

Supporting Information

An investigation of the structural and electronic origins of enhanced chemical looping air separation performance of B-site substituted $\text{SrFe}_{1-x}\text{Co}_x\text{O}_{3-\delta}$ perovskites

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Table S1. Amount of metal nitrates used in the sol-gel synthesis of perovskite oxygen carriers.

Sample	Metal nitrate precursors					
	Sr(NO ₃) ₂		Fe(NO ₃) ₃ ·9H ₂ O		Co(NO ₃) ₂ ·6H ₂ O	
	Mass (g)	Amount (mmol)	Mass (g)	Amount (mmol)	Mass (g)	Amount (mmol)
SrFeO _{3-δ} (SF)	2.116	10.0	4.040	10.0	-	-
SrFe _{0.75} Co _{0.25} O _{3-δ} (SFC ₂₅)	2.116	10.0	3.030	7.5	0.728	2.5
SrFe _{0.5} Co _{0.5} O _{3-δ} (SFC ₅₀)	2.116	10.0	2.020	5.0	1.455	5.0
SrFe _{0.25} Co _{0.75} O _{3-δ} (SFC ₇₅)	2.116	10.0	1.010	2.5	2.183	7.5

Table S2. The oxygen stoichiometry (3-δ) of the perovskite oxygen carriers determined by iodometric titration and N₂-TPD method.

Sample	3-δ (iodometric titration)	3-δ (N ₂ -TPD)
SF	2.83	2.81
SFC ₂₅	2.75	2.77
SFC ₅₀	2.73	2.73
SFC ₇₅	2.68	2.69

Table S3. Oxygen carrying capacity of the perovskite oxygen carriers during the 50 redox swing cycles.

Sample	Oxygen carrying capacity (wt%)					
	Cycle 1	Cycle 10	Cycle 20	Cycle 30	Cycle 40	Cycle 50
SF	0.61	0.63	0.64	0.65	0.65	0.65
SFC ₂₅	0.75	0.84	0.84	0.84	0.85	0.85
SFC ₅₀	1.02	1.23	1.28	1.30	1.32	1.31
SFC ₇₅	1.34	1.33	1.31	1.33	1.32	1.32

Oxygen carrying capacity = sample mass (ox) - sample mass (re), where (ox) and (re) represent the sample mass measured after the 10 min oxidation stage in air and 30 min reduction stage in N₂ in each cycle, respectively. For example, during cycle 1, Oxygen carrying capacity = sample mass (10 min) - sample mass (40 min).

Table S4. Summary of XRD refinement results of as-synthesized perovskite samples.

Sample	Space group	Lattice constant $a = b = c$ (Å)	Volume (Å ³)	Mean crystallite size D (nm)	Dislocation density $\delta \times 10^{14}$ (lines/m ²)	Microstrain $\varepsilon \times 10^{-3}$	R_{wp} (%)
SF	P m -3 m	3.867	57.832	49.37	4.10	2.02	3.20
SFC ₂₅	P m -3 m	3.866	57.796	44.96	4.95	2.35	3.74
SFC ₅₀	P m -3 m	3.865	57.742	44.87	4.97	2.57	4.22
SFC ₇₅	P m -3 m	3.864	57.692	46.66	4.59	2.81	4.36

The dislocation density (δ) was estimated using the equation: $\delta = 1/D^2$ (lines/m²)¹

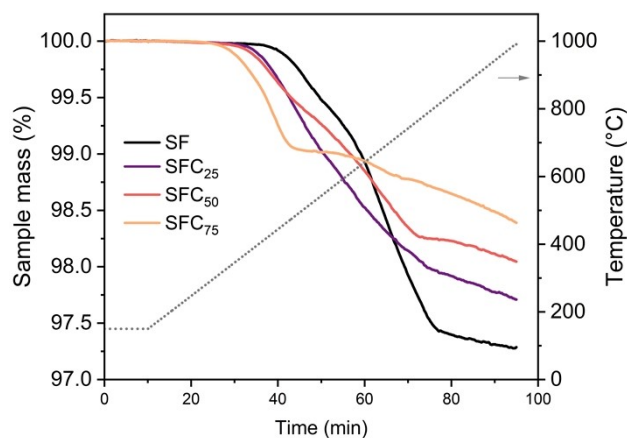


Figure S1. Weight loss curves in TGA during the temperature programmed desorption experiment in N₂.

