ELECTRONIC SUPPLEMENTARY INFORMATIONSHEET

Spin, valence variation and half metallicity in Cobalt doped Barium Strontium Titanate Ceramics

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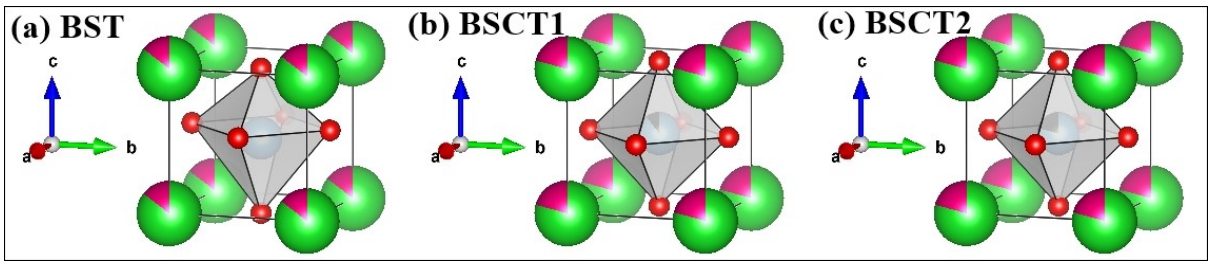
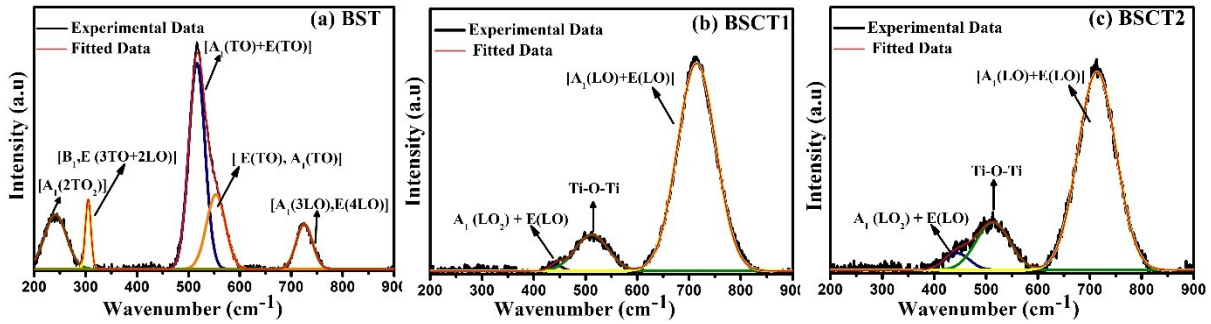
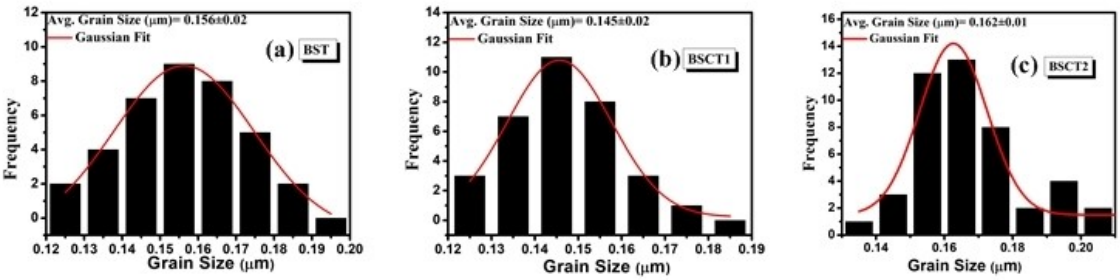
FIGURES:



