Supplementary Information

Discovery of TaFeSb-based half-Heuslers with high thermoelectric performance

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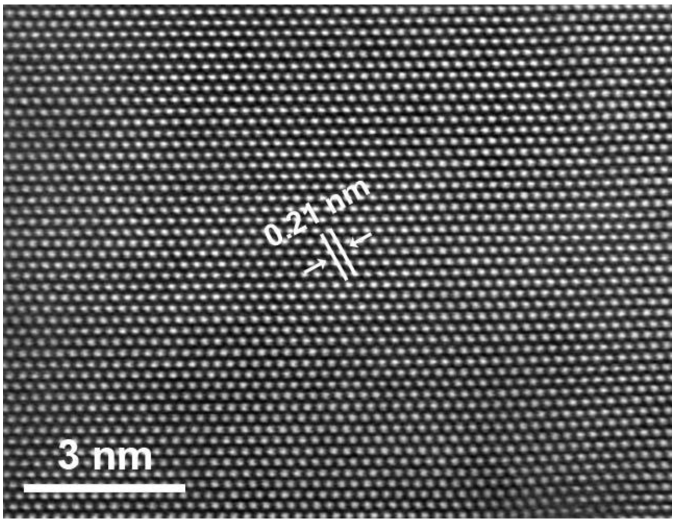
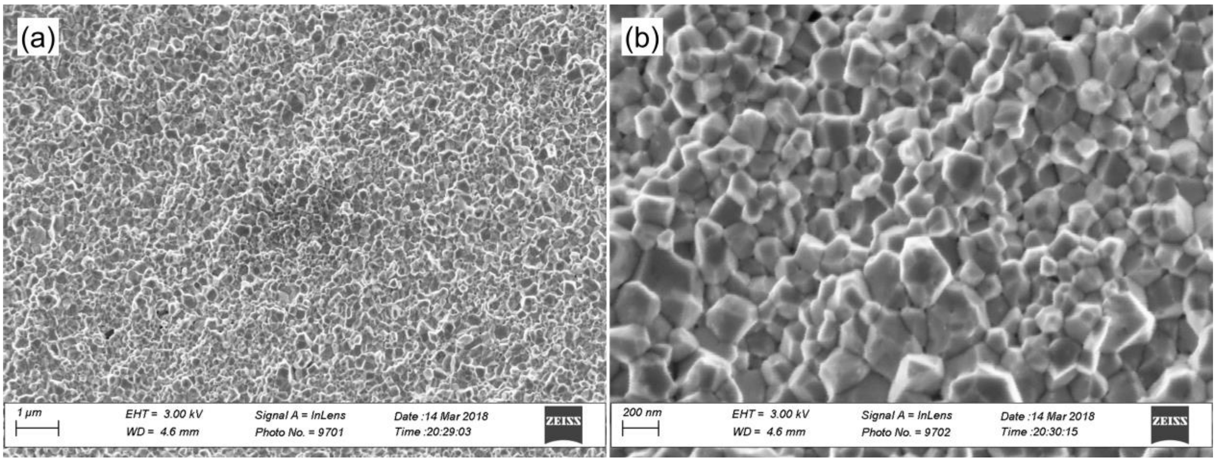
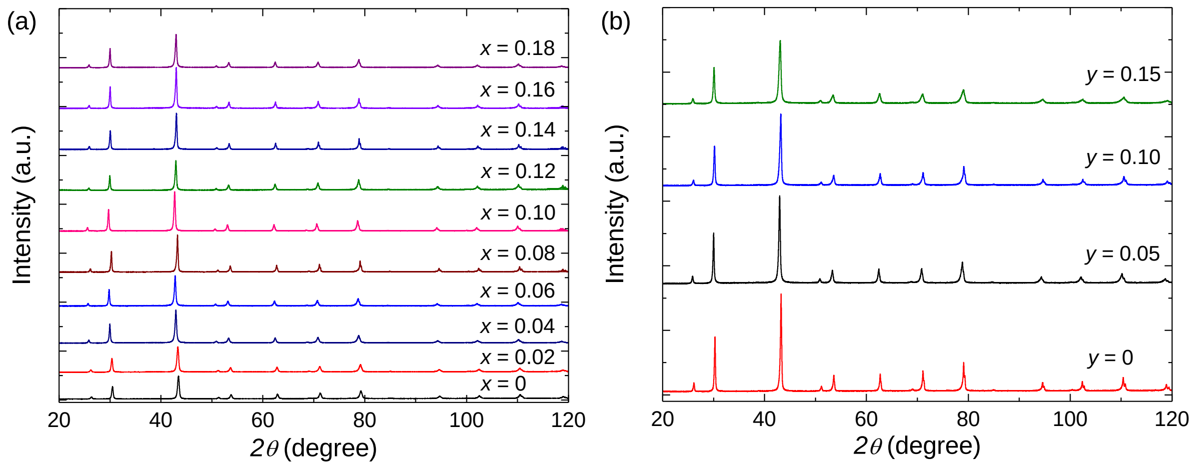
Supplementary Figures



