Supporting Information for:

Structural and thermodynamic analysis of triple conducting ceramic materials $BaCo_{0.4}Fe_{0.4}Zr_{0.2-X}Y_XO_{3-\delta}$

Jack H. Duffy[*a], Nancy Birkner[*a], Chiyoung Kim[b], Ryan Jacobs[b], Dane Morgan[b], Shivani Sharma[c], Scott T. Misture[c], Erik M. Kelder[d], Harry W. Abernathy[e], Kyle S. Brinkman[#a,e]

a. Department of Materials Science and Engineering, Clemson University, Clemson, South Carolina 29634, United States

b. Department of Materials Science and Engineering, University of Wisconsin – Madison, Madison, Wisconsin 54706, United States

c. Kazuo Inamori School of Engineering, Alfred University, Alfred, New York 14802, United States

d. Department of Radiation Science & Technology, Delft University of Technology, 2629 JB Delft, The Netherlands

e. National Energy Technology Laboratory, United States Department of Energy, Morgantown, West Virginia 26507, United States

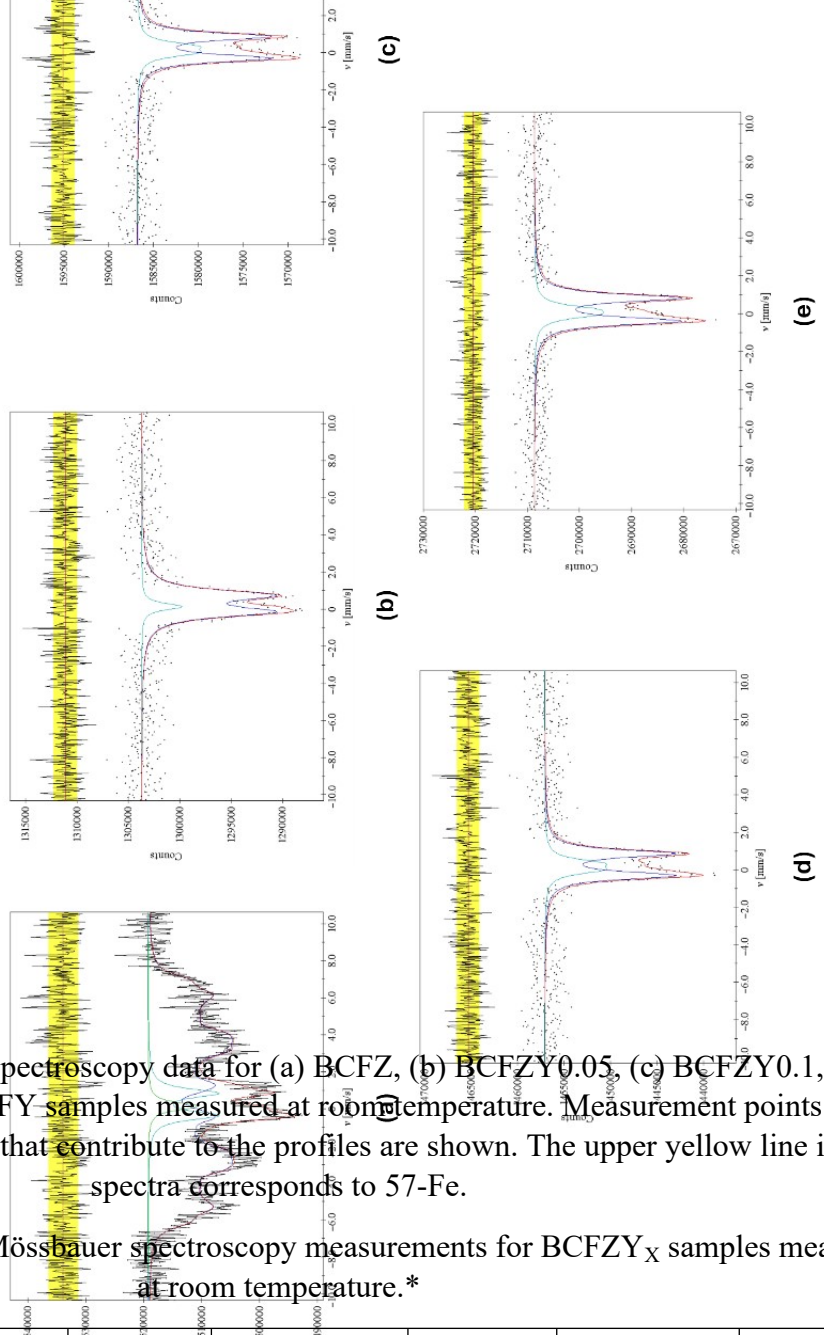

Figure S1: Mössbauer spectroscopy data for (a) BCFZ, (b) BCFZY0.05, (c) BCFZY0.1, (d) BCFZY0.15, and (e) BCFY samples measured at room temperature. Measurement points and different spectral fit lines that contribute to the profiles are shown. The upper yellow line in the spectra corresponds to 57-Fe.

