Supporting Information

Enhancement of Thermoelectric Performance via Weak Disordering of Topological Crystalline Insulator and Band Convergence by Se Alloying in $Pb_{0.5}Sn_{0.5}Te_{1-x}Se_x$ Compounds

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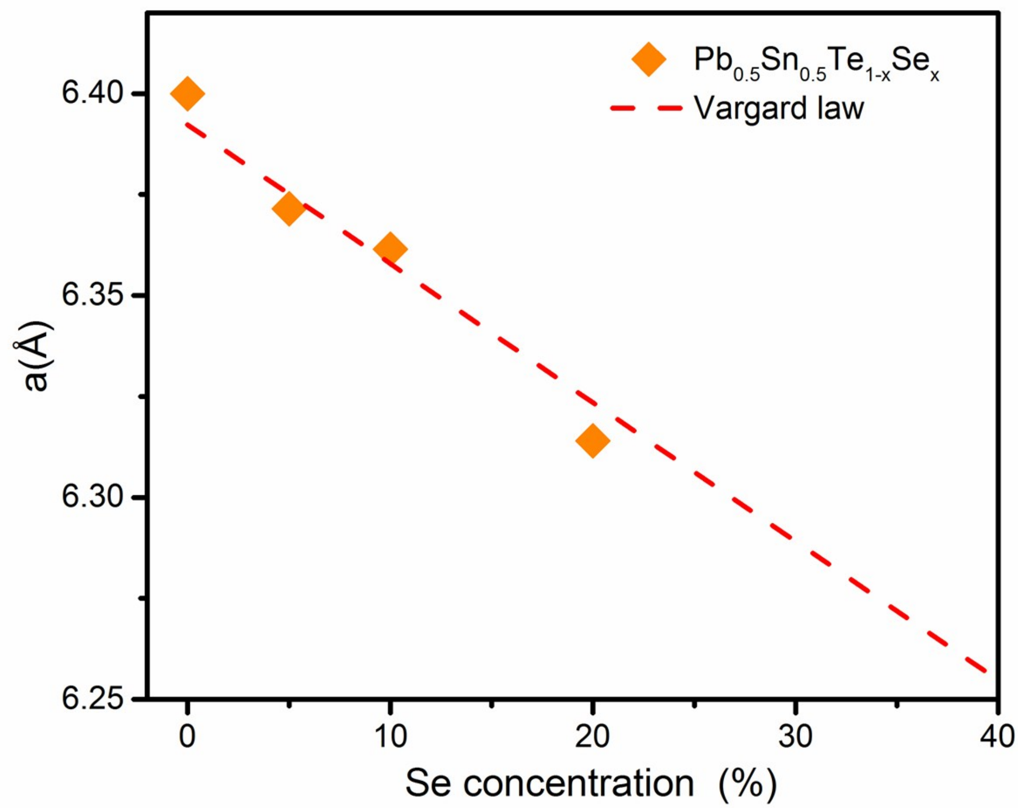

Figure S1: The lattice parameter content against Se content of Se and Vargard law

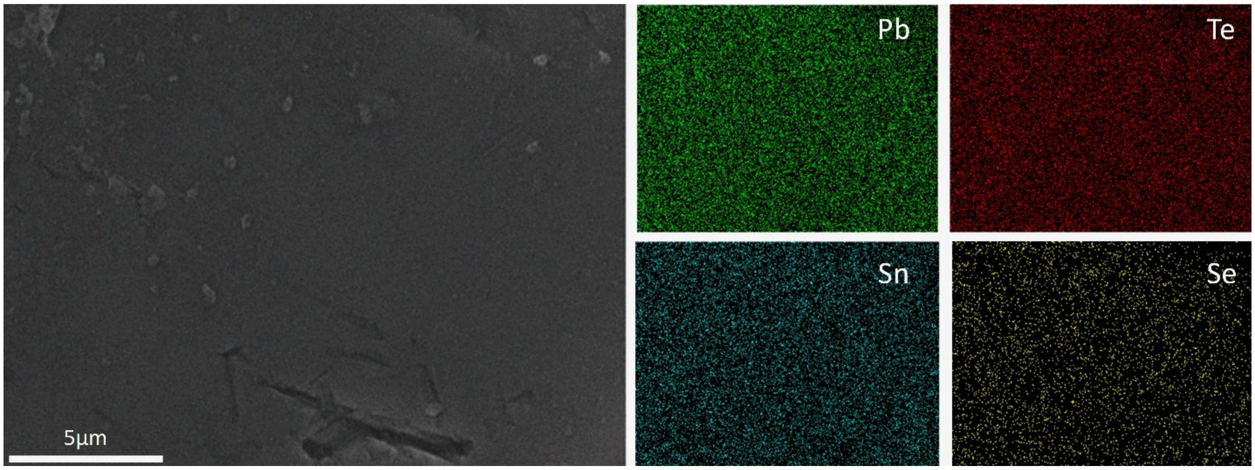

Figure S2. The SEM image of $Pb_{0.5}Sn_{0.5}Te_{0.95}Se_{0.05}$ and its SEM-EDS elemental maps of Pb, Sn, Te, and Se.