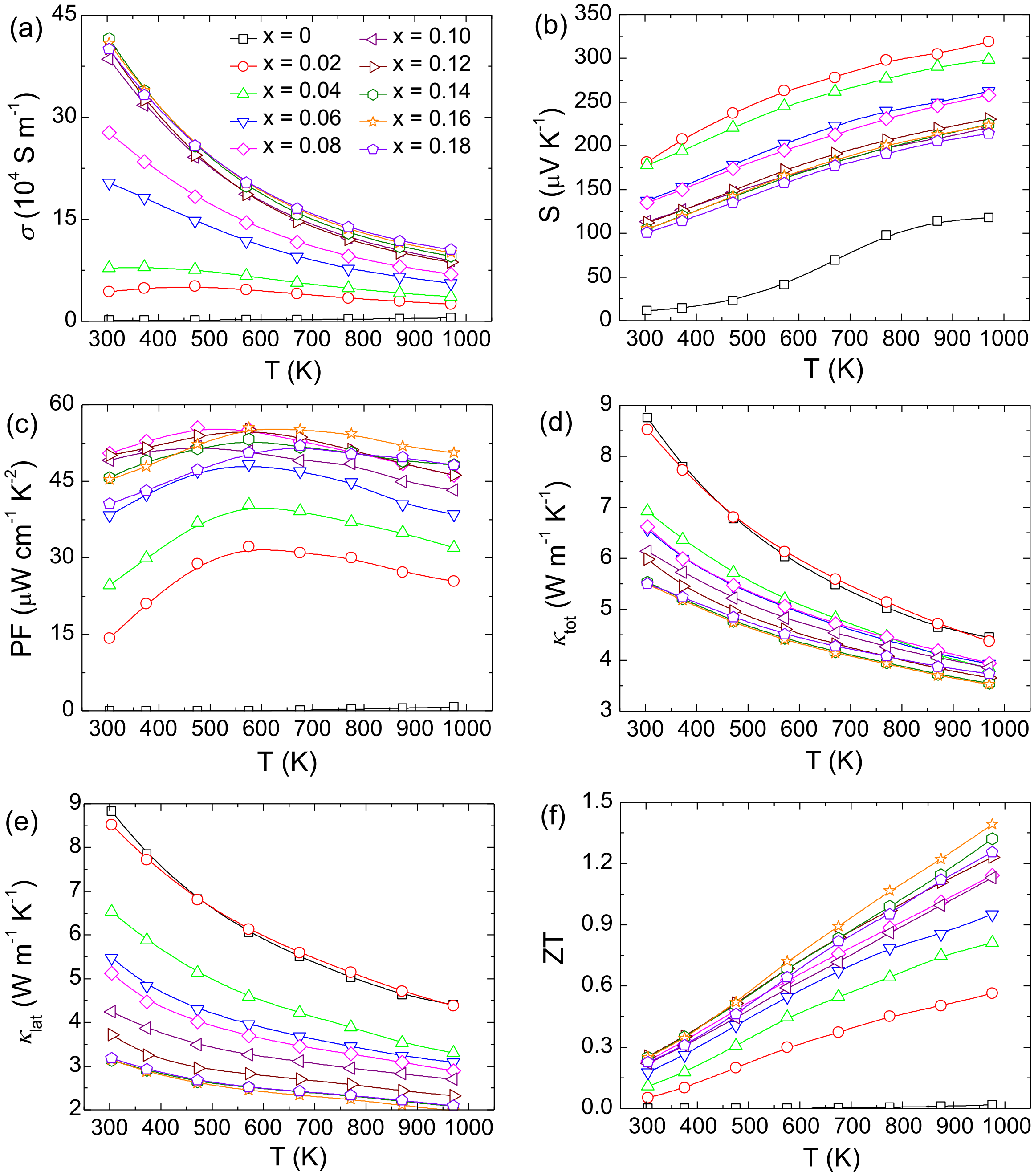
Supplementary Figure 1. STEM image of the prepared TaFeSb half-Heusler. The $\left(2\bar{2}0\right)$ plane with a spacing of ~0.21 nm has been verified.



