

## A, B site doping strategy enhances $\text{Sr}_{0.9}\text{Y}_{0.1}\text{Fe}_{1-x}\text{Ni}_x\text{O}_{3-\delta}$ structural stability, electrical and magnetic properties driven by Fe (IV) ions

Ruihang Yao, Hongyuan Song\*, Haorong Wu, Xiaolong Yang, Kun Dong, Xingcan Chen, Zhenhua Ge, Liangwei Chen, Bin Liu, Lan Yu\*

Faculty of Materials Science and Engineering, Kunming University of Science and Technology, Kunming, 650093, PR China

\* Corresponding Authors: songhongyuan0227@outlook.com (Hongyuan Song), yulan000@hotmail.com (Lan Yu)

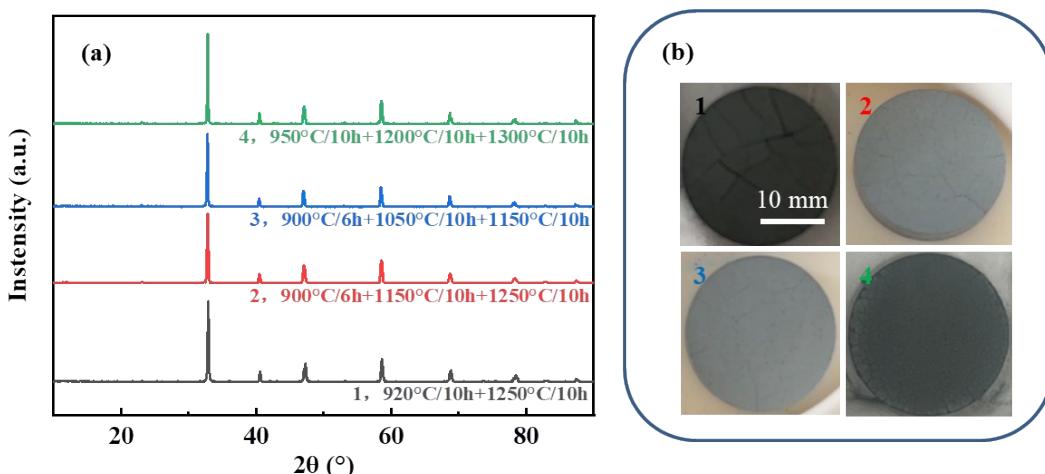


Fig. S1 (a) XRD patterns of different sintering processes for  $\text{SrFeO}_{3-\delta}$ . (b) Corresponding optical photographs.

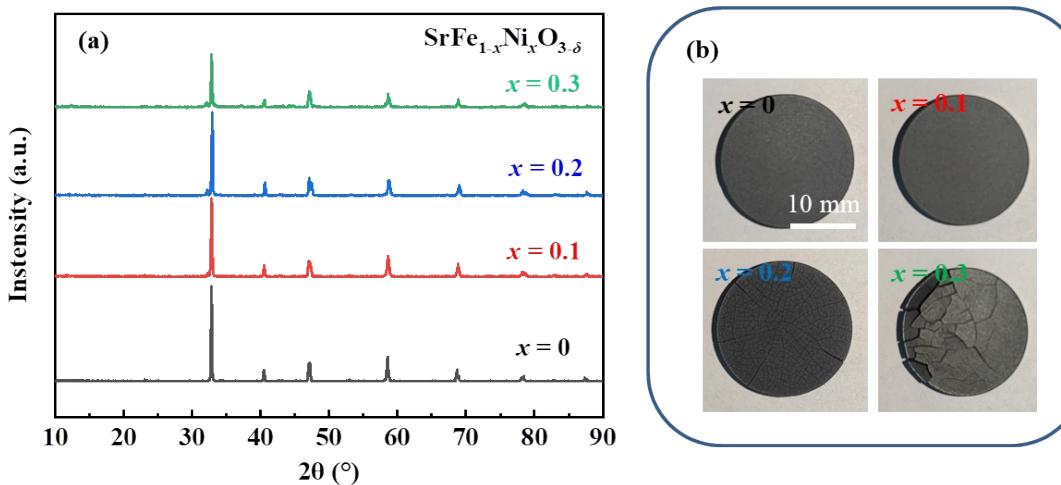


Fig. S2 (a) XRD patterns of  $\text{SrFe}_{1-x}\text{Ni}_x\text{O}_{3-\delta}$  ( $x = 0\sim0.3$ ) polycrystals. (b) Corresponding optical photographs.