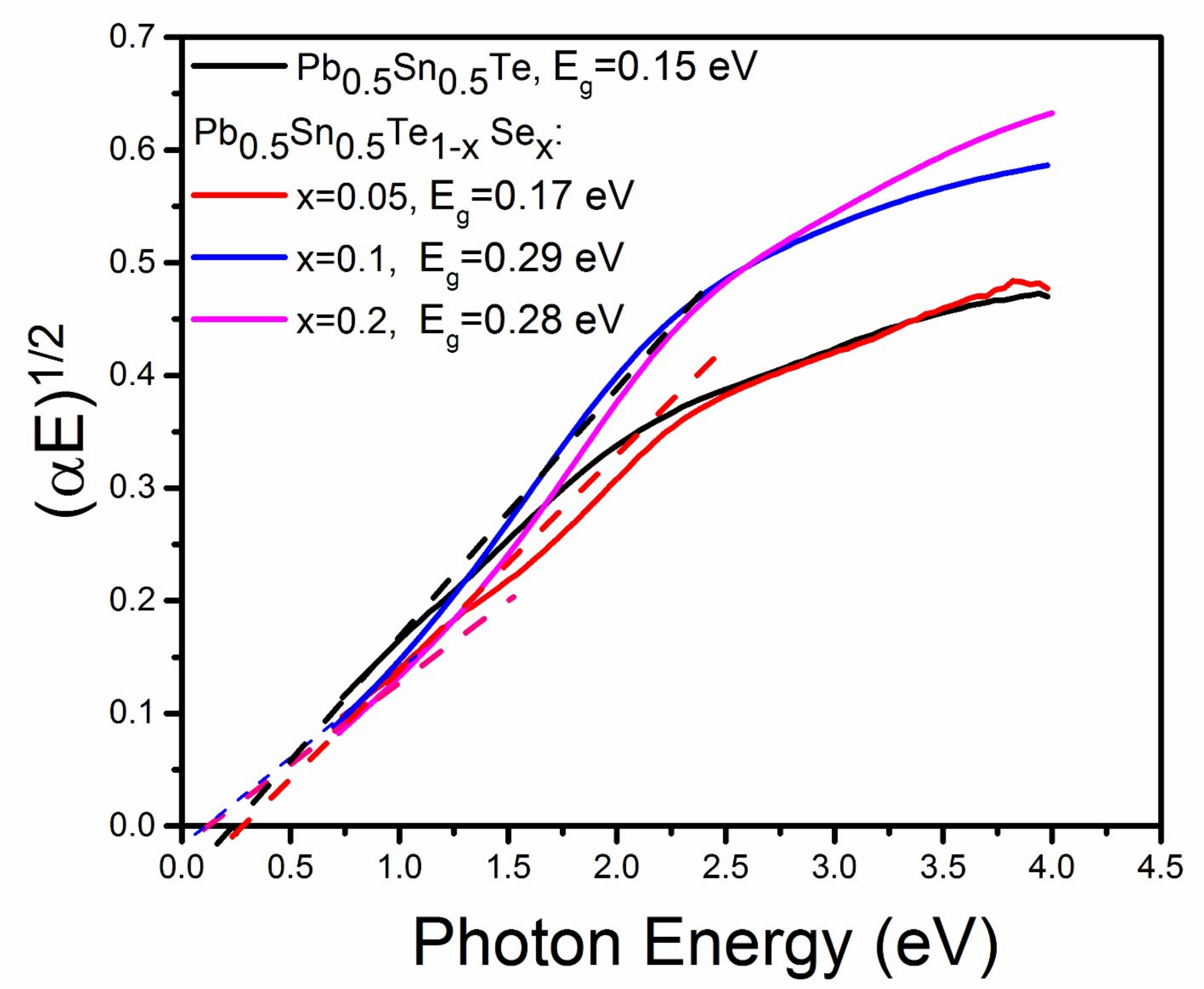

Figure S3: Band gap at room temperature for *x*=0.00, 0.05, 0.1, and 0.2

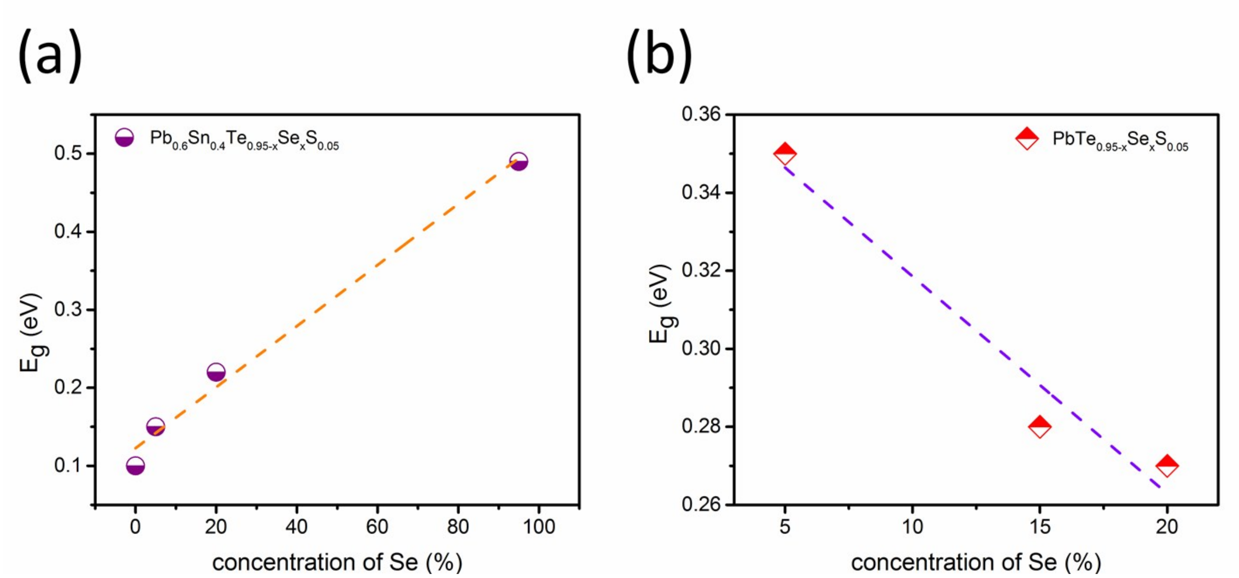

Figure S4 : Band gap of TCIs $Pb_{0.6}Sn_{0.4}Te_{0.95-x}Se_xS_{0.05}$ (a)[1] band gap of $PbT_{0.95}Se_xS_{0.05}$(b)[1]

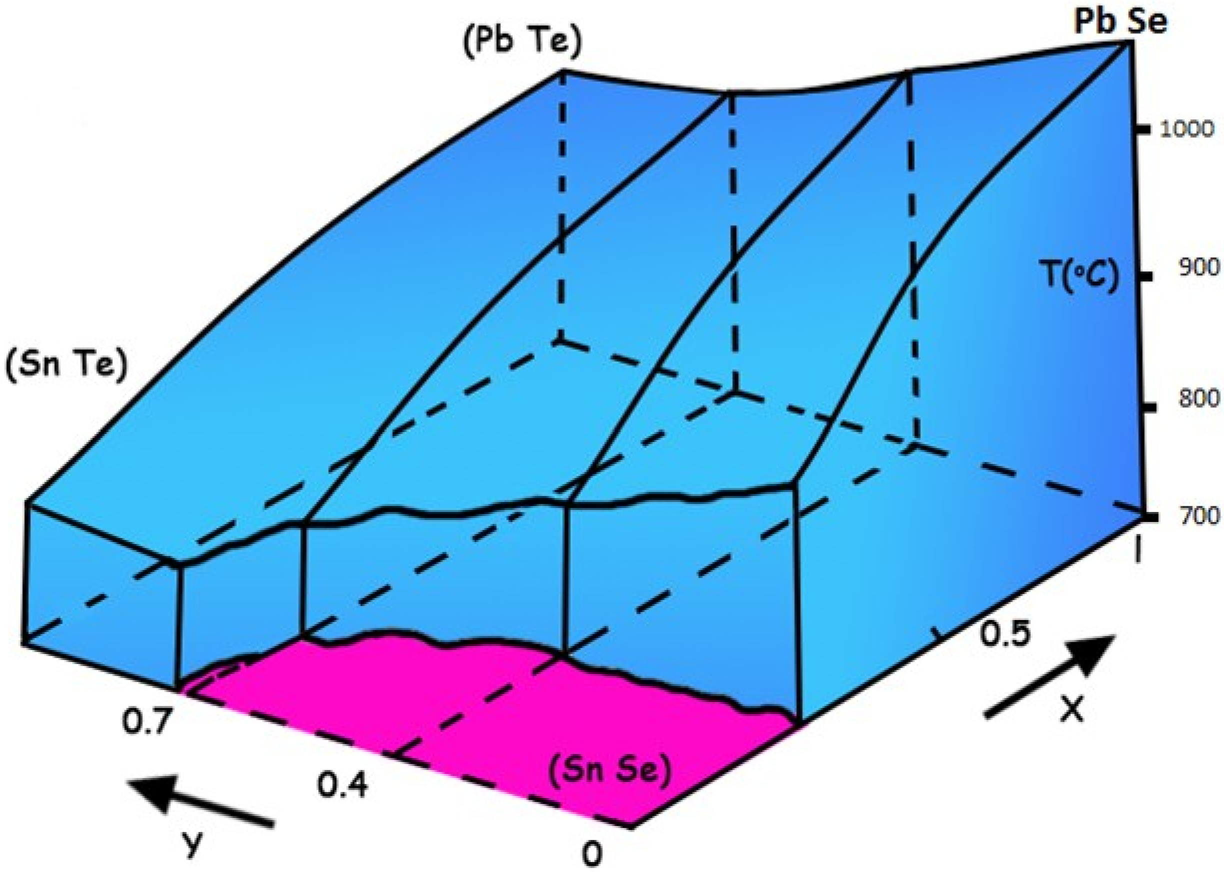

Figure S5: Three-dimensional representation of the liquidus surface of the stoichiometric system of $Pb_zSn_{1-z}Te_ySe_{1-y}$ from reference[2]

