Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

High Thermoelectric Performance of $Ba_3Cu_{16-x}(S,Te)_{11}$

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Supplementary Information

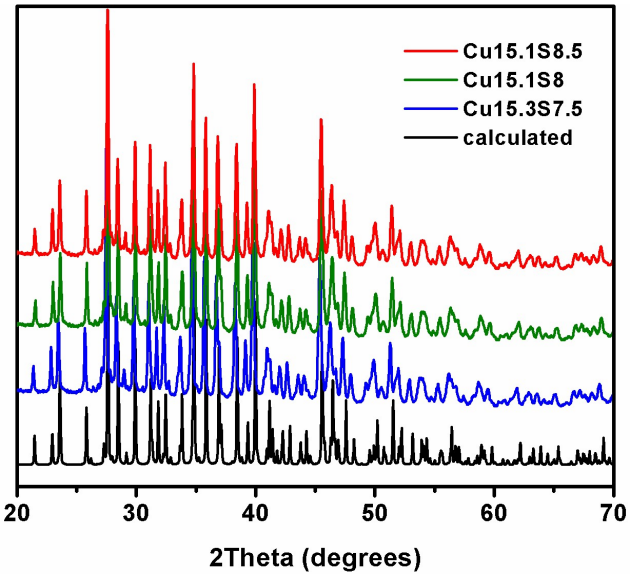

Fig. S1. Experimental X-ray patterns. The calculated pattern is from the single crystal data of $Ba_3Cu_{15.09}S_{7.9}Te_{3.09}$.

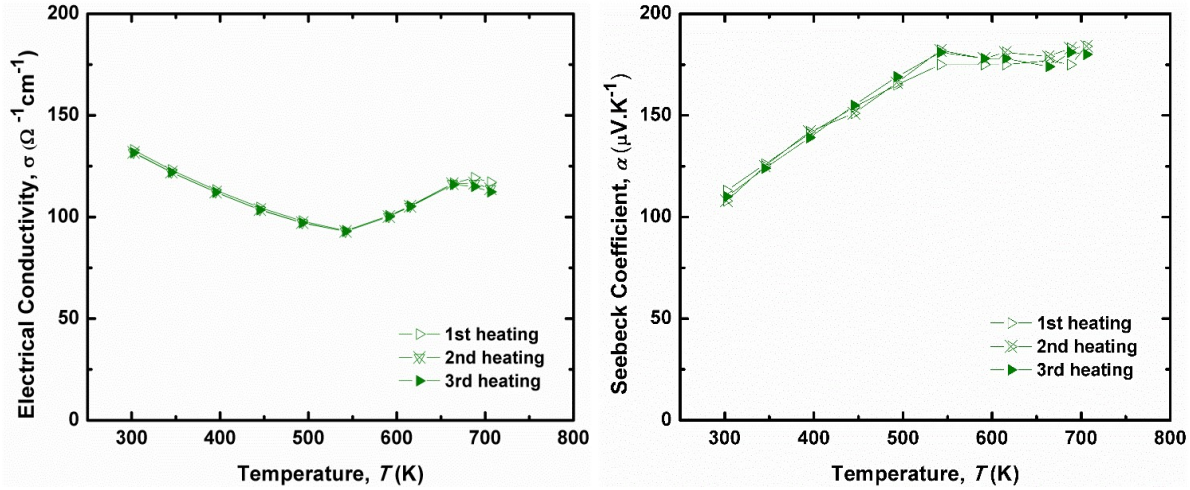

Fig. S2. Stability of the electrical transport properties of $Ba_3Cu_{15.1}S_8Te_3$.