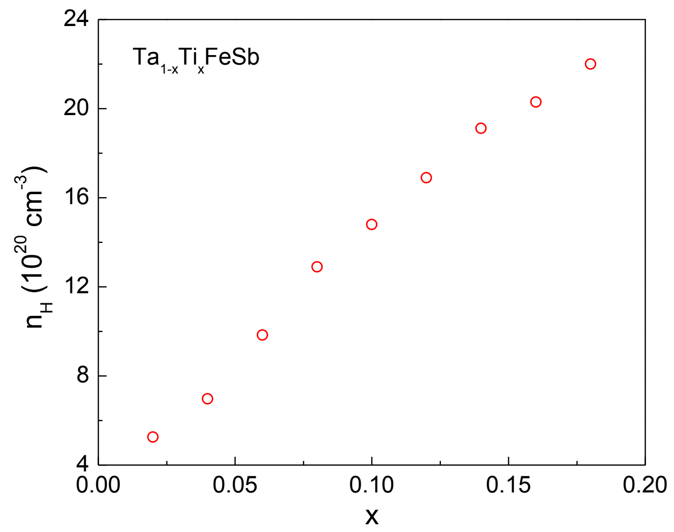
Supplementary Figure 2. Microstructures of the pristine TaFeSb half-Heusler. (a) and (b) Scanning electron microscopy images.



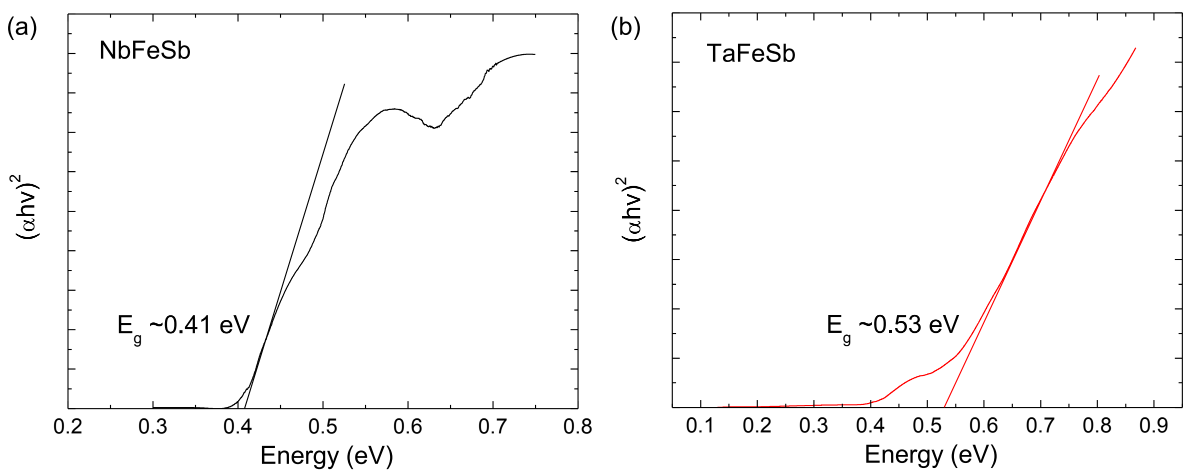
Supplementary Figure 3. Phase composition of TaFeSb-based half-Heuslers. XRD patterns of the prepared (a) $Ta_{1-x}Ti_xFeSb$ (x = 0, 0.02, 0.04, 0.06, 0.08, 0.10, 0.12, 0.14, 0.16, and 0.18) and (b) $Ta_{0.84-y}V_yTi_{0.16}FeSb$ (y = 0, 0.05, 0.10, and 0.15).