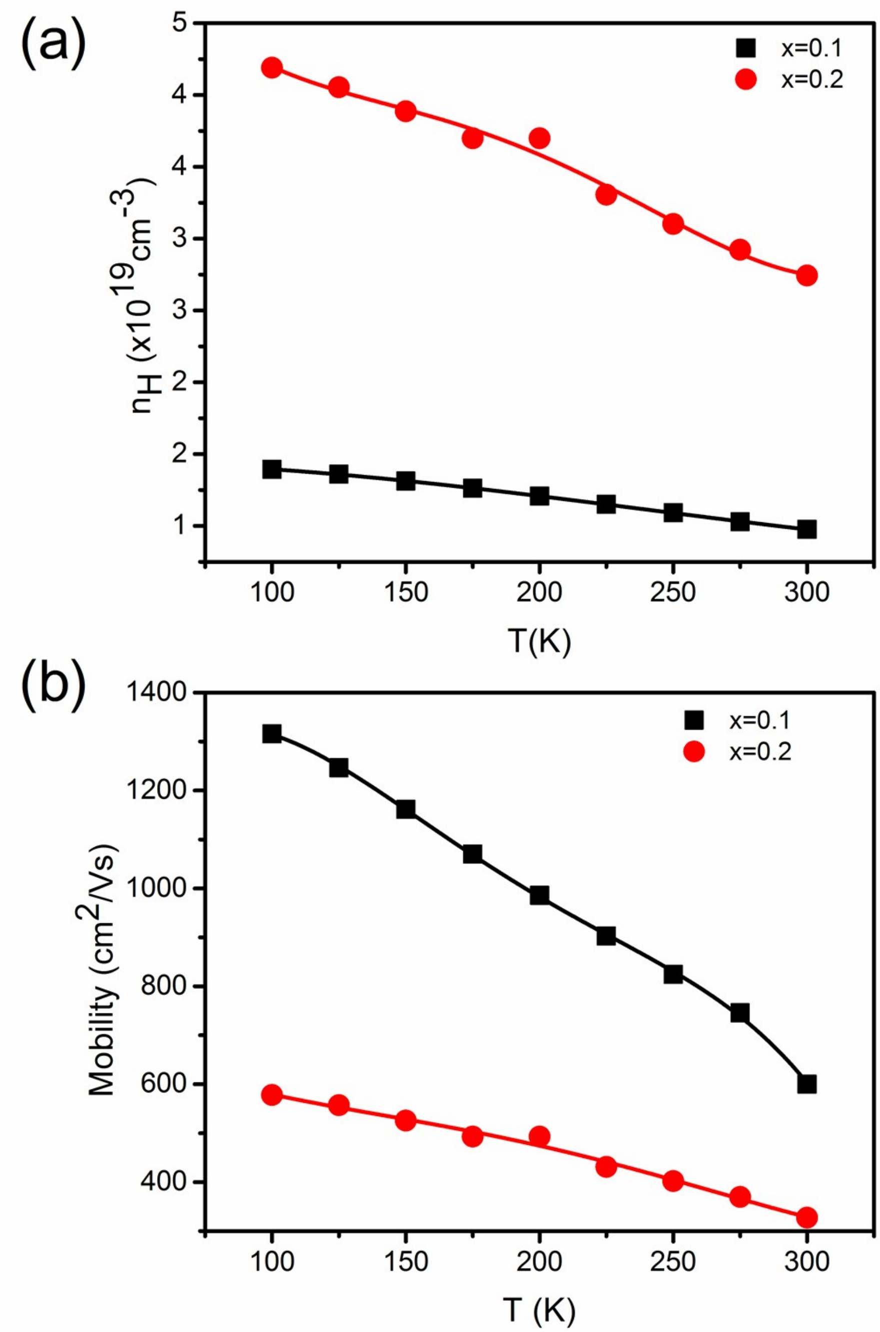

Figure S6: hall carrier concentration and mobility for *x*=0.1 and 0.2 at 200K-300K

