

**Doping Fe at the Co-tetrahedra site to improve the microstructure, optical,  
and Na-ion migrations in  $\text{Na}_2\text{Co}_{1-x}\text{Fe}_x\text{SiO}_4$**

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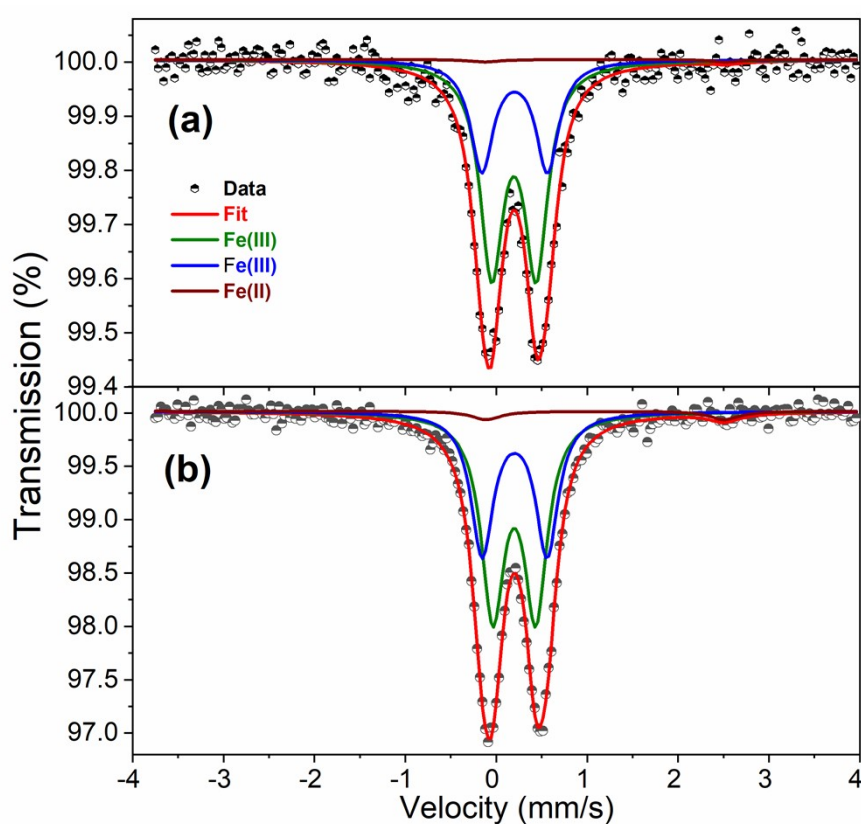


Fig.1S. The Mössbauer spectra recorded at room temperature of a)  $\text{Na}_2\text{Co}_{0.9}\text{Fe}_{0.1}\text{SiO}_4$  and (b)  $\text{Na}_2\text{Co}_{0.8}\text{Fe}_{0.2}\text{SiO}_4$ .

Table 1S Fractional atom coordinates and isotopic atomic displacement parameters ( $\text{\AA}^2$ ) for  $\text{Na}_2\text{Co}_{1-x}\text{Fe}_x\text{SiO}_4$ , with  $x=0.1$  and  $0.2$  from x-ray powder diffraction data at 300 K.

Samples	Atom	x	y	z	$O_{cc}$	$U_{iso}$ ( $\text{\AA}^2$ )
	Co	0.1448(8)	0.2744(2)	0.6139(9)	0.89954	0.115(8)
	Fe	0.1448(8)	0.2744(2)	0.6140(10)	0.098	0.115(8)
	Si	0.4050(10)	0.2670(10)	0.8760(1)	1	-0.031(7)
	Na(1)	0.1248(1)	0.2540(8)	0.0741(7)		-0.035(1)

NCFS1	Na(2)	0.3909(8)	0.2819(3)	0.3661(10)		-0.001(6)
	O(1)	0.3202(1)	0.3882(3)	0.7057(3)		0.112(4)
	O(2)	0.1000(1)	0.4470(1)	0.4080(10)		0.001(2)
	O(3)	0.0510(1)	0.2890(1)	0.8940(10)		0.186(8)
	O(4)	0.1420(2)	0.8800(3)	0.5757(1)		-0.085(3)
NCFS2	Co	0.1527(1)	0.2580(3)	0.6370(1)	0.79748	0.012(6)
	Fe	0.1527(1)	0.2580(3)	0.6370(1)	0.1999	0.012(6)
	Si	0.4050(10)	0.2670(9)	0.8760(4)	1	-0.028(2)
	Na(1)	0.1669(8)	0.2540(8)	0.0741(7)		-0.041(8)
	Na(2)	0.4070(2)	0.2819(3)	0.3646(1)		-0.001(10)
	O(1)	0.3220(2)	0.4020(10)	0.7057(3)		0.122(5)
	O(2)	0.1000(10)	0.4470(7)	0.4080(10)		0.001(2)
	O(3)	0.051(2)	0.2830(5)	0.8840(10)		0.185(5)
O(4)	0.1420(7)	0.880(3)	0.5770(9)		-0.085(2)	

Table 2S: Selected distances of NCFS1 and NCFS2 (Å)

	NCFS1	NCFS2
Co/Fe–O1	2.970	1.885
Co/Fe–O2	3.749	2.931
Co/Fe–O3	1.946	3.976
Co/Fe–O4	3.431	3.314
Si– O1	2.707	3.210
Si– O2	1.785	1.884
Si– O3	2.102	2.211
Si– O4	2.870	2.912
Na1– O1	2.759-3.604	2.789-3.712
Na1– O2	2.801-3.599	2.811-3.727
Na1– O3	2.178-3.995	2.188-4.205
Na1– O4	2.115-4.222	2.225-4.284
Na2– O1	2.793-4.004	2.793-4.231
Na2– O1	2.202-4.236	2.402-4.076
Na2– O1	2.640-4.462	2.669-4.462
Na2– O1	2.464-4.048	2.475-4.033

Table 3S: Selected angles of NCFS1 and NCFS2 (°)

	NCFS1	NCFS2
O4–Co–O1	116.08	93.54
O1–Co/Fe–O2	112.06	118.39
O1–Co/Fe–O3	91.90	105.14
O4– Co/Fe –O2	91.16	104.75
O4– Co/Fe –O3	116.50	103.34
O2– Co/Fe –O3	129.05	125.62

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O3-Si-O1	124.15	122.03
O3-Si-O2	129.76	81.65
O3-Si-O4	117.76	107.4
O1-Si-O2	117.82	91.71
O1-Si-O4	79.52	125.20
O2-Si-O4	114.55	101.55
O3-Na1-O4	116.54	113.95
O3-Na2-O1	125.96	98.75
O2-Na2-O4	118.84	116.28

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