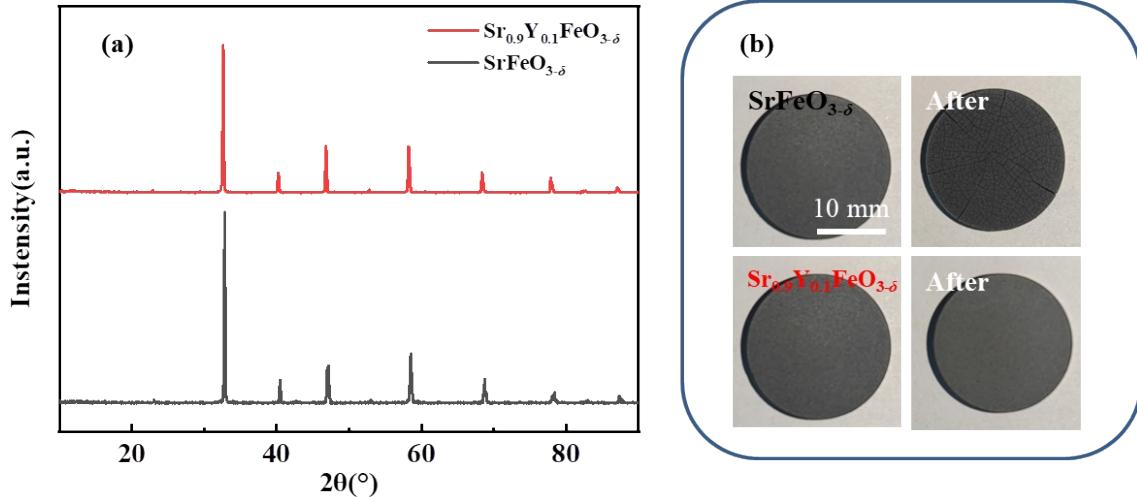


Fig. S3 (a) XRD patterns of  $\text{SrFeO}_{3-\delta}$  and  $\text{Sr}_{0.9}\text{Y}_{0.1}\text{FeO}_{3-\delta}$ . (b) Comparison of finished sintering and after sitting.

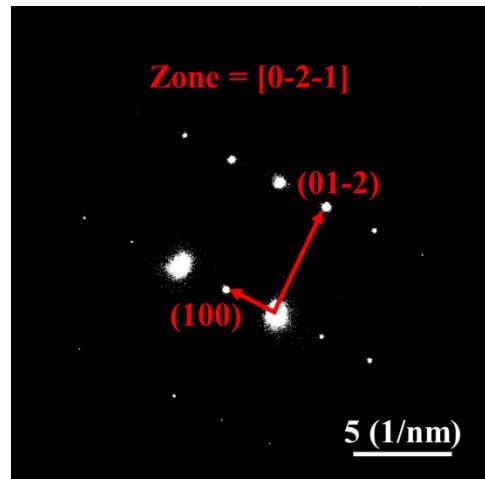


Fig. S4 The selected area electron diffraction (SAED) pattern of  $\text{Sr}_{0.9}\text{Y}_{0.1}\text{Fe}_{0.9}\text{Ni}_{0.1}\text{O}_{3-\delta}$

Table S1 Crystal parameters of  $\text{Sr}_{0.9}\text{Y}_{0.1}\text{Fe}_{1-x}\text{Ni}_x\text{O}_{3-\delta}$  ( $x = 0\sim 0.3$ )

Sample	Phase structure	Space group	$a / \text{\AA}$
$x = 0$	CP (97.5%) + T (2.5%)	$Pm\bar{3}m + I4/mmm$	3.86518
$x = 0.05$	CP	$Pm\bar{3}m$	3.85615
$x = 0.1$			3.83091
$x = 0.2$	CP (98.9%) + NiO (1.1%)	$Pm\bar{3}m + Fm\bar{3}m$	3.85507
$x = 0.3$	CP (84.19%) + NiO (5.39%) + T (10.42%)	$Pm\bar{3}m + Fm\bar{3}m + I4/mmm$	3.85978

Table S2 Atomic parameters of the Rietveld refinement

Sample	Phase structure	Atoms	Site	x	y	z	Occ
$x = 0$	CP	Sr <sub>1</sub>	1b	0.5	0.5	0.5	0.9
		Y <sub>1</sub>	1b	0.5	0.5	0.5	0.1
		Fe <sub>1</sub>	1a	0	0	0	1
		O <sub>1</sub>	3d	0.5	0	0	0.93
$x = 0.1$	T – SrFeO <sub>3-<math>\delta</math></sub>	Sr <sub>1</sub>	8i	0.258	0	0	1
		Sr <sub>2</sub>	8j	0.2519	0	0.5	1
		Fe <sub>1</sub>	4e	0	0	0.2546	1
		Fe <sub>2</sub>	8f	0.25	0.25	0.25	1
		Fe <sub>3</sub>	4d	0.5	0	0.25	1
		O <sub>1</sub>	2b	0	0	0.5	1
		O <sub>2</sub>	16m	0.1201	0.1201	0.2227	1
		O <sub>3</sub>	8h	0.2398	0.2398	0.5	1
		O <sub>4</sub>	16k	0.1238	0.6238	0.25	1
		O <sub>5</sub>	4c	0.5	0	0	1
$x = 0.3$	CP	Sr <sub>1</sub>	1b	0.5	0.5	0.5	0.9
		Y <sub>1</sub>	1b	0.5	0.5	0.5	0.1
		Fe <sub>1</sub>	1a	0	0	0	0.9
		Ni <sub>1</sub>	1a	0	0	0	0.1
		O <sub>1</sub>	3d	0.5	0	0	0.93
	T – Sr <sub>3</sub> Fe <sub>2</sub> O <sub>7</sub>	Sr <sub>1</sub>	1b	0.5	0.5	0.5	0.9
		Y <sub>1</sub>	1b	0.5	0.5	0.5	0.1
		Fe <sub>1</sub>	1a	0	0	0	0.7
		Ni <sub>1</sub>	1a	0	0	0	0.3
		O <sub>1</sub>	3d	0.5	0	0	0.93
		Sr <sub>1</sub>	2b	0	0	0.5	1
		Sr <sub>2</sub>	4e	0	0	0.3171	1
		Fe <sub>1</sub>	4e	0	0	0.0979	1
		O <sub>1</sub>	8g	0	0.5	0.0916	1
		O <sub>2</sub>	4e	0	0	0.195	1
		O <sub>3</sub>	2a	0	0	0	1