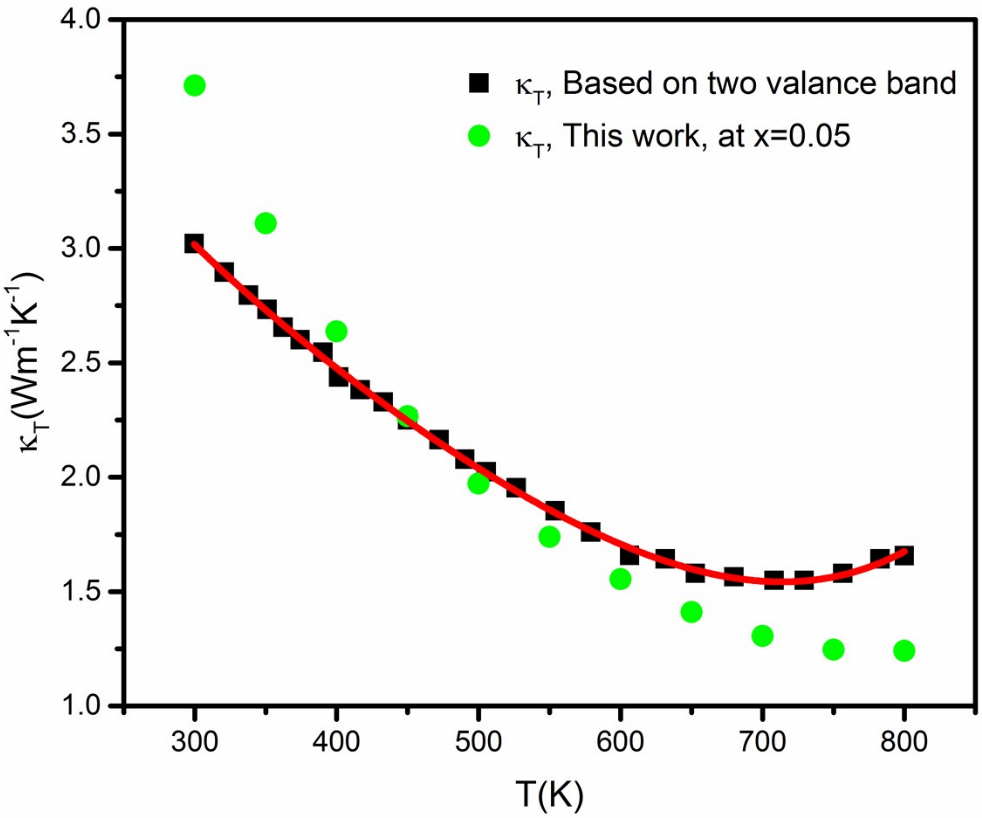

Figure S7: Two band total thermal conductivity of $Pb_{0.5}Sn_{0.5}Te$ from refence[3] with this work at x=0.05

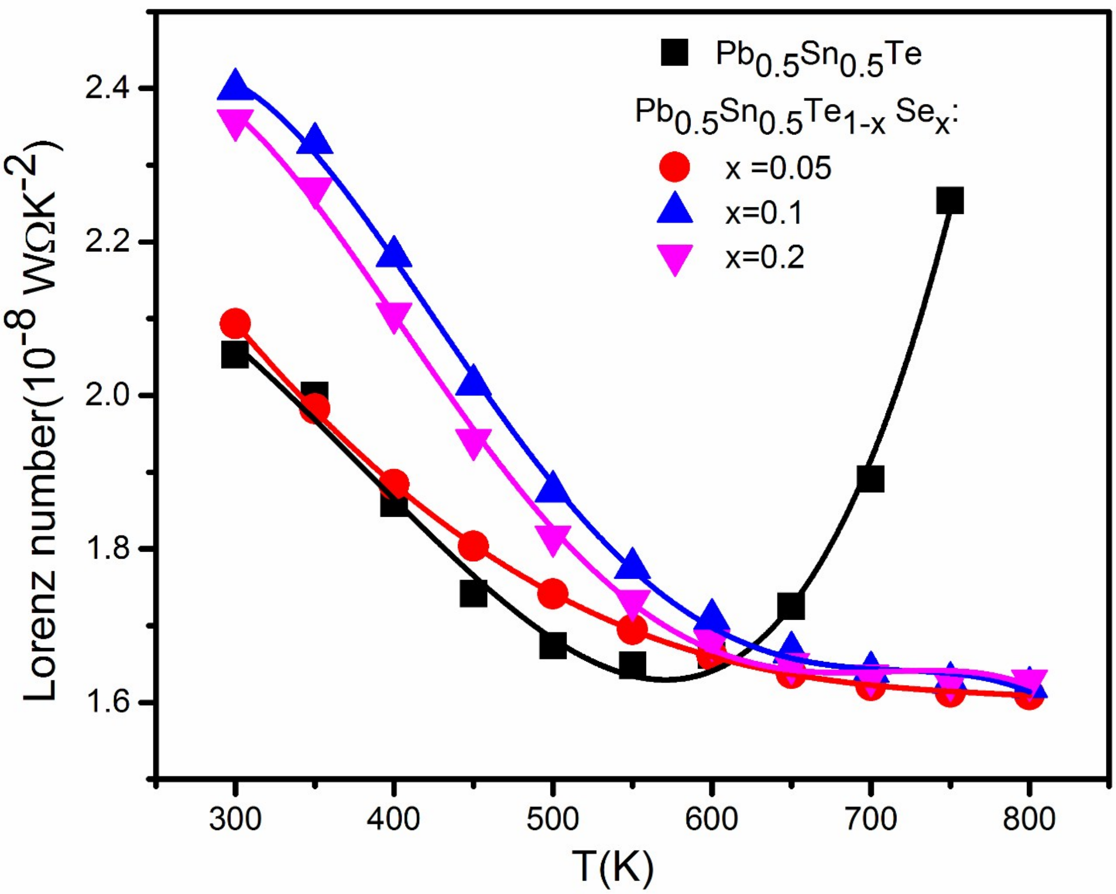

Figure S8. Temperature-dependent Lorenz number for $Pb_{0.5}Sn_{0.5}Te_{1-x}Se_x$ (x = 0.0, 0.05, 0.1, and 0.2) compounds obtained from the single parabolic band model (see text).