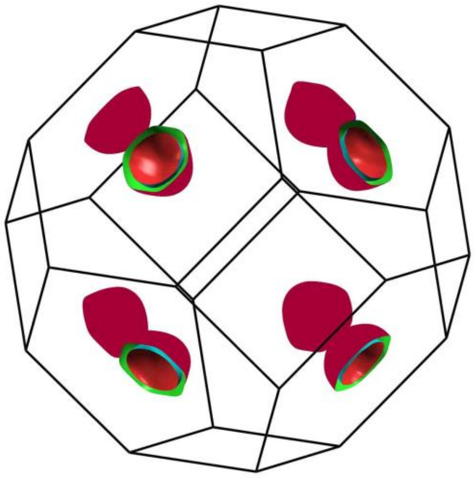
Supplementary Figure 4. Thermoelectric properties of $Ta_{1-x}Ti_xFeSb$ (x = 0, 0.02, 0.04, 0.06, 0.08, 0.10, 0.12, 0.14, 0.16, and 0.18). (a) Electrical conductivity, (b) Seebeck coefficient, (c) power factor, (d) total thermal conductivity, (e) lattice thermal conductivity, and (f) *ZT*.



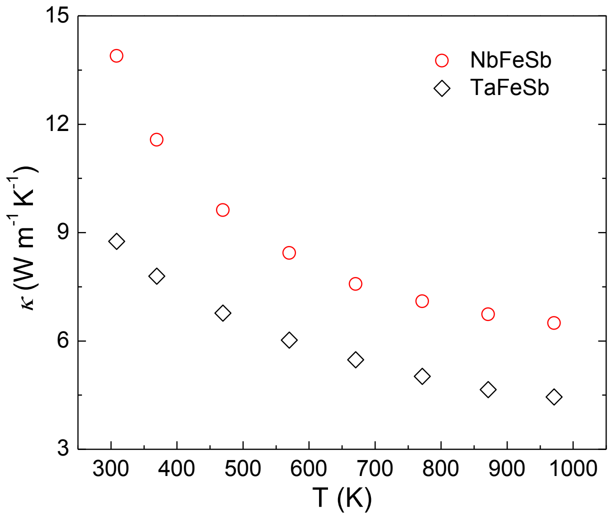
Supplementary Figure 5. Composition-dependent room-temperature hole concentration.



