

Effect of Mixed Occupancies on The Thermoelectric Properties of $\text{BaCu}_{6-x}\text{Se}_{1-y}\text{Te}_{6+y}$ Polychalcogenides

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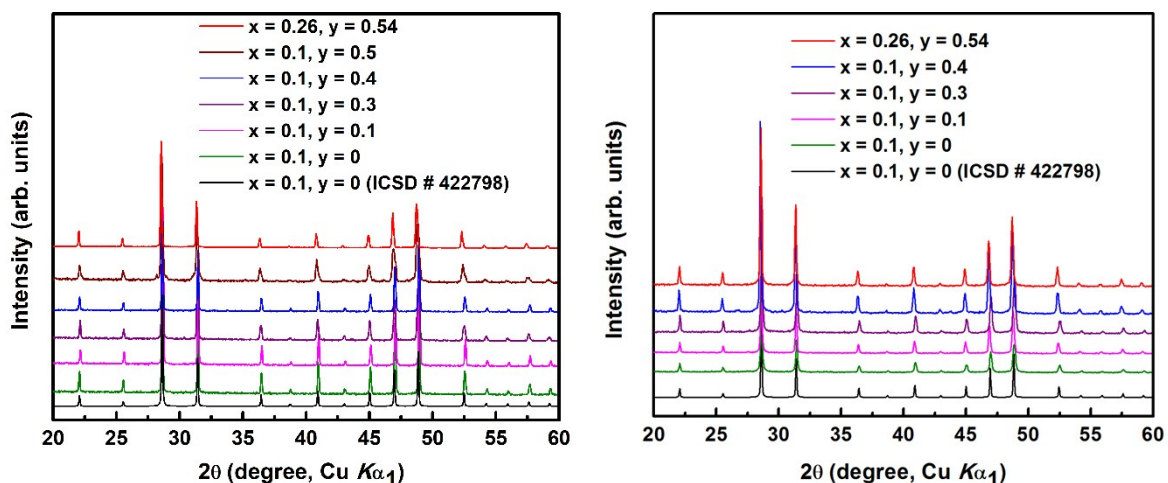


Fig. S1 Room temperature powder XRD patterns of $\text{BaCu}_{6-x}\text{Se}_{1-y}\text{Te}_{6+y}$. Left: before hot-pressing; right: after hot-pressing.

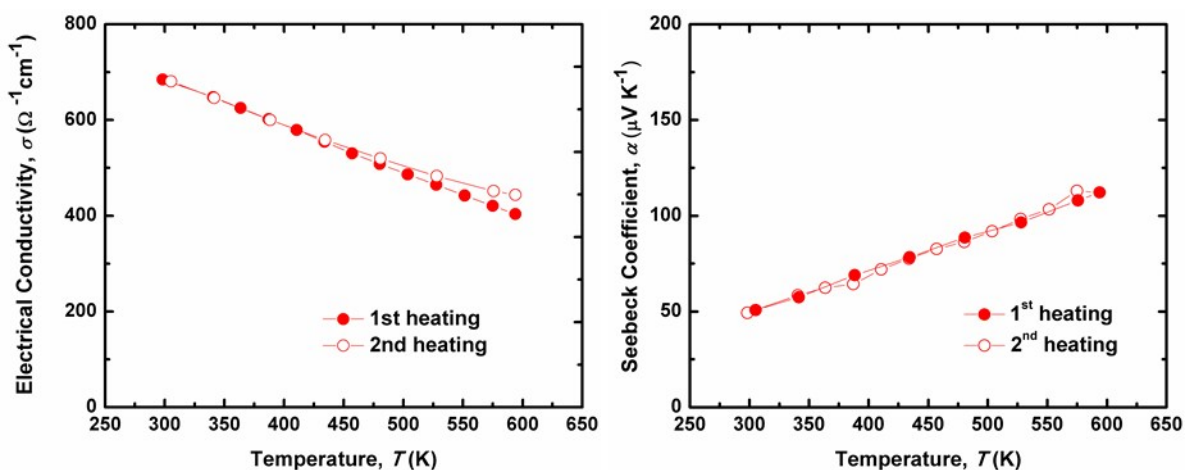


Fig. S2 Stability of the electrical transport properties of “ $\text{BaCu}_{5.74}\text{Se}_{0.46}\text{Te}_{6.54}$ ”.