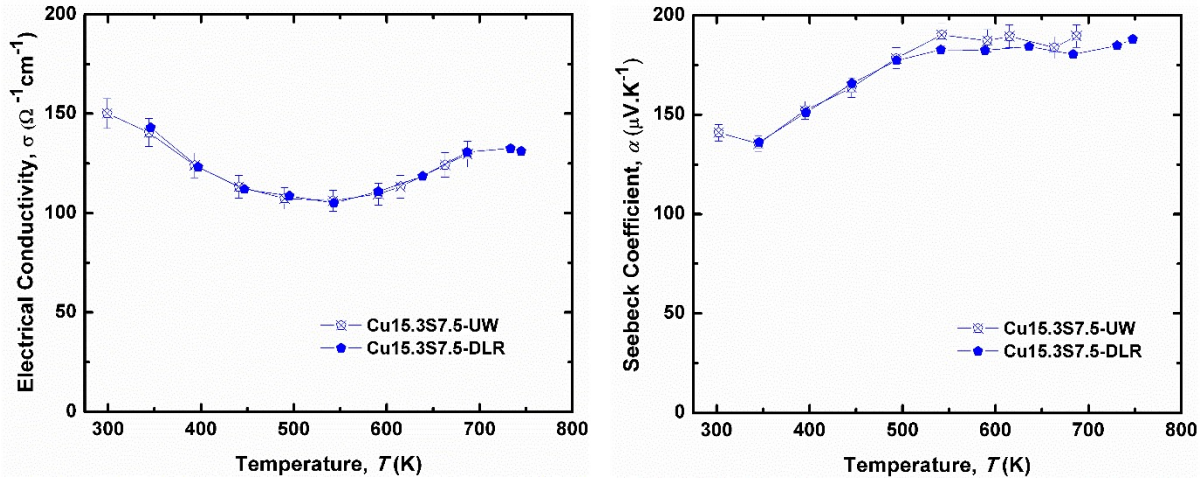

Fig. S3. Reproducibility of the electrical transport properties of two different samples of $Ba_3Cu_{15.3}S_{7.5}Te_{3.5}$. UW: measured at the University of Waterloo; DLR: measured at the German Aerospace Center.

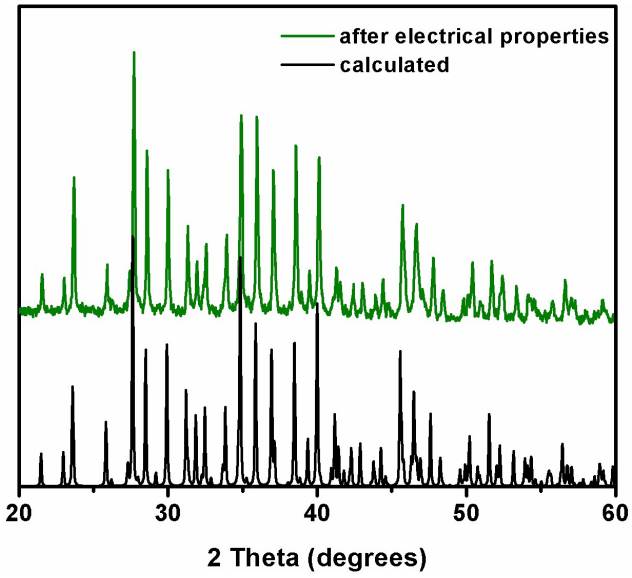

Fig. S4. X-ray pattern of $Ba_3Cu_{15.1}S_8Te_3$ after three consecutive electrical transport property measurements.