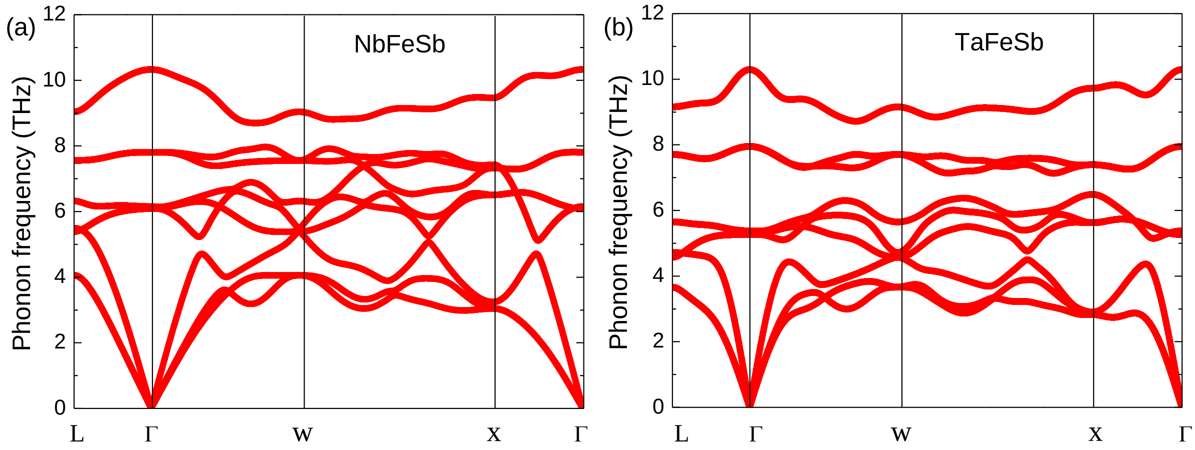
Supplementary Figure 6. Measured bandgap of the pristine (a) NbFeSb and (b) TaFeSb.



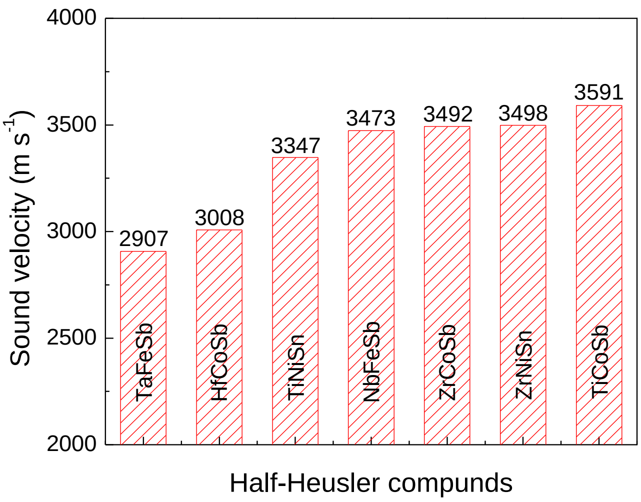
Supplementary Figure 7. The iso-energy carrier pockets of TaFeSb at 0.1 eV below the valence band maximum.