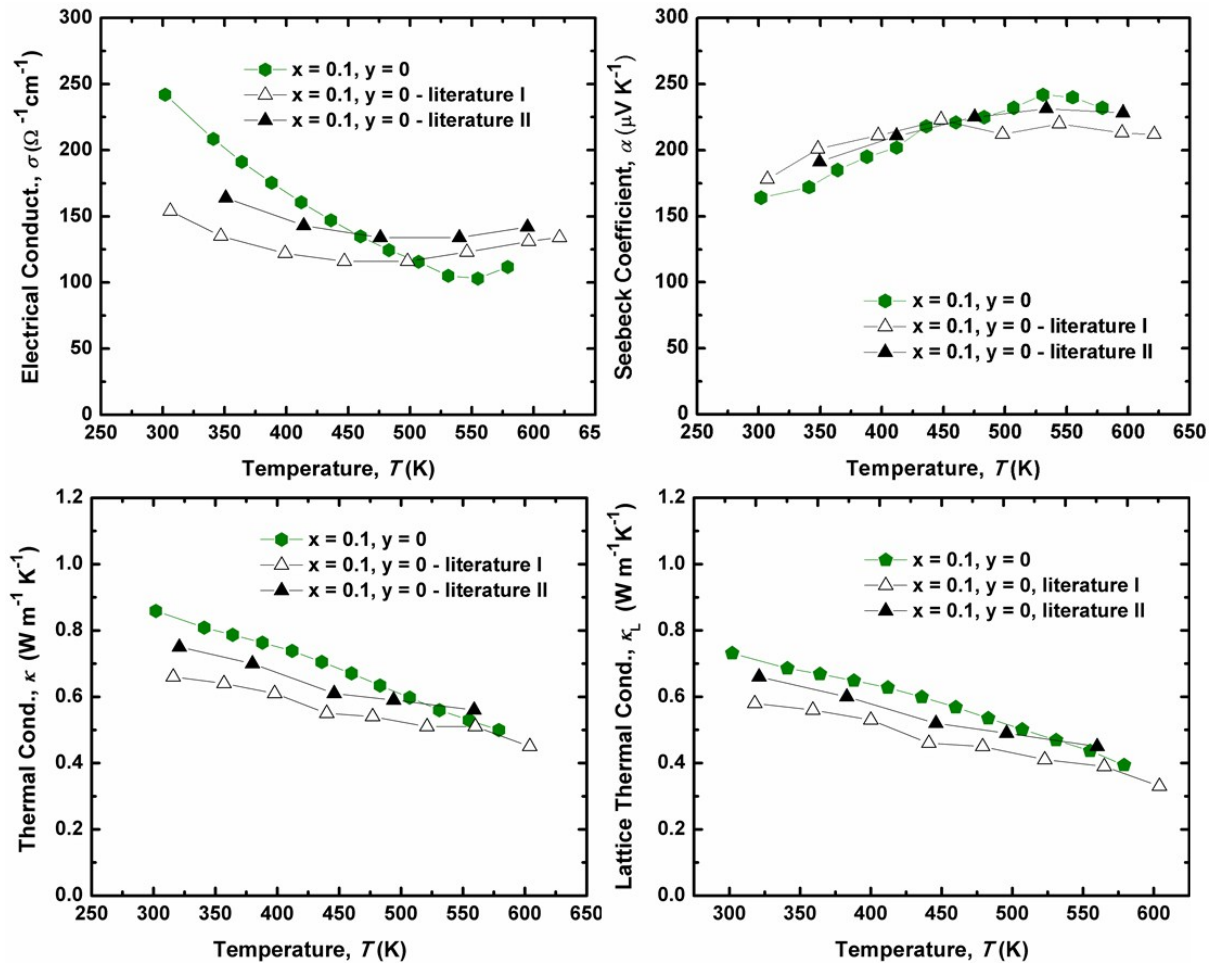


Fig. S3 Physical properties of “BaCu_{5.9}SeTe₆”.