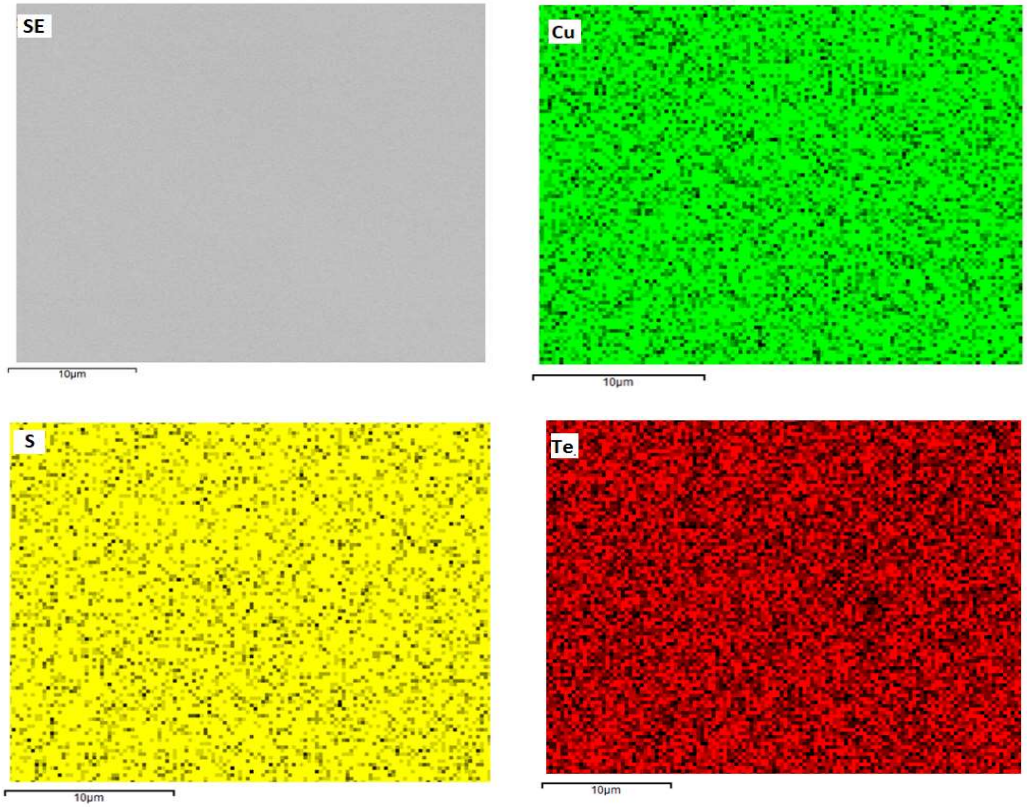

Fig. S5. EDX maps of $Ba_3Cu_{15.1}S_8Te_3$. Top left: secondary electron image; top right: Cu map; bottom left: S map; bottom right: Te map.

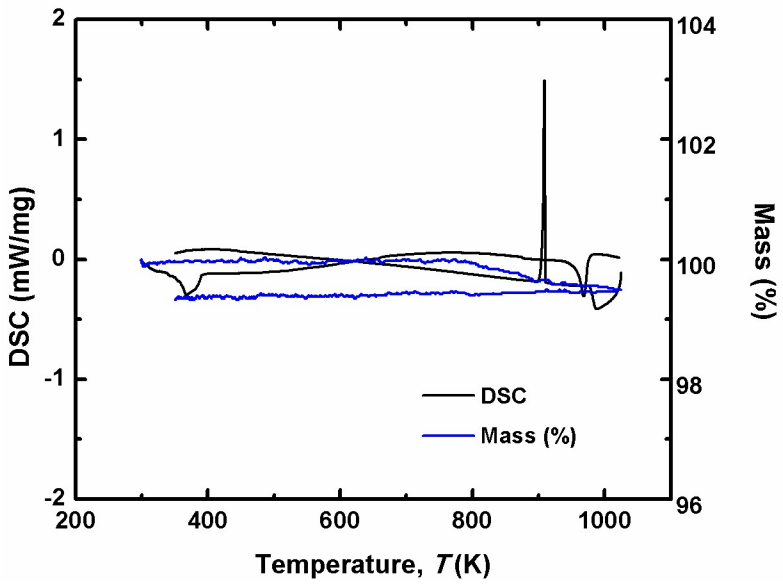

Fig. S6. DSC/TG of $Ba_3Cu_{15.3}S_{7.5}Te_{3.5}$.