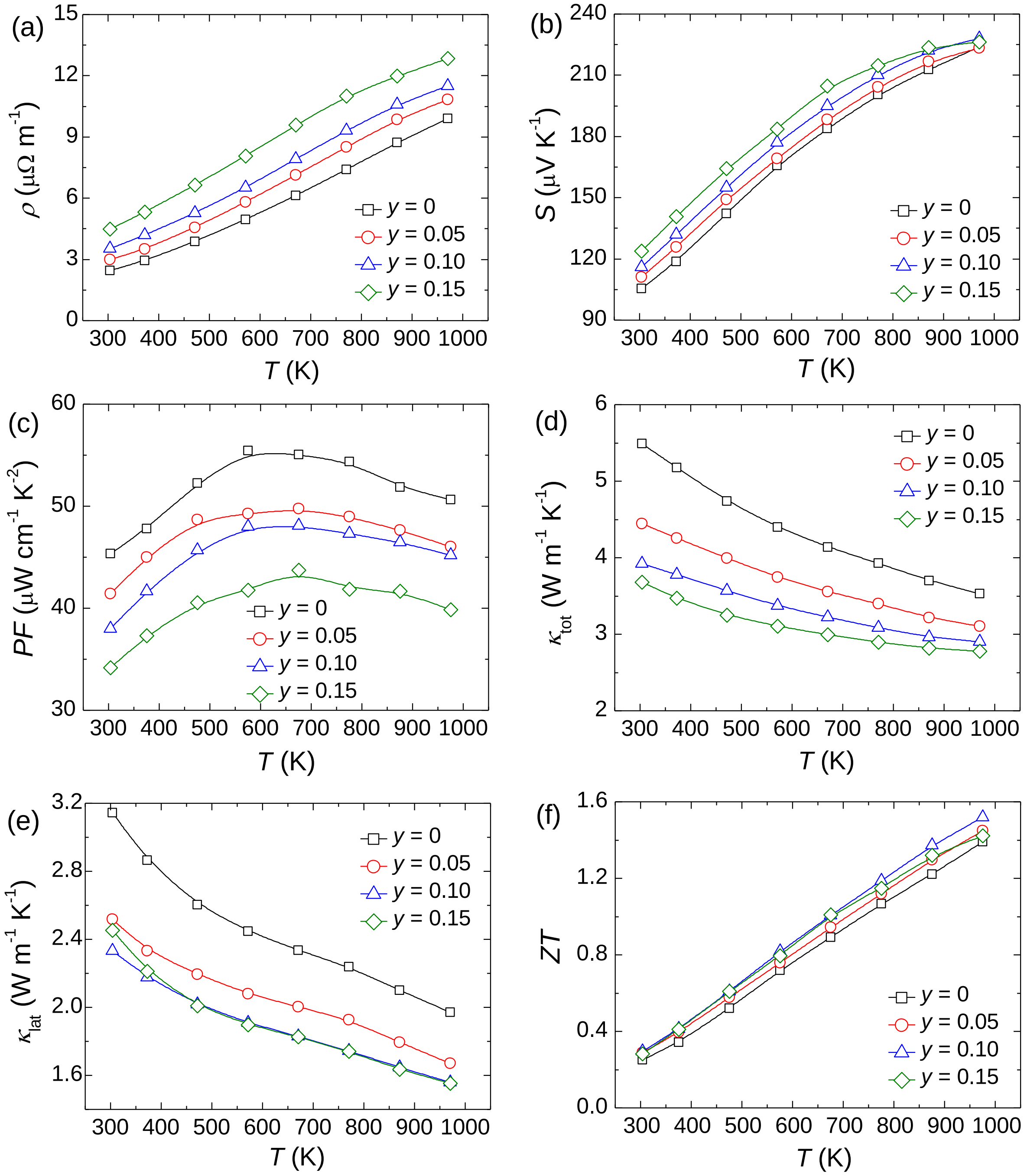
Supplementary Figure 8. The thermal conductivity of the undoped NbFeSb and TaFeSb. The samples are both prepared by the identical ball-milling and hot-pressing method.