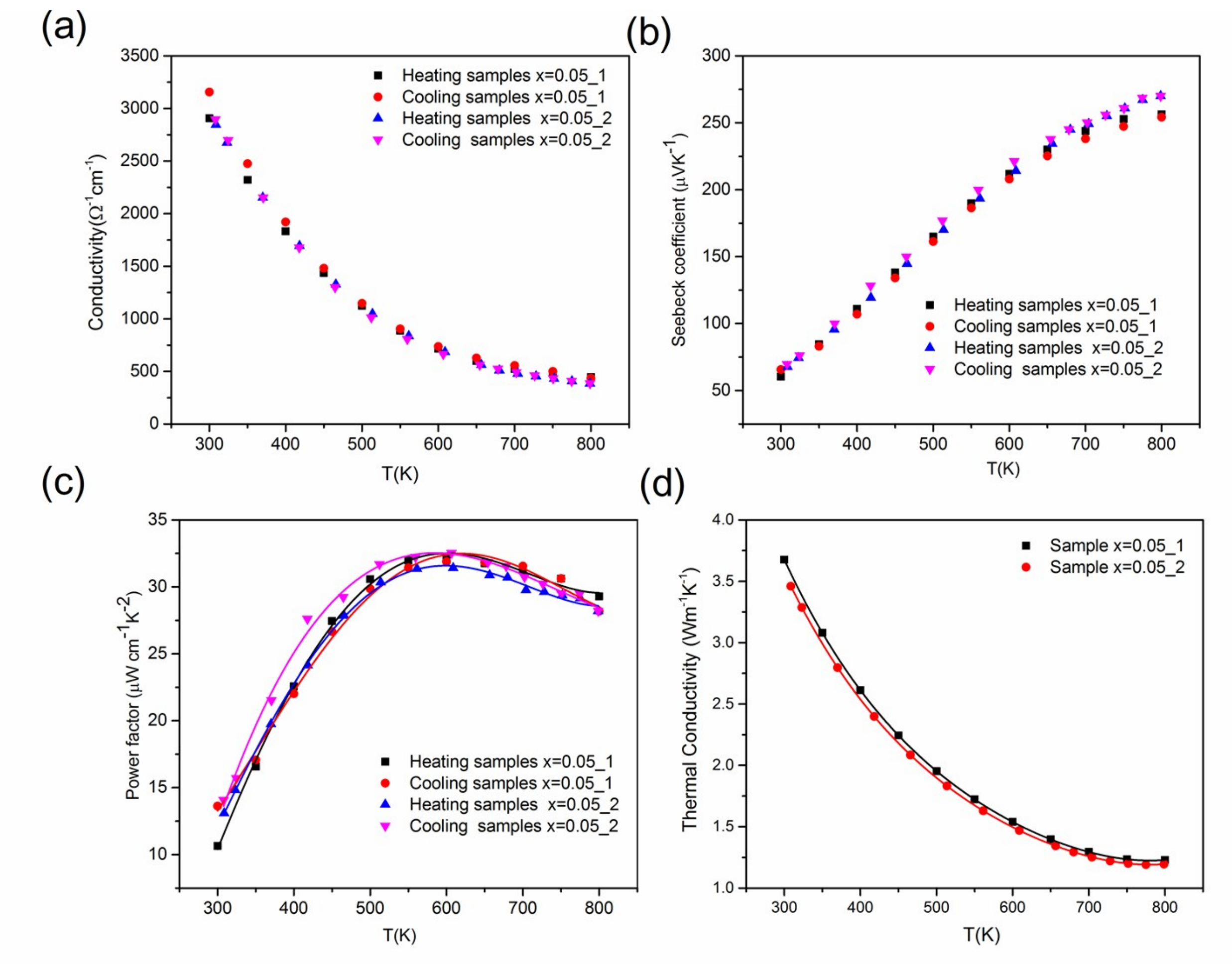

Figure S9. Reproducible measurements of the $Pb_{0.5}Sn_{0.5}Te_{1-x}Se_x$ (x = 0.05) compound for different samples with heat cycling. It shows reasonable reproducibility of the sample.