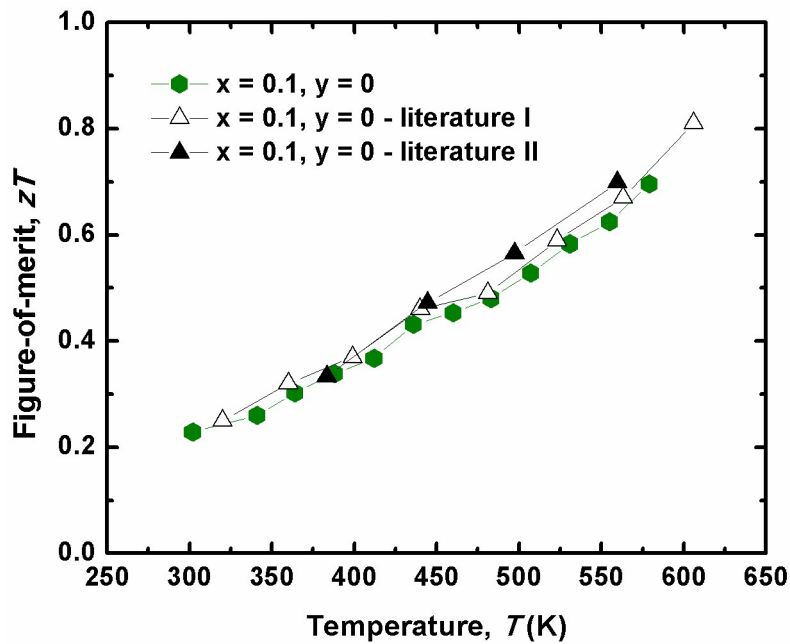


Fig S4 Reproducibility of the zT values of “BaCu_{5.9}SeTe₆”.

Table S1. Fractional atomic coordinates, equivalent isotropic displacement parameters and occupancies of $\text{BaCu}_{5.74(2)}\text{Se}_{0.69(1)}\text{Te}_{6.31}$.

	Site	x	y	z	$U_{eq}/\text{\AA}^2$
Ba1	1b	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0.0209(2)
Cu1	8i	0.19980(7)	x	x	0.0254(3)
Te1	6f	0.30021(5)	0	$\frac{1}{2}$	0.0172(1)
Q (Se2, Te2)	1a	0	0	0	0.0428(6)

Table S2. Fractional atomic coordinates, equivalent isotropic displacement parameters and occupancies of $\text{BaCu}_{5.80(3)}\text{Se}_{0.64(2)}\text{Te}_{6.36}$.

	Site	x	y	z	$U_{eq}/\text{\AA}^2$
Ba1	1b	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0.0216(4)
Cu1	8i	0.2001(1)	x	x	0.0274(6)
Te1	6f	0.30031(8)	0	$\frac{1}{2}$	0.0183(3)
Q (Se2, Te2)	1a	0	0	0	0.046(1)

Table S3. Fractional atomic coordinates, equivalent isotropic displacement parameters and occupancies of $\text{BaCu}_{5.74(2)}\text{Se}_{0.43(2)}\text{Te}_{6.57}$.

	Site	x	y	z	$U_{eq}/\text{\AA}^2$
Ba1	1b	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0.0211(2)
Cu1	8i	0.20018(6)	x	x	0.0269(2)
Te1	6f	0.30031(8)	0	$\frac{1}{2}$	0.0175(1)
Q (Se2, Te2)	1a	0	0	0	0.0578(5)

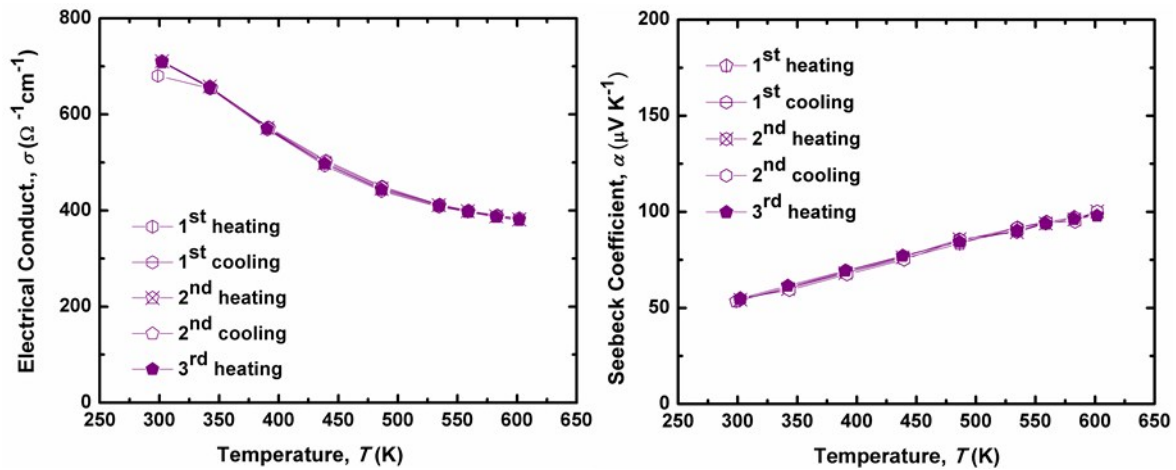


Fig. S5 Stability of the electrical transport properties of “ $\text{BaCu}_{5.74}\text{Se}_{0.6}\text{Te}_{6.4}$ ”.