Table S1: Fit data of the Mössbauer spectroscopy measurements for $BCFZY_X$ samples measured at room temperature.*

Sample	T (°C)	IS ($mm \cdot s^{-1}$)	QS ($mm \cdot s^{-1}$)	Hyperfine Field (T)	Γ ($mm \cdot s^{-1}$)	Phase	Spectral Contribution
BCFZ	25	0.13 0.23 0.41	-- 1.20 --	-- -- 30.3	0.50 0.58 0.70	Fe^{II} (LS) Fe^{3+} Fe^{3+} (M)	4% 12% 84%
BCFZY0.05	25	0.12 0.29	-- 0.91	-- --	0.43 0.67	Fe^{II} (LS) Fe^{3+}	10% 90%
BCFZY0.1	25	0.15 0.26	0.36 1.18	-- --	0.52 0.49	Fe^{II} (LS) Fe^{3+}	27% 73%
BCFZY0.15	25	0.15 0.26	0.36 1.18	-- --	0.52 0.49	Fe^{II} (LS) Fe^{3+}	27% 73%

BCFY	25	0.08 0.21	0.28 1.22	-- --	0.53 0.51	Fe^{II} (LS) Fe^{3+}	25% 75%

**Experimental uncertainties of the fits are as follows: Isomer shift (IS): ± 0.03 mm·s^{-1}; Quadrupole shift (QS): ± 0.05 mm·s^{-1}; Line Width (Γ): ± 0.05 mm·s^{-1}; Spectral contribution (mol %): ± 3%.*

