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Supplementary Information

Substitution driven Structural and Magnetic properties and Evidence of Spin Phonon Coupling in Sr-doped $BiFeO_3$ nanoparticles

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Table S1 Rietveld refined parameters of $Bi_{1-x}Sr_xFeO_3$ nanostructured samples.

Samples	Lattice parameters	Atoms Positions	x	y	z	R-factors (%)
x=0	a =5.57516 (6) (Å)	Fe	0.0	0.0	0.01903(92)	R_{wp} = 3.17
	c =13.85908(20)(Å)	Bi	0.0	0.0	0.29745(85)	R_p = 2.49
R3c	V = 373.061(8) (Å^3)	O	0.23075(15)	0.35815(209)	0.0833	R_f = 1.75
						R_{Bragg} = 1.17
x=0.05	a = 5.57663 (6) (Å)	Fe	0.0	0.0	0.01629(108)	R_{wp} = 4.86
R3c	c = 13.83109(38) (Å)	Bi/Sr	0.0	0.0	0.29309(104)	R_p = 3.84
	V = 372.504(12)(Å^3)	O	0.24008(283)	0.35873(220)	0.0833	χ^2 = 2.03
x=0.10	a = 5.57645(5) (Å)	Fe	0.0	0.0	0.01981(95)	R_{wp} = 4.52
R3c	c = 13.84578 (29) (Å)	Bi/Sr	0.0	0.0	0.29738(86)	R_p = 3.56
	V = 372.875(9) (Å^3)	O	0.23943(255)	00.37170(181)	0.0833	χ^2 = 1.98
x=0.15	a = 5.57536 (6) (Å)	Fe	0.0	0.0	0.01674(109)	R_{wp} = 4.44
R3c	c = 13.83676 (40) (Å)	Bi/Sr	0.0	0.0	0.29589(107)	R_p = 3.53
	V = 372.487(12) (Å^3)	O	0.25005(319)	0.40282(229)	0.0833	χ^2 = 1.95
x=0.20	a = 5.57475 (6)(Å)	Fe	0.0	0.0	0.01415(109)	R_{wp} = 4.15
R3c	c = 13.83385 (36) (Å)	Bi/Sr	0.0	0.0	0.29138(105)	R_p = 3.32
	V = 372.326 (11) (Å^3)	O	0.24293(297)	0.37768(215)	0.0833	χ^2 = 1.67
x=0.25	a = 5.58034 (26) (Å)	Fe	0.0	0.0	0.02896(175)	R_{wp} = 4.54
***R3c* (65.25%)**	c = 13.84518 (76) (Å)	Bi/Sr	0.0	0.0	0.30717(163)	R_p = 3.57
	V = 373.380 (32) (Å^3)	O	0.25597(406)	0.35376(285)	0.0833	R_{fl} = 1.94
***P4/mmm* (34.75%)**	a = 3.93373 (22) (Å)	Bi/Sr	0	0	0	R_{Bragg1} = 2.16
	c = 3.97941 (31) (Å)	Fe	0.5	0.5	0.5	R_{f2} = 1.69
		O	0.5	0.5	0	R_{Bragg2} = 2.47
	V = 61.578 (7) (Å^3)	O	0.5	0	0.5	χ^2 = 1.86

Table S2 Selected bond lengths, angles and bond valence sums (BVS) of $Bi_{1-x}Sr_xFeO_3$ nanoparticles.

Bonds	**x=0.00**	**x=0.05**	**x=0.10**	**x=0.15**	**x=0.20**	**x=0.25**
Fe-Oshort	1.966(16)	1.995(16)	2.021(15)	1.900(13)	1.963(16)	1.920(16)
Fe-Olong	2.078(15)	2.054(16)	2.039(11)	2.170(16)	2.082(16)	2.213(20)
Bi-O1	2.243(15)	2.290(16)	2.201(15)	2.118(16)	2.224(16)	2.185(20)
Bi-O2	2.586(18)	2.525(17)	2.583(17)	2.618(17)	2.561(17)	2.481(15)
Bi-O3	3.149(16)	3.184(18)	3.159(17)	3.141(18)	3.148(18)	3.328(15)
Bi-O4	3.447(14)	3.397(15)	3.478(13)	3.537(16)	3.421(16)	3.57(2)
Fe-O-Fe	156.8(7)	155.9(8)	154.7(8)	153.2(8)	151.3(8)	146.9(13)
Bi-O-Bi	110.1(6)	110.6(7)	111.5(6)	113.0(7)	113.8(7)	116.1(1)
BVS Bi	2.798(45)	2.635(46)	2.914(47)	3.310(63)	3.342(50)	3.399(83)
BVS Fe	2.981(46)	2.863(46)	2.762(42)	2.840(49)	2.981(49)	2.821(70)
BVS Sr	-	2.812(46)	3.110(50)	3.531(63)	3.541(53)	3.627(89)
BVS O	1.926(32)	1.883(33)	1.977(31)	2.204(42)	2.215(33)	2.092(50)

Table S3 Raman modes positions and FWHMs of $Bi_{1-x}Sr_xFeO_3$ nanoparticles.