Table S1. Crystallographic details of the refinement of $Ba_3Cu_{15.1}S_{8.5}Te_{2.5}$.

Formula	$Ba_3Cu_{15.26(7)}S_{8.31(1)}Te_{2.69}$[a]	$Ba_3Cu_{15.38(7)}S_{8.35(1)}Te_{2.65}$[b]
Formula Weight	1991.67	1994.36
Crystal System	Rhombohedral	Rhombohedral
Space group	$R\bar{3}m$ (no. 166)	$R\bar{3}m$ (no. 166)
a, c [Å]	11.901(1), 27.433(2)	11.899(2), 27.449(4)
V [Å^3]	3364.80(6)	3365.5(1)
Z	6	6
Density [g cm^{-3}]	5.90	5.90
Absorption coefficient [mm^{-1}]	23.49	23.53
F(000)	5301	5311
Crystal size [mm]	0.01 × 0.02 × 0.04	0.01 × 0.02 × 0.04
Temperature [K]	296(2)	296(2)
Radiation [Å]	0.71073	0.71073
Total, unique data, R(int)	7819, 1243, 0.026	6505, 1246, 0.038
Observed data [I > 2σ(I)]	1104	1016
$R(F_o)$,[c] $R_w(F_o^2)$,[d] GOF (obs. Data)	0.037, 0.085, 1.04	0.038, 0.085, 1.04
Min., max. residual electron density [e Å^{-3}]	-2.3, 4.48	-2.29, 4.26

[a] before hot pressing;

[b] after the electrical property measurements;

[c] $R(F_o) = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$;

[d] $R_w(F_o^2) = [\ \Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\ ]^{1/2}$, with F_o and F_c being the observed and calculated structure factors, respectively.

Table S2. Fractional atomic coordinates, equivalent isotropic displacement parameters and occupancies of $Ba_3Cu_{15.1}S_{8.5}Te_{2.5}$.

	x [a]	***y*** [a]	***z*** [a]	U_{eq}/Å^2 [a]	U_{eq}/Å^2 [b]	**occ.** [a]	**occ.** [b]
Ba1	0.47177(3)	0.52823(3)	0.08655(2)	0.0161(2)	0.0165(2)	1	1
Cu1	0.2325(2)	0.0134(1)	0.13515(6)	0.0391(6)	0.0414(7)	0.816(6)	0.816(7)
Cu1B	0.137(1)	-0.0175(9)	0.1503(3)	0.046(4)	0.041(4)	0.138(6)	0.135(6)
Cu2	0.4237(1)	0.5762(1)	0.35185(9)	0.0586(9)	0.060(1)	0.945(9)	0.968(9)
Cu3	0.52396(8)	0.47604(8)	0.28215(5)	0.0243(5)	0.0248(5)	0.996(7)	0.991(8)
Cu4	0.54640(9)	0.45360(9)	0.37995(6)	0.0339(6)	0.0348(7)	0.961(8)	0.970(8)
Cu5	0	0	0.1688(2)	0.042(2)	0.045(2)	0.63(2)	0.66(2)
Cu6	1/3	2/3	0.4340(6)	0.033(5)	0.035(5)	0.20(1)	0.23(1)
*Q*1(S, Te)	0.77521(4)	0.22479(4)	0.11060(3)	0.0124(3)	0.0129(3)	0.435(6), 0.565(6)	0.451(6), 0.549(6)
S3	0.3197(2)	0	0	0.0135(4)	0.0144(5)	1	1
S4	0	0	0.3595(2)	0.0162(8)	0.0172(9)	1	1
S5	0.4781(1)	0.5219(1)	0.20550(8)	0.0170(5)	0.0180(5)	1	1
Te2	0	0	0.07669(4)	0.0168(2)	0.0170(3)	1	1

[a] before hot pressing;

[b] after the electrical property measurements.