Supporting information

Optimizing Thermoelectric Performance of Mixed Crystals $Bi_2O_2Se_{1-x}Te_x$ in the Bi_2O_2Se/Bi_2O_2Te Pseudobinary Bulk System

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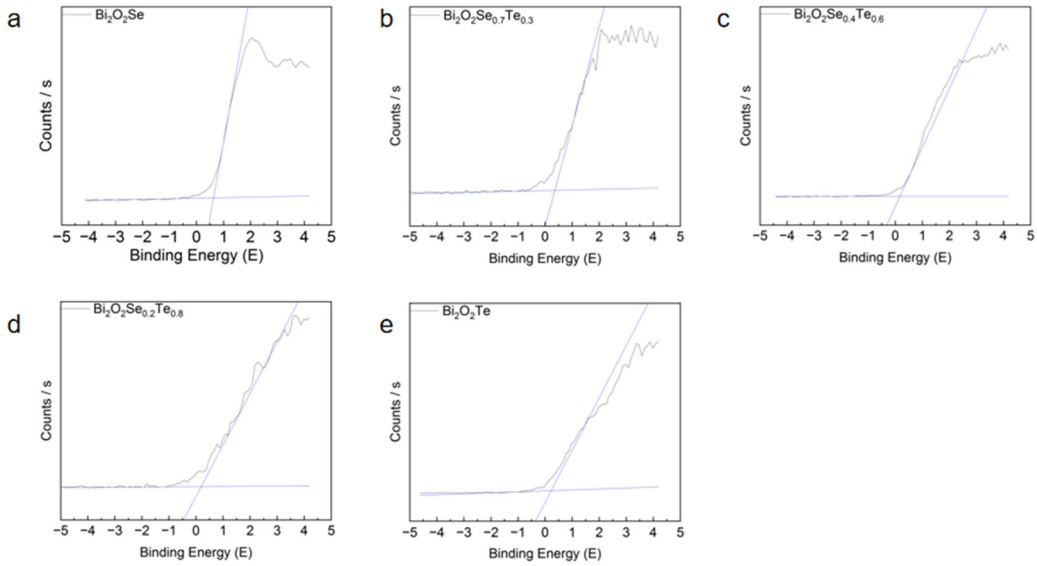

Figure S1. The valence band of samples. The valence band of Bi_2O_2Se(a), $Bi_2O_2Se_{0.7}Te_{0.3}$(b), $Bi_2O_2Se_{0.4}Te_{0.6}$(c), $Bi_2O_2Se_{0.2}Te_{0.8}$(d) and Bi_2O_2Te(e).

