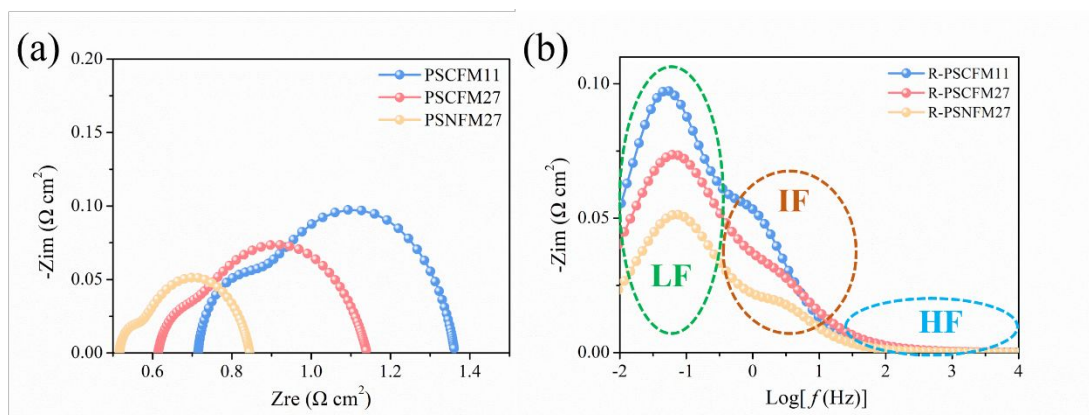
**Figure S1.** XRD patterns and the corresponding lattice parameters of (a) PSCFM11 and R-PSCFM11, (b) PSCFM27 and R-PSCFM27, and (c) PSNFM27 and R-PSNFM27



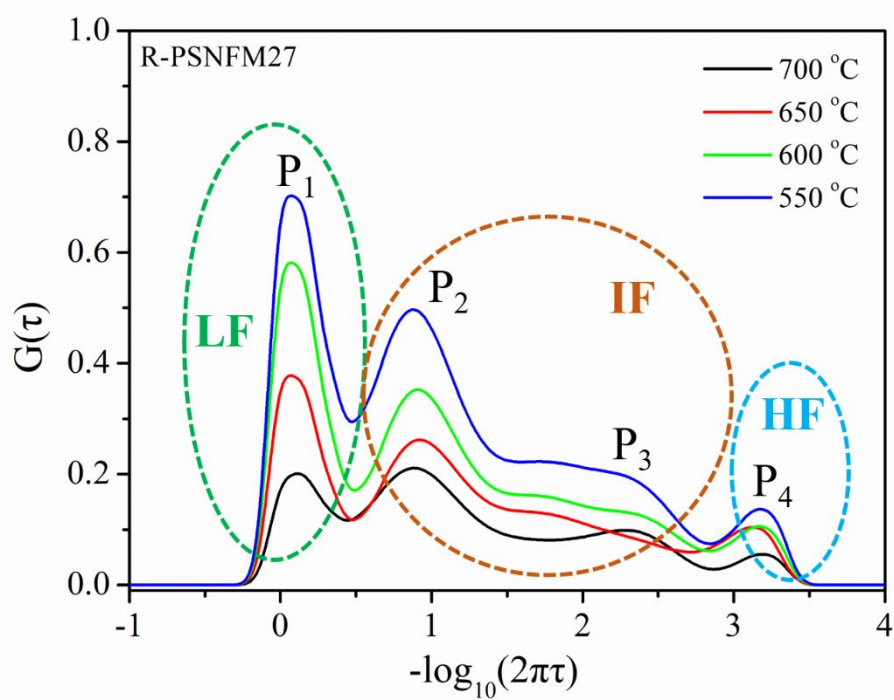
**Figure S2.** XPS spectra of (a) full spectra, (b) Ni 2p<sub>3/2</sub>, (c) Co 2p, (d) Mo 3d, (e) Fe 2p, (f) O 1s of R-PSCFM11, R-PSCFM27 and R-PSNFM27, and (g) adsorbed oxygen content of various sample powders.