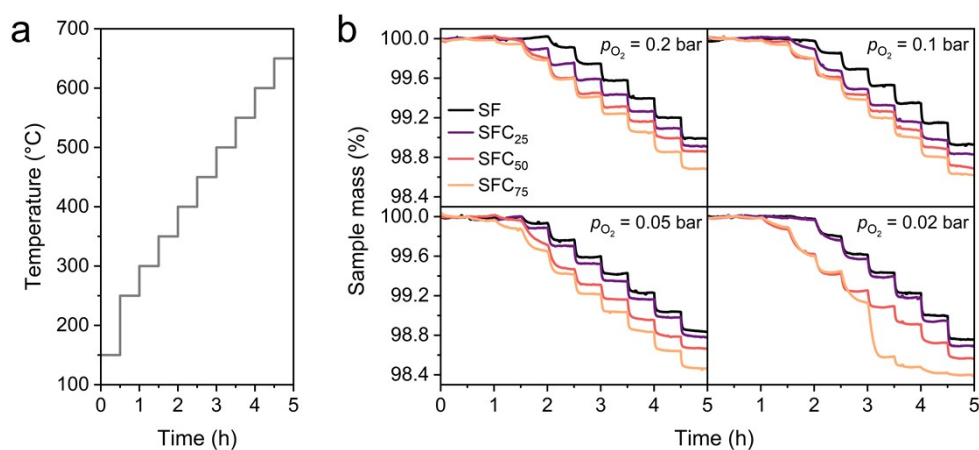


Figure S2. (a) Temperature program and (b) weight loss curves of the isothermal experiments under different oxygen partial pressure.

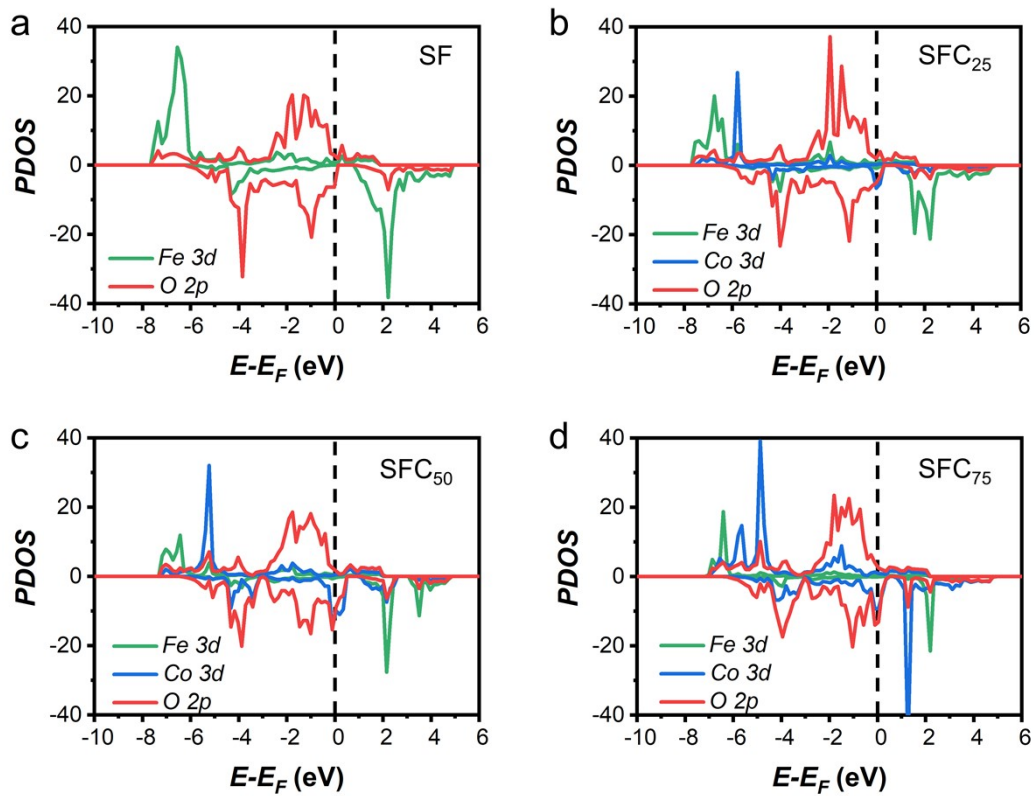


Figure S3. Calculated PDOS of the (a) SF, (b) SFC₂₅, (c) SFC₅₀, and (d) SFC₇₅ perovskite oxygen carriers.

1. L. K. Parmar, R. Joshi, P. Yadav, T. Garg, A. Kumar and A. Yadav, *Chemical Physics Impact*, 2024, **8**, 100603.