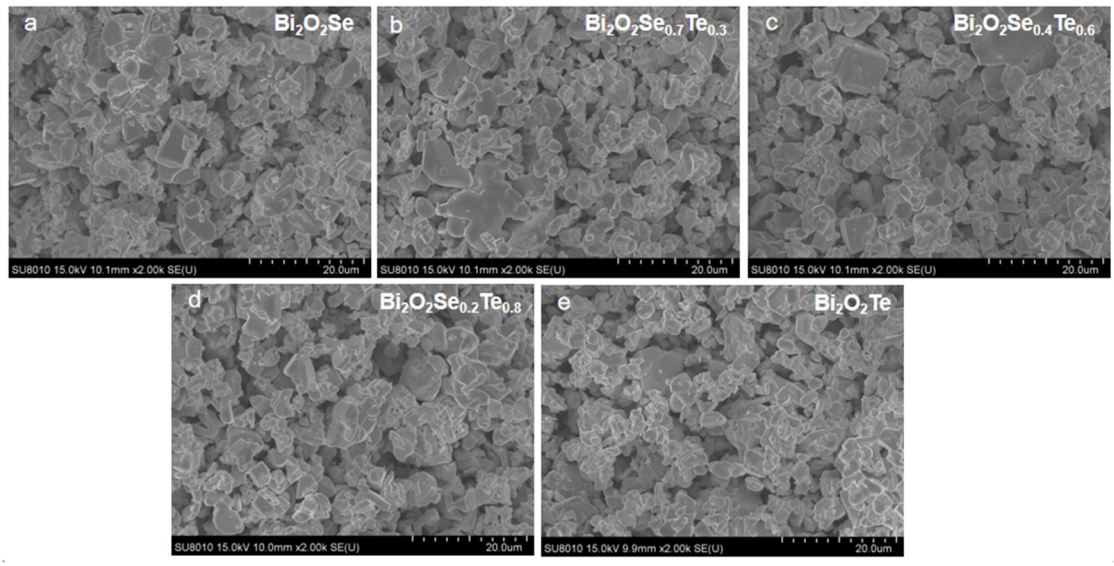

Figure S2. SEM of samples. SEM images of all $Bi_2O_2Se_{1-x}Te_x$ samples including Bi_2O_2Se (a), $Bi_2O_2Se_{0.7}Te_{0.3}$ (b), $Bi_2O_2Se_{0.4}Te_{0.6}$ (c), $Bi_2O_2Se_{0.2}Te_{0.8}$ (d) and Bi_2O_2Te (e). We measured the average size of each sample from the SEM plots, and the average size of these particles was calculated to be 3.4±0.7, 3.2±0.9, 3.9±1.0, 4.2±0.8, and 2.6±0.6 μm for different Te doping levels of $Bi_2O_2Se_{1-x}Te_x$ (x=0, 0.2, 0.4, 0.7, 1).

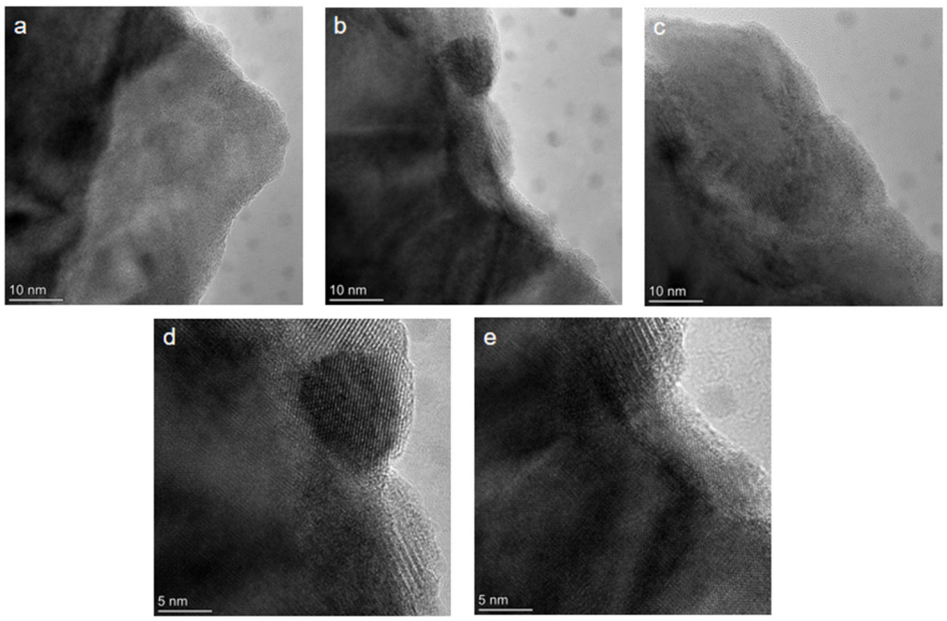

Figure S3. (**a-e**) TEM of $Bi_2O_2Se_{0.4}Te_{0.6}$. TEM images of $Bi_2O_2Se_{0.4}Te_{0.6}$ compounds.

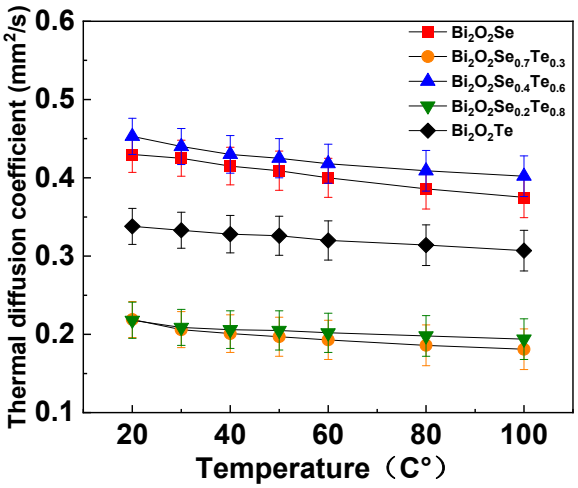

Figure S4. The thermal diffusion coefficient of Bi_2O_2Se, $Bi_2O_2Se_{0.7}Te_{0.3}$, $Bi_2O_2Se_{0.4}Te_{0.6}$, $Bi_2O_2Se_{0.2}Te_{0.8}$ and Bi2O2Te at different temperatures.