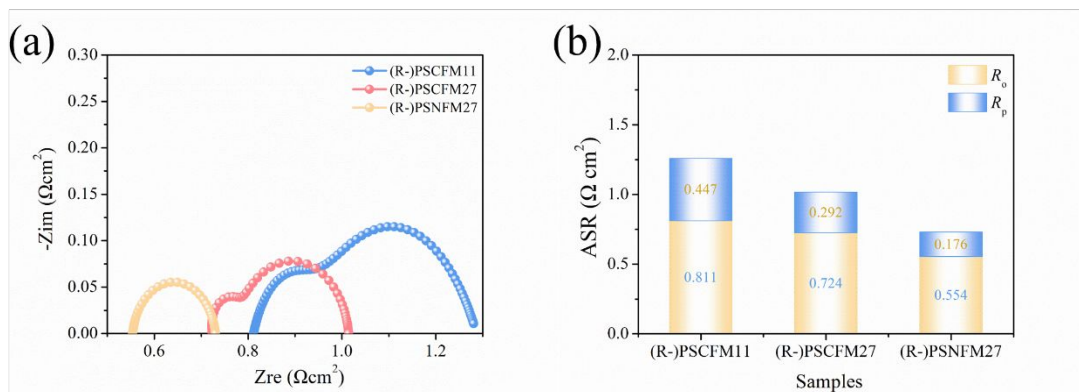
**Figure S3.** (a) Nyquist plot and (b) the corresponding ASR values of the SCFCs composed of (R-)PSCFM11, (R-)PSCFM27, and (R-)PSNFM27 oxides at 700 °C. (hydrogen side:  $\text{H}_2$ ; oxygen side:  $\text{O}_2$ )



**Figure S4.** (a) Nyquist plots and (b) Bode plots of the SCFCs composed of R-PSCFM11, R-PSCFM27, and R-PSNFM27 oxides at 700 °C in  $\text{H}_2$  atmosphere.