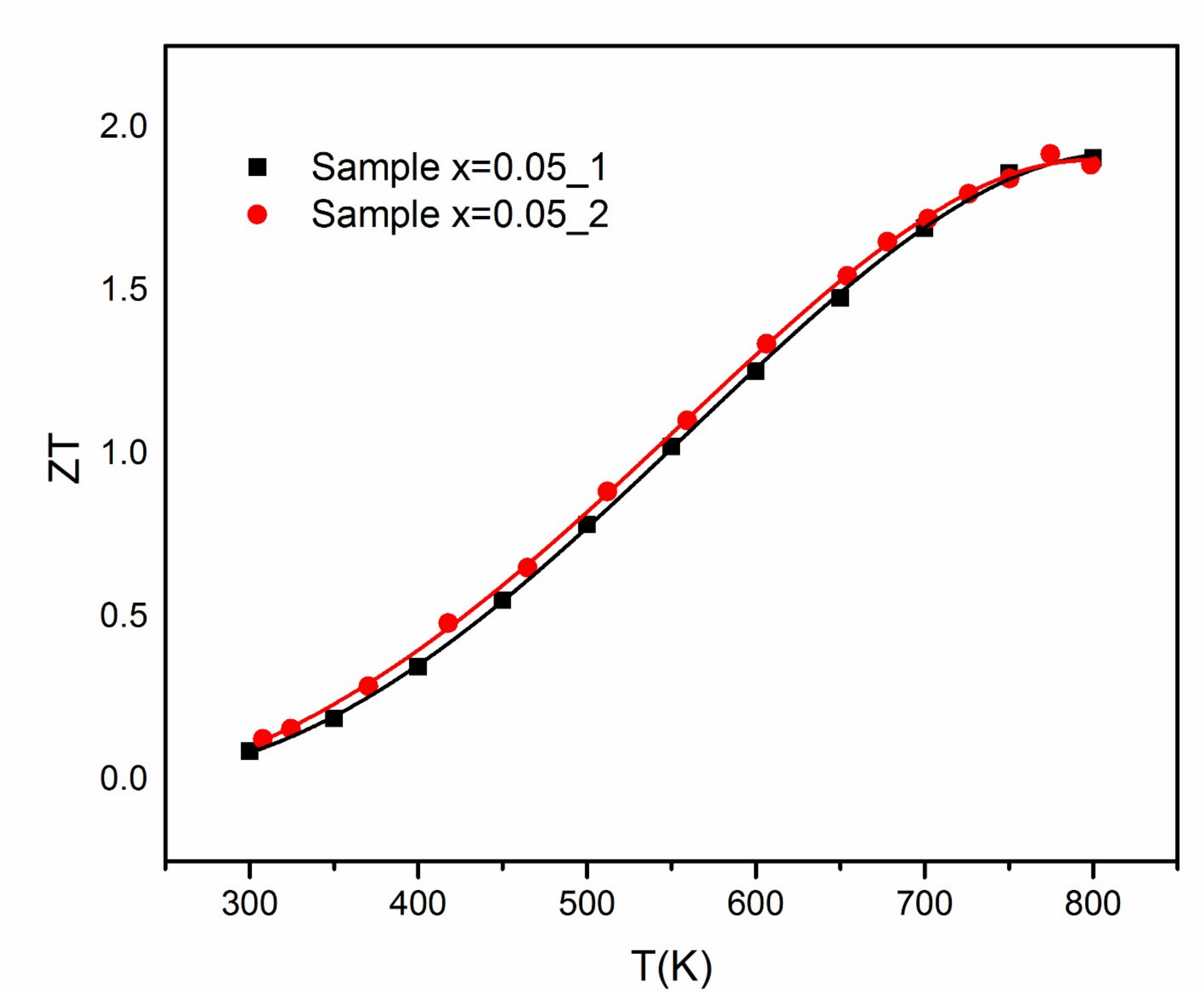

Figure S10. Reproducibility of the temperature-dependent *ZT* value for $Pb_{0.5}Sn_{0.5}Te_{1-x}Se_x$ (x = 0.05) compound.

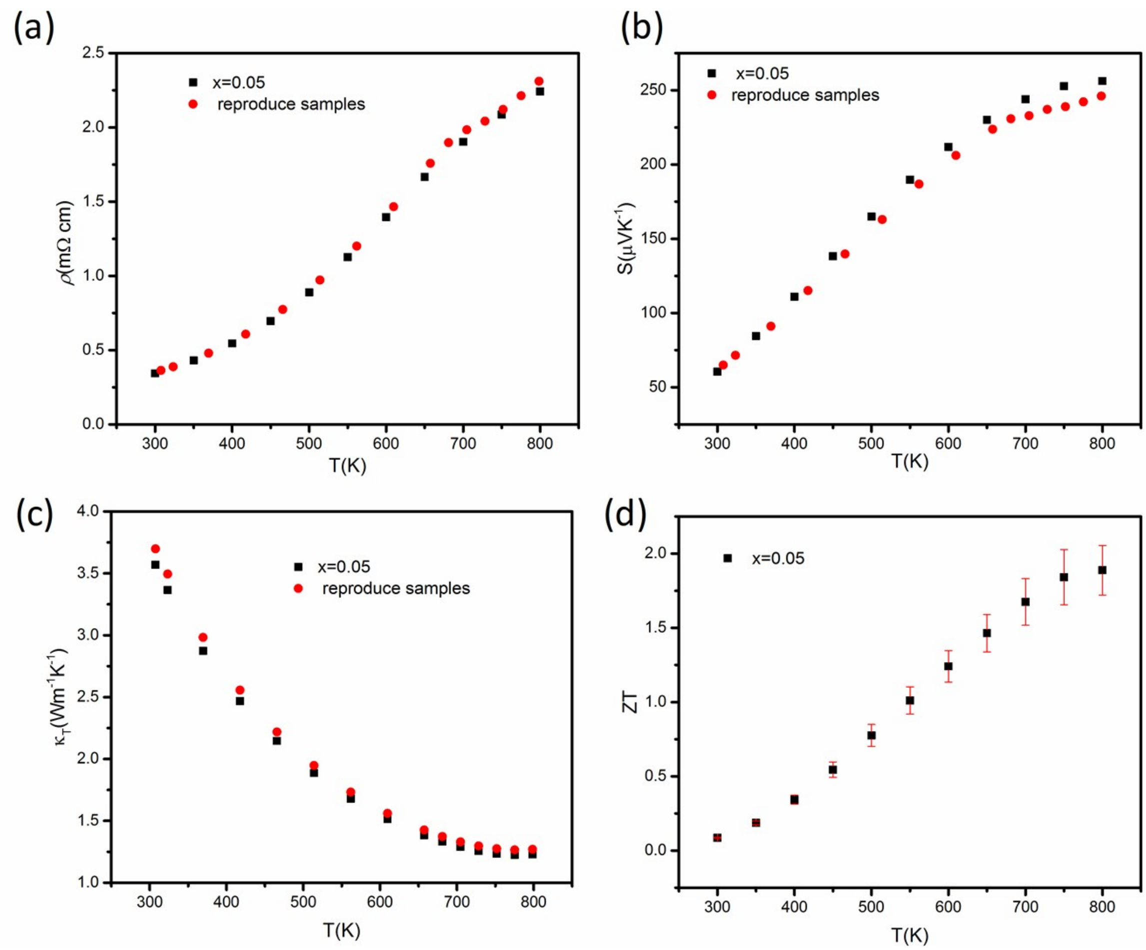

Figure S11. Reproducible measurements of the $Pb_{0.5}Sn_{0.5}Te_{1-x}Se_x$ (x = 0.05) compound for different batch: electric resistivity (a), Seebeck coefficient (b), thermal conductivity (c), temperature-dependent *ZT* value for $Pb_{0.5}Sn_{0.5}Te_{1-x}Se_x$ (x = 0.05) compound with error bar from reproducibility samples with different batch (d).