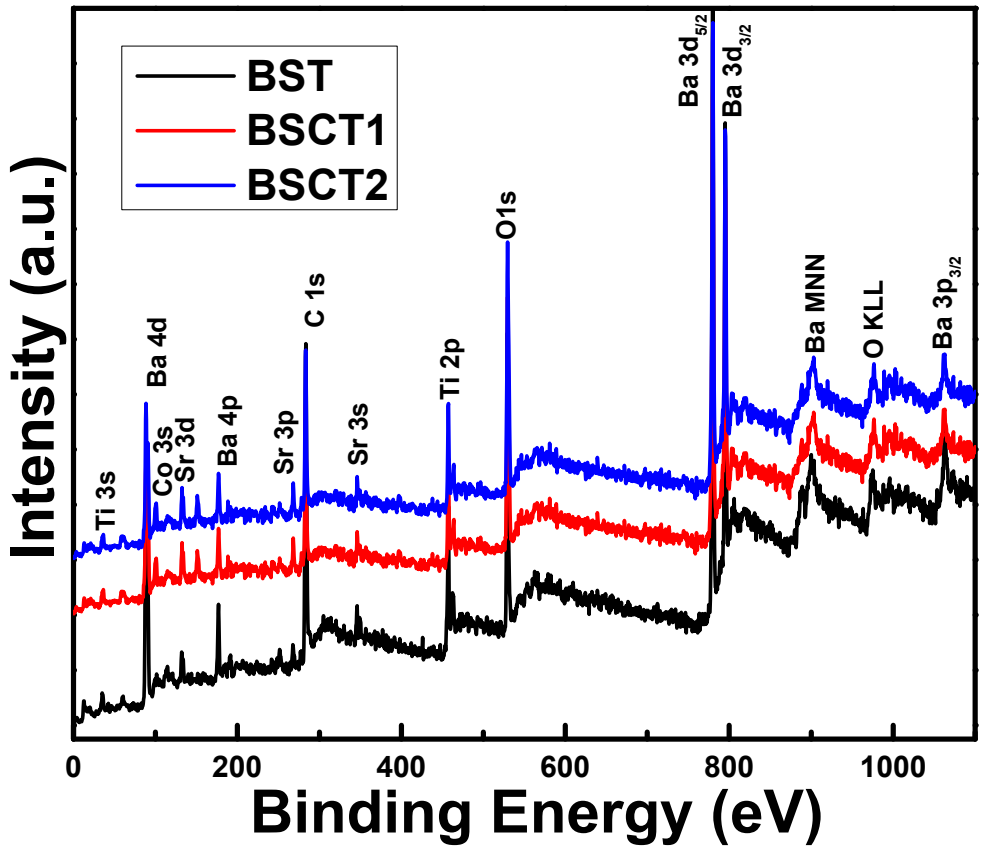
ESF 1: Crystal Structure of BST, BSCT1 and BSCT2 generated using vista software



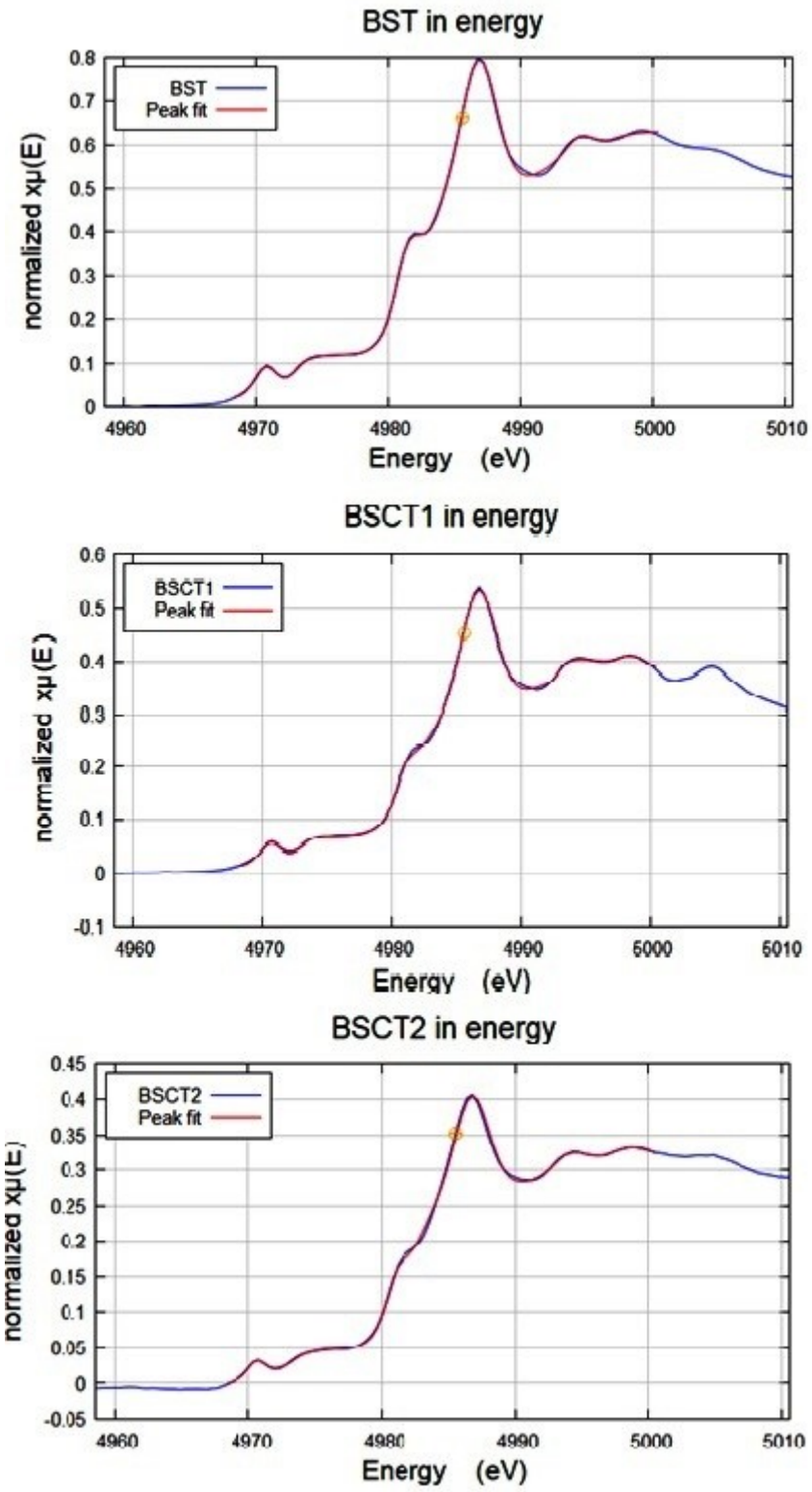
ESF 2: Deconvoluted Raman Spectra of BST, BSCT1 and BSCT2