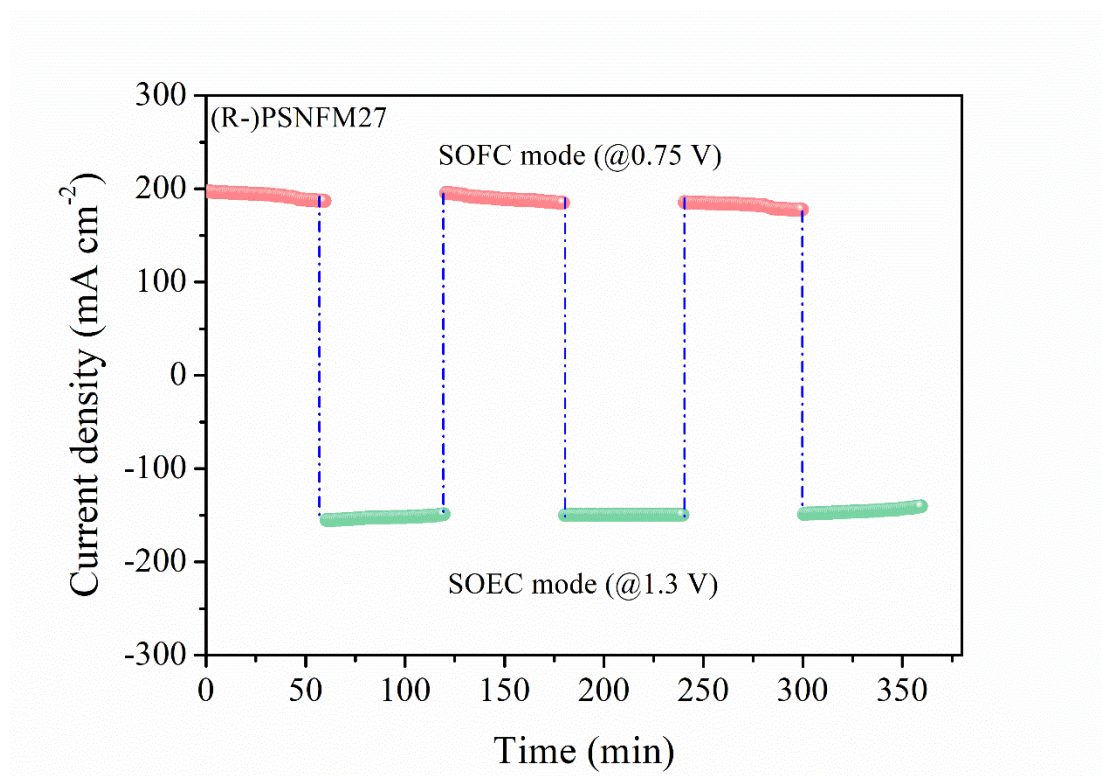


**Figure S5.** DRT spectra of the SCFC composed of R-PSNFM27 at various temperatures in  $H_2$  atmosphere.



**Figure S6.** (a) Nyquist plot and (b) the corresponding ASR values of the cells composed of (R-)PSCFM11, (R-)PSCFM27, and (R-)PSNFM27 oxides at 700 °C in SOEC mode at a voltage of 1.3 V. (hydrogen side: 70% $\text{H}_2$ -30% $\text{H}_2\text{O}$ ; oxygen side:  $\text{O}_2$ )





**Figure S7.** Short-term interval reversibility of the RSCCs composed of (R-)PSNFM27 in two modes (SOFC and SOEC) at 600 °C.



**Table S1** Elements content of R-PSCFM11, R-PSCFM27 and R-PSNFM27 (calculated from SEM-EDX)

Samples	Element content (Atomic) (%)						
	Pr	Sr	Co	Ni	Fe	Mo	O
R-PSCFM11	6.73	7.96	7.35		8.42	2.68	66.87
R-PSCFM27	7.63	9.16	4.26		14.24	2.63	62.09
R-PSNFM27	11.83	9.9		6.77	22.59	3.26	45.64

**Table S2** Relative areas derived from curve deconvolutions of Fe 2p, Co 2p, Ni 2p and O 1s spectra for PSCFM11, PSCFM27 and PSNFM27

samples	Relative area (%)										
	Fe <sup>2+</sup>	Fe <sup>3+</sup>	Co <sup>2+</sup>	Co <sup>3+</sup>	Ni <sup>2+</sup>	Ni <sup>3+</sup>	Mo <sup>5+</sup>	Mo <sup>6+</sup>	surface O	adsorbed O	lattice O
PSCFM11	39.1	60.9	39.5	60.5	/	/	44.0	56.0	56.5	21.1	22.4
PSCFM27	50.2	49.8	64.5	35.5	/	/	47.3	52.7	49.9	26.9	23.2
PSNFM27	57.3	42.7	/	/	44.5	55.5	53.2	46.8	51.0	28.1	20.9

**Table S3** Relative areas derived from curve deconvolutions of Fe 2p, Co 2p, Ni 2p and O 1s spectra for R-PSCFM11, R-PSCFM27 and R-PSNFM27

samples	Relative area (%)													
	Fe <sup>0</sup>	Fe <sup>2+</sup>	Fe <sup>3+</sup>	Co <sup>0</sup>	Co <sup>2+</sup>	Co <sup>3+</sup>	Ni <sup>0</sup>	Ni <sup>2+</sup>	Ni <sup>3+</sup>	Mo <sup>5+</sup>	Mo <sup>6+</sup>	surface O	adsorbed O	lattice O
R-PSCFM11	17.5	28.7	53.8	19.3	30.4	50.3	/	/	/	46.9	53.1	61.2	23.0	15.8
R-PSCFM27	26.4	36.0	37.6	34.3	44.6	21.1	/	/	/	53.8	46.2	49.7	28.2	22.1
R-PSNFM27	29.6	32.3	38.1	/	/	/	9.3	39.5	51.2	57.3	42.7	53.0	31.0	16.0