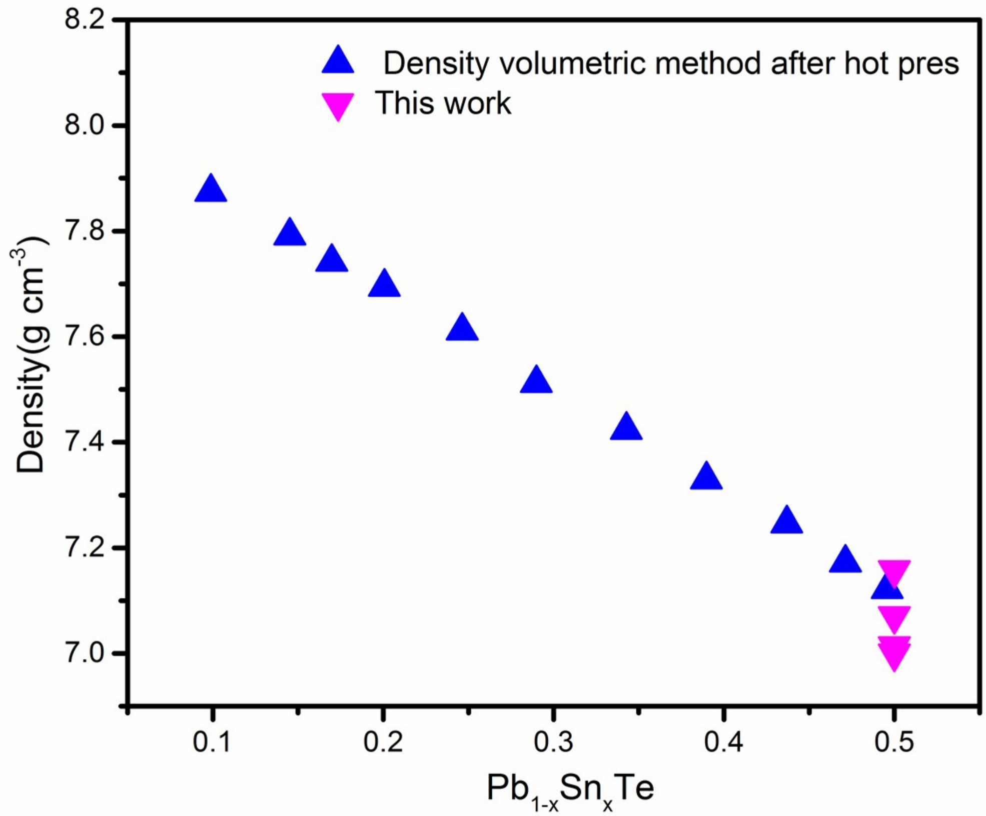

Figure 12: Density volumetric method after hot press for $Pb_{1-x}Sn_xTe$ from reference[4] with density this work by Archimedes method

Table S1. Density Volumetric of $Pb_{1-x}Sn_xTe$[4] and density $Pb_{0.5}Sn_{0.5}Te_{1-x}Se_x$ by Archimedes method.

$Pb_{1-x}Sn_xTe$	Density volumetric	$Pb_{0.5}Sn_{0.5}Te_{1-x}Se_x$	Density by Archimedes method
0.2	7.68	0	7.014
0.3	7.486	0.05	7
0.4	7.298	0.1	7.071
0.5	7.112	0.2	7.158

Table S1. Theoretical density D_T, experimental density D_{exp}, relative density D_R, heat

x	D_t (g cm^{-3})	D_{exp} (g cm^{-3}	D_R(%)	Cp (Jg^{-1}K^{-1})	λ (mm^2 s^{-1})
0	7.100(Gelbstein, 2007 #460)	7014	98.7	0.1757	1.7328
0.05	7.150	7.000	97.90	0.1758	3.0496
0.1	7.200	7.071	98.20	0.1759	1.0190
0.2	7.300	7.158	98.05	0.1762	1.0603

capacity, and thermal diffusivity λ at room temperature.

Reference:

1. C. C. L. D. Ginting, L. Rathnam, G. Kim, J. H. Yun, H. S. So, H. Lee, B. Kyu Yu, S -J. Kim, K. Ahn, and J-S Rhyee, *sumitted*, 2018.
2. C. A. Kennedy and K. J. Linden, *Journal of Applied Physics*, 1970, **41**, 252-253.
3. Y. Gelbstein, Z. Dashevsky and M. P. Dariel, *Physica B: Condensed Matter*, 2007, **391**, 256-265.
4. Y. Gelbstein, Z. Dashevsky, Y. George and M. P. Dariel, 2006.