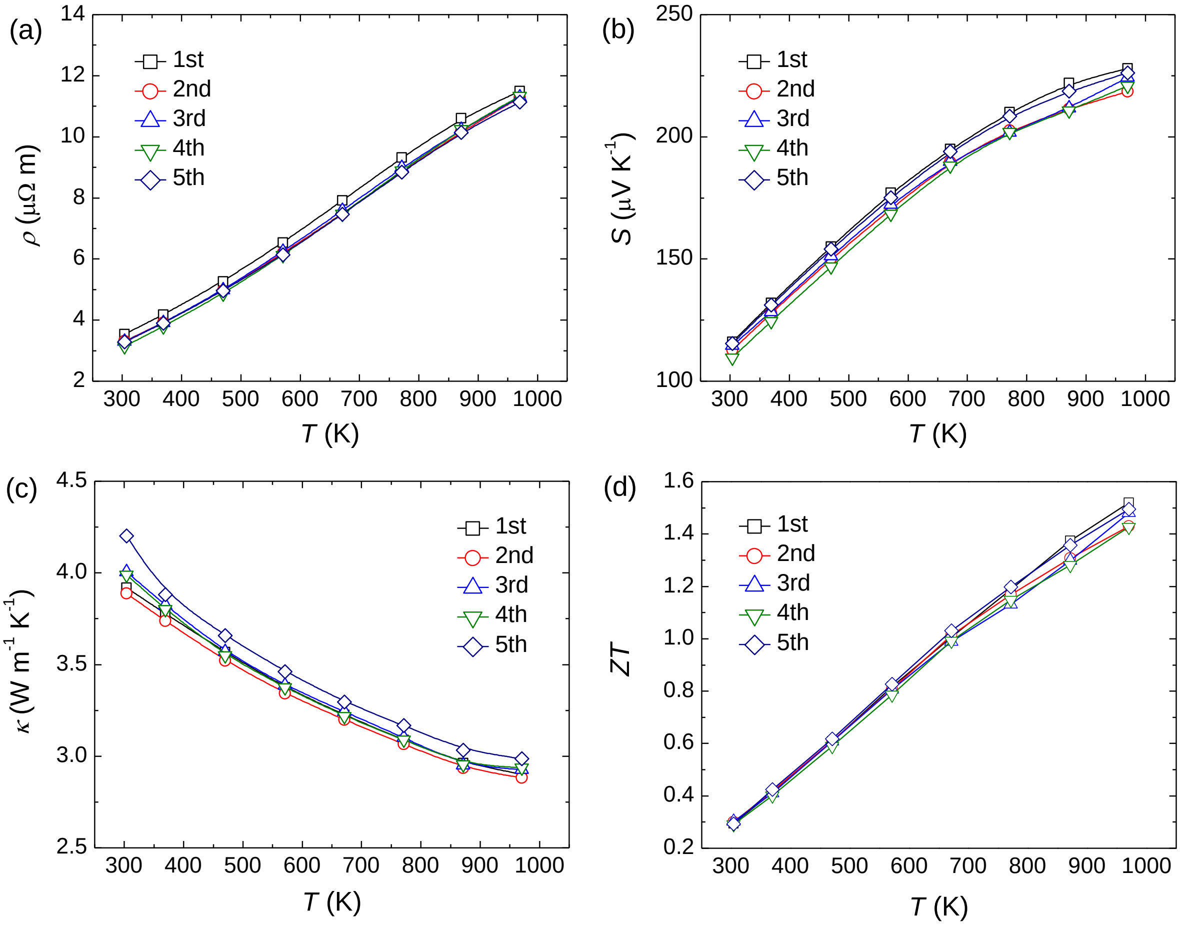
Supplementary Figure 9. Comparison of the phonon dispersion between (a) NbFeSb and (b) TaFeSb.