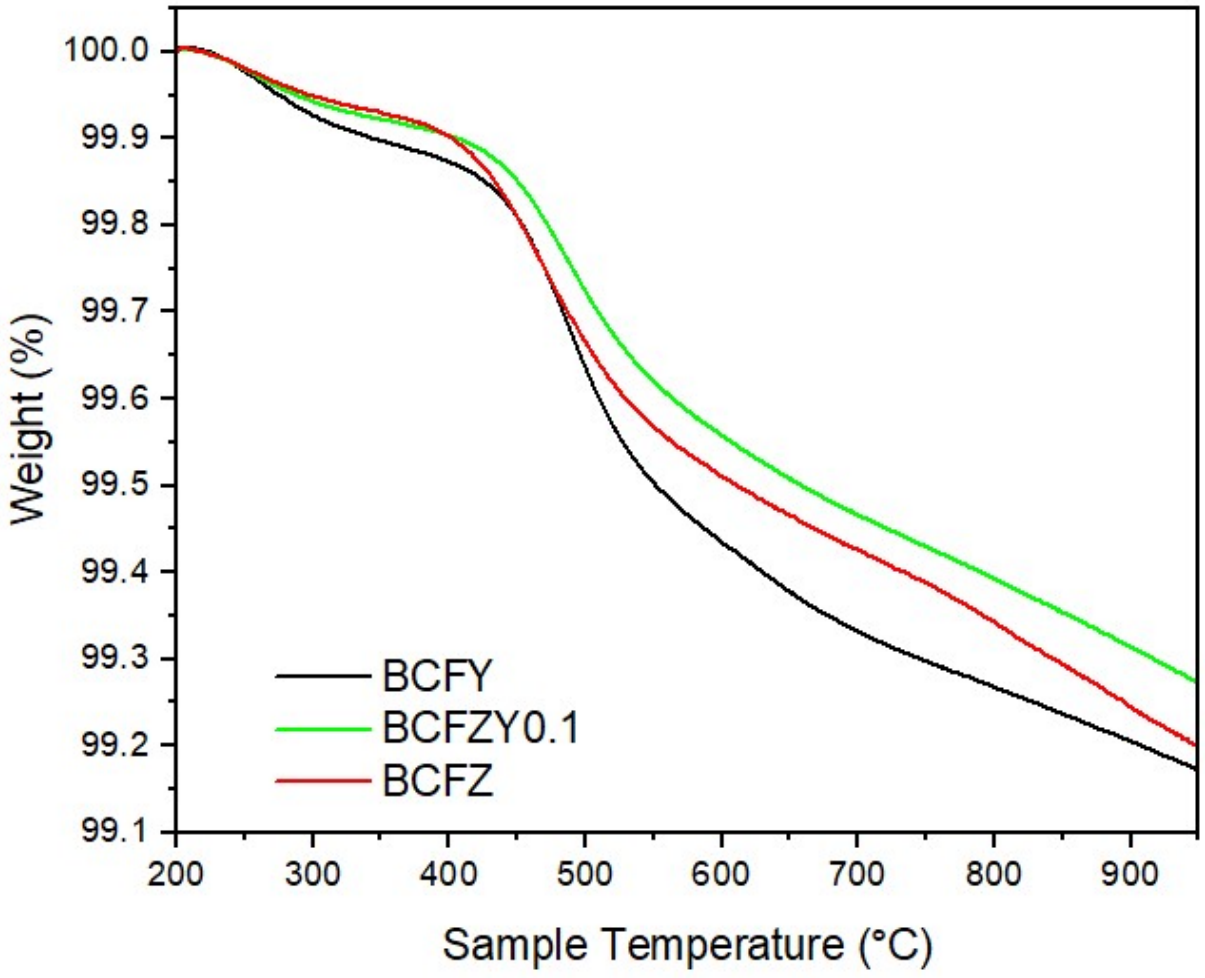

Figure S2: TG plot of $BCFZY_X$ under inert (N_2) conditions. This measurement does not show oxidizing weight increase at 400°C unlike the measurement performed in air.

Table S2: Composition of $BCFZY_X$ materials using ICP-MS, normalizing the B-site to a composition of one.

Shorthand	Target Stoichiometry	ICP-MS Stoichiometry
BCFZ	$BaCo_{0.4}Fe_{0.4}Zr_{0.2}O_{3-\delta}$	$Ba_{0.959}Co_{0.404}Fe_{0.416}Zr_{0.180}O_{2.376}$
BCFZY0.05	$BaCo_{0.4}Fe_{0.4}Zr_{0.15}Y_{0.05}O_{3-\delta}$	$Ba_{0.988}Co_{0.398}Fe_{0.415}Zr_{0.140}Y_{0.046}O_{2.361}$
BCFZY0.1	$BaCo_{0.4}Fe_{0.4}Zr_{0.1}Y_{0.1}O_{3-\delta}$	$Ba_{0.991}Co_{0.409}Fe_{0.410}Zr_{0.090}Y_{0.091}O_{2.346}$
BCFZY0.15	$BaCo_{0.4}Fe_{0.4}Zr_{0.05}Y_{0.15}O_{3-\delta}$	$Ba_{1.005}Co_{0.410}Fe_{0.408}Zr_{0.046}Y_{0.136}O_{2.322}$
BCFY	$BaCo_{0.4}Fe_{0.4}Y_{0.2}O_{3-\delta}$	$Ba_{1.029}Co_{0.408}Fe_{0.408}Y_{0.184}O_{2.298}$