S. No.	Mode	x = 0.0		x = 0.05		x = 0.10		x = 0.15		x = 0.20		x = 0.25	
		Center ω_i cm^{-1}	FWHM Γ_i cm^{-1}	Center ω_i cm^{-1}	FWHM Γ_i cm^{-1}	Center ω_i cm^{-1}	FWHM Γ_i cm^{-1}	Center ω_i cm^{-1}	FWHM Γ_i cm^{-1}	Center ω_i cm^{-1}	FWHM Γ_i cm^{-1}	Center ω_i cm^{-1}	FWHM Γ_i cm^{-1}
1	$E(TO_1)$	71.1	8.9	69.9	8.7	66.7	8.3	65.5	8.4	64.9	5.9	63.6	8.9
2	$E(LO_1)$	76.6	5.3	75.4	5.4	74.1	8.8	74.6	7.1	74.5	9.1	73.6	13.2
3	$E(TO_2)$	139.2	27.7	138.9	28.9	139.9	33	140	32	140.3	29.8	141.4	32.6
4	$A_1(TO_1)$	172.3	10.9	170.9	12.4	170.3	14.1	170.4	14.1	170.1	13	169.1	20.4
5	$A_1(TO_2)$	218.4	17.9	217	15	216	13.4	218.6	18.4	222.1	18.4	221.4	15.5
6	$E(TO_3)$	232.2	23.5	228.8	21.1	226.2	17.4	229.4	19.2	246	10.8	233.2	20.9
7	$E(TO_4)$	261.2	19.3	260.2	22.4	257.3	29.4	256.8	27.6	263	20.8	257.9	24.9
8	$E(TO_5)$	278.1	23.8	277.1	25.8	275.3	24.4	274.3	24.3	283.5	22.3	286.6	22.2
9	$A1(TO_3)$	302.4	37.3	303.7	36.4	305	36.4	294.1	27	300.7	11.4	297.8	19
10	$E(TO_6)$	346.6	27.5	344.6	26.8	341.1	32.1	342.5	36.8	329.9	22.9	327.6	26.4
11	$E(TO_7)$	369.7	10.9	368.1	12.6	367.7	16.6	367.4	16.7	362.4	11.6	364.7	17.8
12	$E(TO_8)$	436.3	11.4	431.6	13.8	441.9	17.9	435.9	46.8	424.1	24.2	428.7	45.9
13	$E(LO_8)$	471.2	32.6	471.3	35.9	473.1	34.1	472.5	41.1	475.6	45.1	477.6	45.8
14	$E(TO_9)$	524.0	29.6	521.1	35.1	516.3	46.7	520.5	47.6	520.3	55.7	525.4	36.7
15	$A_1(TO_4)$	550.8	30.6	544.5	40.2	544.2	35.2	545.6	43.1	553.5	21.6	557	30.1
16	$E(LO_9)$	608.2	42.9	609.4	44.1	614.3	54.8	611.5	45.8	610.4	26.5	618.7	41.5
17	-	-	-	689.3	84.8	676.1	92.9	677.4	105.4	646.8	88.2	680.7	76.9
18	$2E(LO_8)$	938.4	72.9	943.8	89.4	940.9	65.1	947.2	124.9	949.9	97.5	935.4	177.7
19	$2E(TO_9)$	1038.8	102.7	1030.3	78.6	1042.6	103.9	1039.7	70.8	1045.7	66.7	1037.3	73
20	$2A_1(TO_4)$	1101.2	58.7	1095.2	62.4	1101.1	55.1	1100.3	77.9	1109.8	74.2	1097.2	61.9
21	$2A1(LO_4)$	1147.6	47.3	1144.5	55.5	1144.7	55.3	1150.1	76.8	1177.3	116.4	1154.1	81.2
22	$2E(LO_9)$	1264.3	142.4	1266.8	142.83	1268.1	142.7	1283	147.5	1298.5	134.7	1292.2	164.7