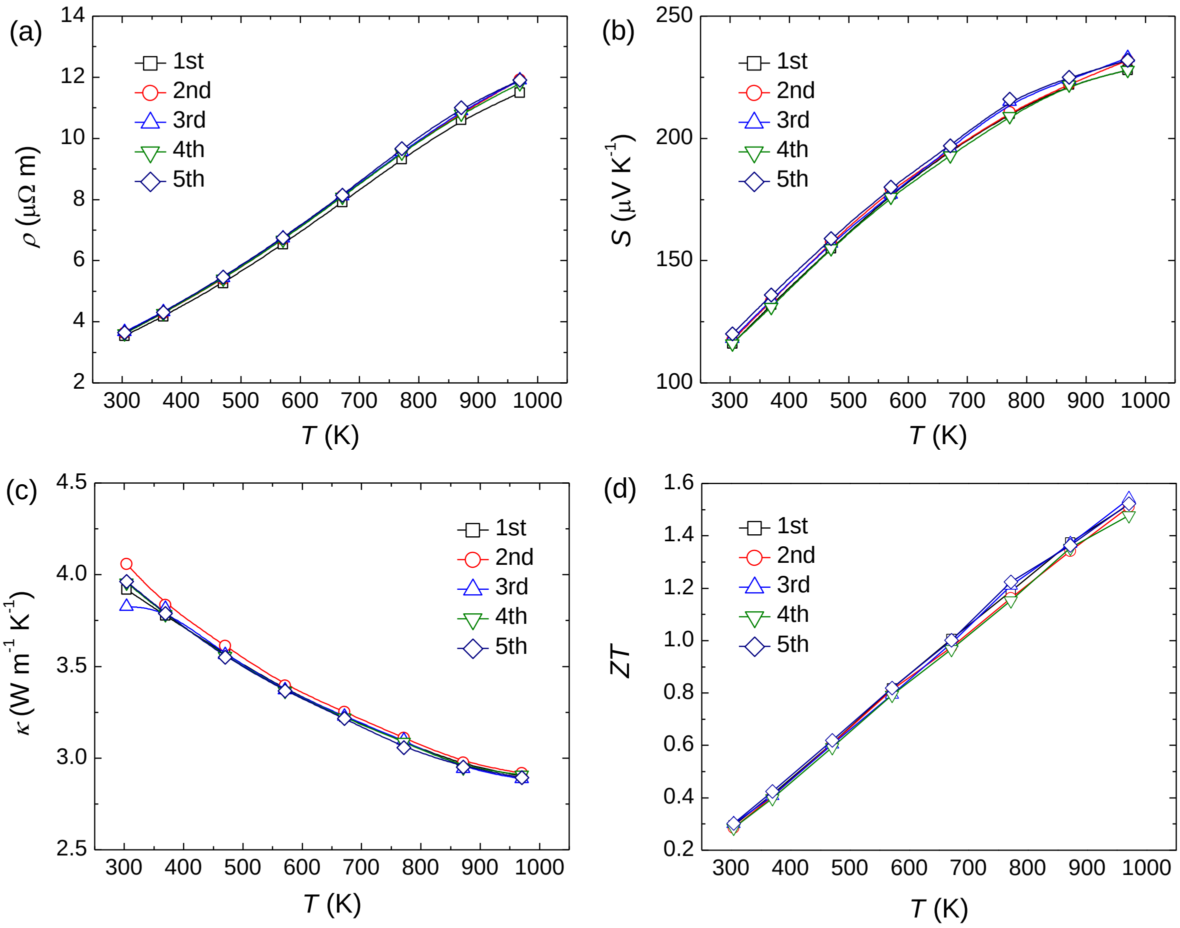
Supplementary Figure 10. Comparison of sound velocity between several half-Heusler compounds.



Supplementary Figure 11. Thermoelectric properties of $Ta_{0.84-y}V_yTi_{0.16}FeSb$ (*y* = 0, 0.05, 0.10, and 0.015). (a) Electrical resistivity, (b) Seebeck coefficient, (c) power factor, (d) total thermal conductivity, (e) lattice thermal conductivity, and (f) *ZT*.



Supplementary Figure 12. Reproducibility of the thermoelectric properties of $Ta_{0.74}V_{0.1}Ti_{0.16}FeSb$. Five different batches of $Ta_{0.74}V_{0.1}Ti_{0.16}FeSb$ were prepared and the thermoelectric properties of the specimens were then characterized. (a) Electrical resistivity, (b) Seebeck coefficient, (c) thermal conductivity, and (d) *ZT*.



Supplementary Figure 13. Thermal stability of $Ta_{0.74}V_{0.1}Ti_{0.16}FeSb$. Thermoelectric properties of the same $Ta_{0.74}V_{0.1}Ti_{0.16}FeSb$ specimen measured five times. (a) Electrical resistivity, (b) Seebeck coefficient, (c) thermal conductivity, and (d) *ZT*.