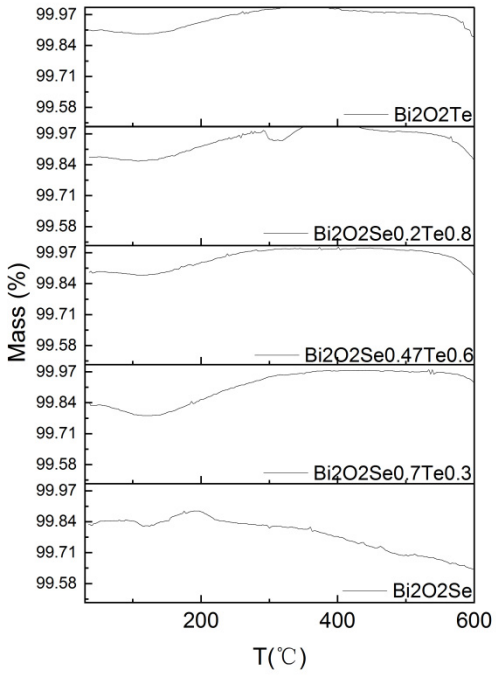

Figure S5. The TGA show the relationship between Mass and temperature of Bi_2O_2Se, $Bi_2O_2Se_{0.7}Te_{0.3}$, $Bi_2O_2Se_{0.4}Te_{0.6}$, $Bi_2O_2Se_{0.2}Te_{0.8}$ and Bi2O2Te. It means that the material is able to efficiently convert waste heat into electricity in a variety of practical scenarios, while maintaining long-term stability and reliability.

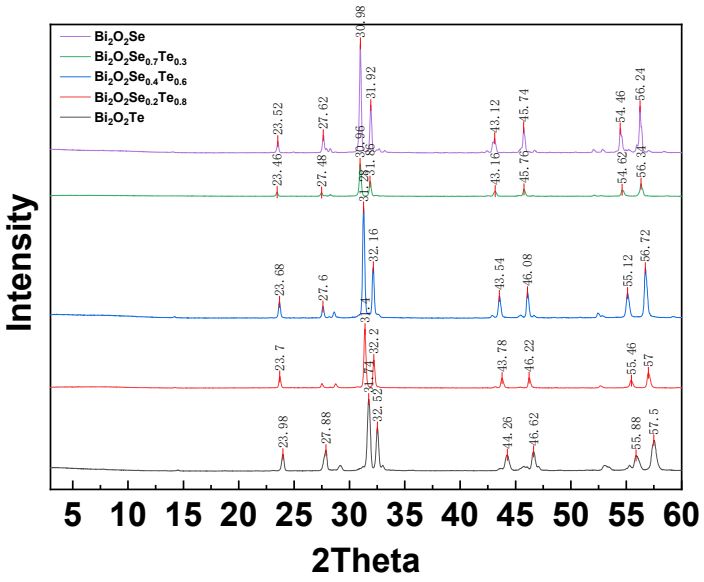

Figure S6. XRD of samples Bi_2O_2Se, $Bi_2O_2Se_{0.7}Te_{0.3}$, $Bi_2O_2Se_{0.4}Te_{0.6}$, $Bi_2O_2Se_{0.2}Te_{0.8}$ and Bi_2O2Te after heating at 600°C.

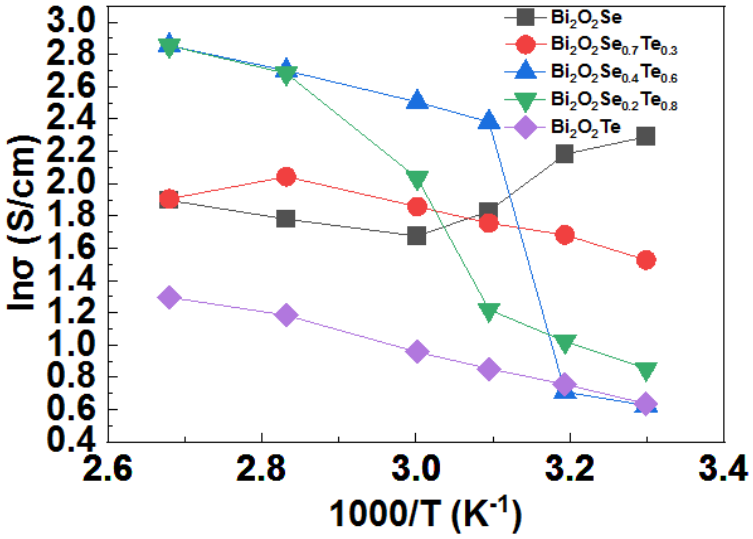

Figure S7. Arrhenius plot of samples.