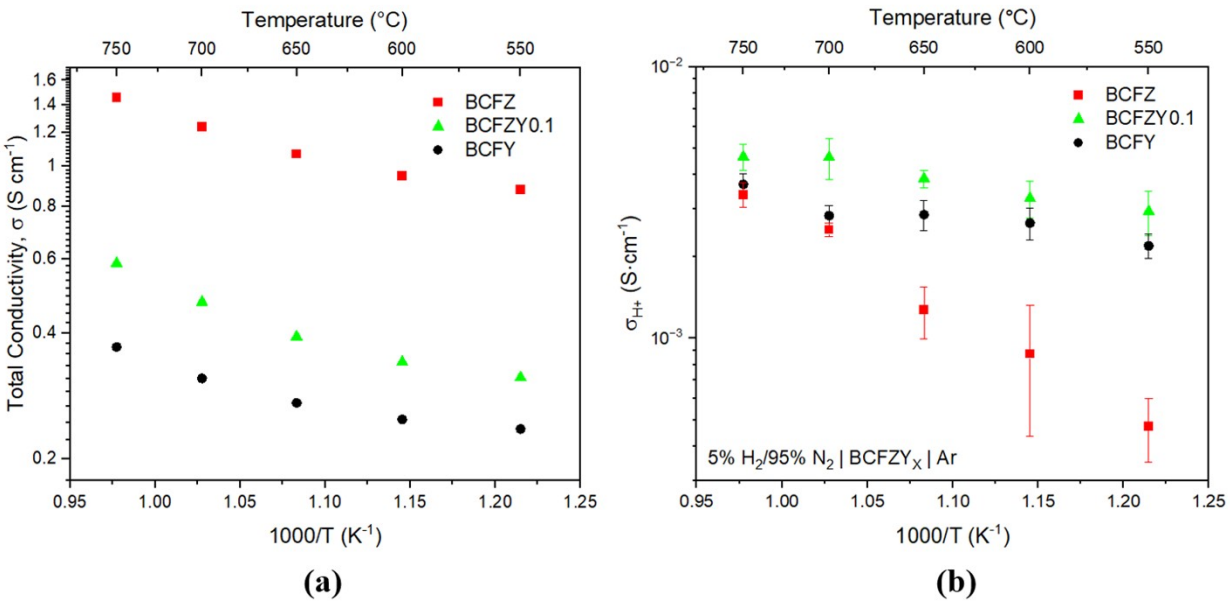

Figure S3: (a) Total conductivity of $BCFZY_X$ under reducing conditions, and (b) proton conductivity under reducing conditions calculated from hydrogen permeation measurements. Reproduced from [19] with permission under Open Access license CC BY 3.0.

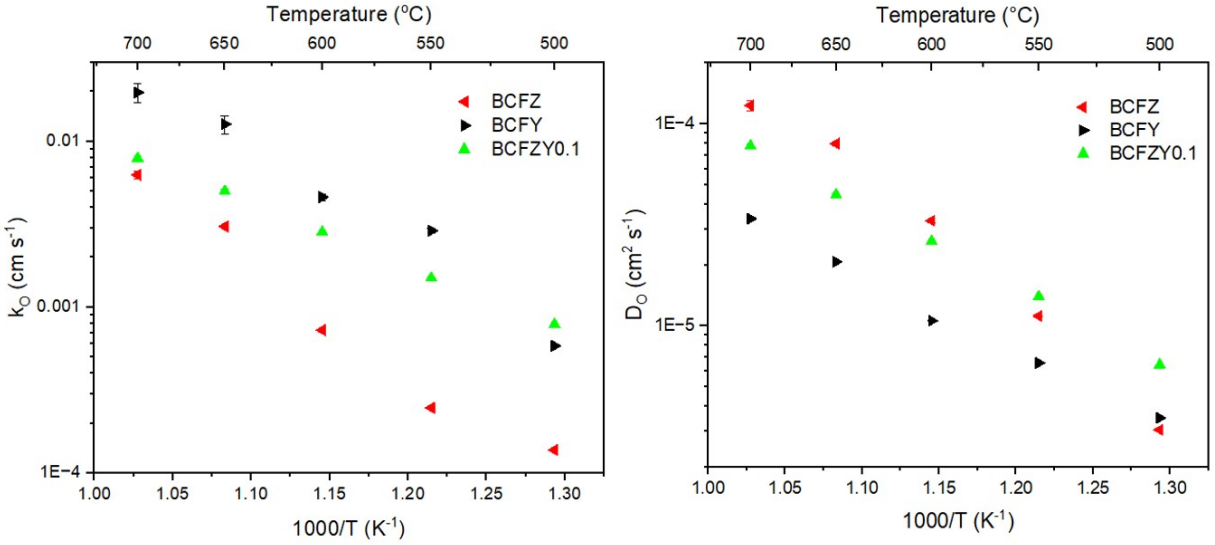

Figure S4: (Left) Surface exchange coefficient as a function of temperature. (Right) Chemical diffusion coefficient as a function of temperature. Reproduced from [19] with permission under Open Access license CC BY 3.0.

Supercell Coordinates for Computational Calculations

POSCAR files used for the vacancy binding energy with yttrium calculations are included in the supplemental information as .cif files. To use these files in the VASP code please remove the position lines with “Vac” in them. These are included just to show where the oxygen was located before being removed to create the vacancy.