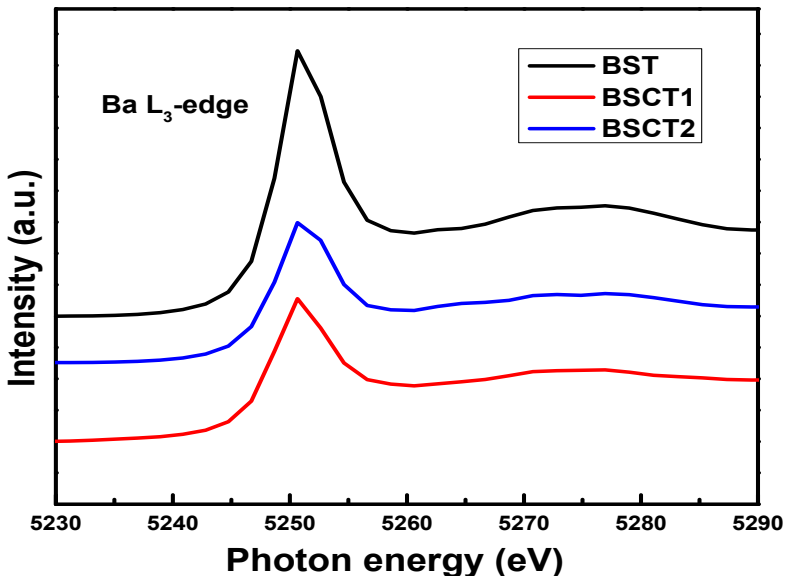
ESF 3: Grain Size calculated from SEM Image for BST, BSCT1 and BSCT2 using ImageJ software



ESF4: Survey Scan for BST, BSCT1 and BSCT2



ESF5: The Fitted spectra for Ti K edge XANES spectra, generated from Athena for BST, BSCT1 and BSCT2



ESF6: Ba L_3-edge XANES Spectra for BSCT, BSCT1 and BSCT2

Tables:

EST1: Refined Parameters of BST, BSCT1 and BSCT2

BST Tetragonal phase with space group *P4mm*,

Cell parameters: a = b = 3.986 (2) Å, c = 4.008 (7) Å Volume = 63.692 (0.004) (Å)^3

Ions	x_T	y_T	z_T	B_{iso}(Å^2)	**Occupancy**
Ba^{2+} (1a)	0.00000	0.00000	0.00000	0.669	0.079
Sr^{2+} (1a)	0.00000	0.00000	0.00000	0.669	0.034
Ti^{4+} (1b)	0.50000	0.50000	0.46900	0.128	0.112
O_I^{2-}(1b)	0.50000	0.50000	-0.04933	0.201	0.125
O_I^{2-}(2c)	0.50000	0.00000	0.54804	0.077	0.250
R-factors	$R_{B(Tetragonal)}$= 6.20	R_p = 7.53	$R_{w\text{-}p}$ = 9.62	R_{exp}= 8.43	χ^2= 1.30

BSCT1 Cubic phase with space group $Pm\bar{3}m$,

Cell parameters: a = b = c = 3.9860 (7) ÅVolume = 63.333 (0.003) (Å)^3

Ions	x_T	y_T	z_T	B_{iso}(Å^2)	**Occupancy**
Ba^{2+} (1a)	0.00000	0.00000	0.00000	0.689	0.017
Sr^{2+} (1a)	0.00000	0.00000	0.00000	0.689	0.004
Ti^{4+} (1b)	0.50000	0.50000	0.50000	0.171	0.019
Co^{2+}(1b)	0.50000	0.50000	0.50000	0.171	0.002
O_I^{2-}(3c)	0.50000	0.50000	0.00000	1.379	0.062
R-factors	$R_{B(Cubic)}$= 9.45	R_p = 11.9	$R_{w\text{-}p}$ = 15.2	R_{exp}= 13.73	χ^2= 1.22

BSCT2 Cubic phase with space group $Pm\bar{3}m$,

Cell parameters: a = b = c = 3.9871 (4) ÅVolume = 63.395 (0.006) (Å)^3

Ions	x_T	y_T	z_T	B_{iso}(Å^2)	**Occupancy**
Ba^{2+} (1a)	0.00000	0.00000	0.00000	0.067	0.017
Sr^{2+} (1a)	0.00000	0.00000	0.00000	0.067	0.004
Ti^{4+} (1b)	0.50000	0.50000	0.50000	0.227	0.017
Co^{2+}(1b)	0.50000	0.50000	0.50000	0.227	0.004
O_I^{2-}(3c)	0.50000	0.50000	0.00000	1.427	0.062
R-factors	$R_{B(Cubic)}$= 6.82	R_p = 8.60	$R_{w\text{-}p}$ = 10.9	R_{exp}= 9.28	χ^2= 1.39

EST2: The parameters obtained from XPS data fitting BST, BSCT1 and BSCT2

BST (Ba $3d_{5/2}$)	**Peak position(eV)**	**FWHM**	**Peak area**
Beta phase	779.6	1.59	12437
Alpha Phase	777.9	2.60	860
BCST1 (Ba $3d_{5/2}$)	**Peak position(eV)**	**FWHM**	**Peak area**
Beta phase	779.6	1.56	11430
Alpha Phase	777.9	2.92	1327
BCST2 (Ba $3d_{5/2}$)	**Peak position(eV)**	**FWHM**	**Peak area**
Beta phase	779.8	1.66	10039
Alpha phase	778.0	2.56	1811
BST	**Peak position(eV)**	**FWHM**	**Peak area**

(Sr $3d_{5/2}$)	132.8	1.18	585
BCST1	**Peak position(eV)**	**FWHM**	**Peak area**
(Sr $3d_{5/2}$)	132.7	1.01	361
BCST2	**Peak position(eV)**	**FWHM**	**Peak area**
(Sr $3d_{5/2}$)	132.9	1.34	270
BCST1	**Peak position(eV)**	**FWHM**	**Peak area**
(Co $2p_{3/2}$) Co^{3+}	779.8	1.67	12526
(Co $2p_{3/2}$) Co^{2+}	777.7	2.36	1797
BCST2	**Peak position(eV)**	**FWHM**	**Peak area**
(Co $2p_{3/2}$) Co^{3+}	779.8	1.39	1487
(Co $2p_{3/2}$) Co^{2+}	777.9	1.89	10002
BST	**Peak position(eV)**	**FWHM**	**Peak area**
(Ti $2p_{3/2}$) Ti^{4+}	457.2	1.24	2210
(Ti $2p_{3/2}$) Ti^{2+}	456.0	2.96	1417
BCST1	**Peak position(eV)**	**FWHM**	**Peak area**
(Ti $2p_{3/2}$) Ti^{4+}	457.2	1.28	1961
(Ti $2p_{3/2}$) Ti^{2+}	456.0	1.68	550
BCST2	**Peak position(eV)**	**FWHM**	**Peak area**
(Ti $2p_{3/2}$) Ti^{4+}	457.3	1.32	903
BST	**Peak position(eV)**	**FWHM**	**Peak area**
(O 1s) O^{2-}	529.7	1.27	4878
(O 1s) V_o (Oxygen vacancy)	531.0	2.93	3683
BCST1	**Peak position(eV)**	**FWHM**	**Peak area**
(O 1s) O^{2-}	530.4	1.46	4498
(O 1s) V_o	532.1	1.88	3809
(O 1s) O^*	528.4	1.11	279
BCST1	**Peak position (eV)**	**FWHM**	**Peak area**
(O 1s) V_o	531.9	1.76	8713
(O 1s) mixed valence state	528.8	2.14	2336

EST3: Deconvoluted peak area fitted from Athena for BST, BSCT1 and BSCT2 sample

Sample	Area under first peak (A)	Area under 2nd peak (B)	Area under 3rd peak (C)	Area under 4th peak (D)
BST	0.03	0.35	0.26	0.94
BSCT1	0.06	2.25	0.42	0.69
BSCT2	0.07	3.50	0.63	0.40