— Supporting Information —

The effects of $Yb_{11}Sb_{10}$ and $Yb_{10}MnSb_9$ secondary phases on the high performing thermoelectric material $Yb_{14}MnSb_{11}$

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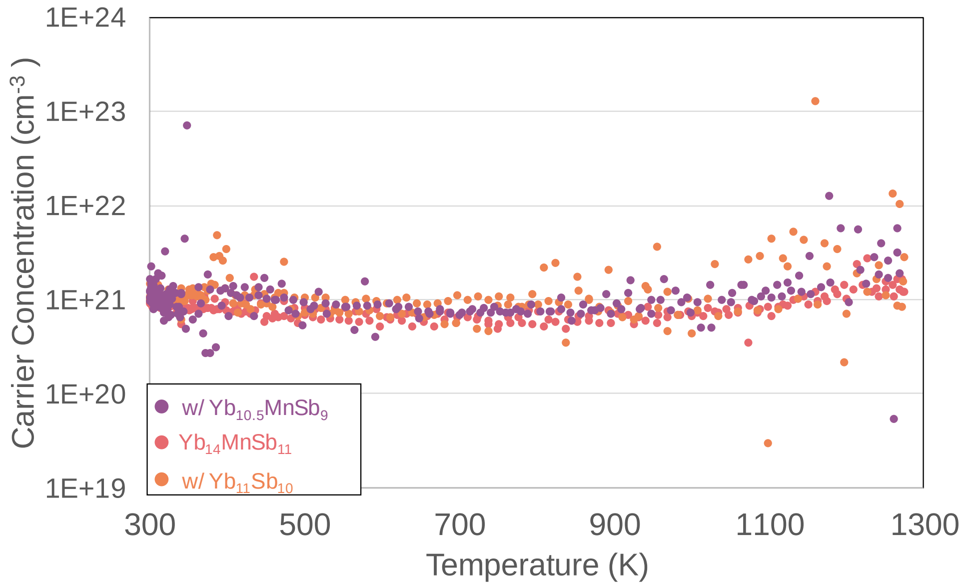

Figure S1: Plots of the carrier concentration as measured at JPL up to 1278K for all three samples. All samples have roughly similar carrier concentrations within the error of the measurement around 1 $\times 10^{21}$ cm^{-3}

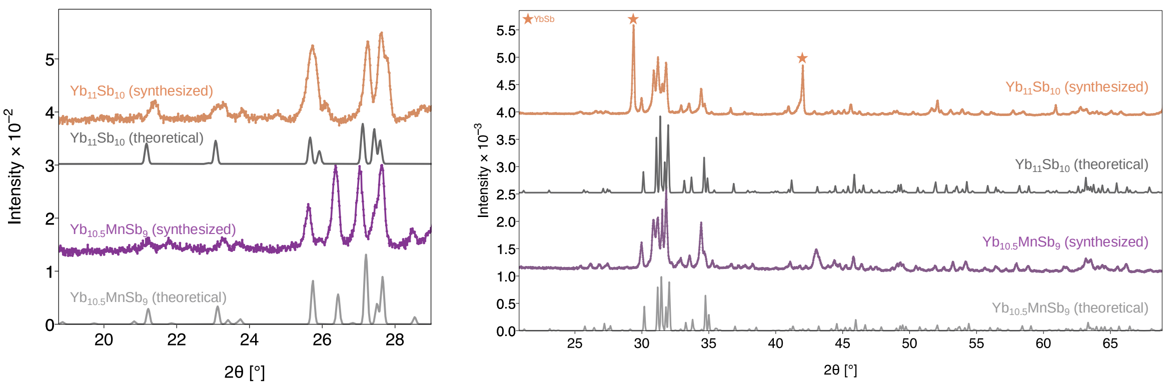

Figure S2: X-ray diffraction patterns for synthesized $Yb_{11}Sb_{10}$ and $Yb_{10}MnSb_9$ pellets that were crushed and added to 14-1-11 powder for samples with purposeful addition of secondary phases. The subfigure on the left shows the low angle zoomed in region, clearly showing that the $Yb_{11}Sb_{10}$ sample does not contain the additional peaks that are seen in the $Yb_{10}MnSb_9$, validating the successful formation of the correct phases. The subfigure on the right depicts longer range XRD pattern. Here it can be seen that the as-synthesized $Yb_{11}Sb_{10}$ material has two starred peaks corresponding to the YbSb phase. However, this YbSb phase is calculated to be unstable (has a formation energy above the Hull[1,2]) and does not appear in the final synthesized 14-1-11 sample with powder added from this pellet. These samples were studied in greater detail in a previous study[3]

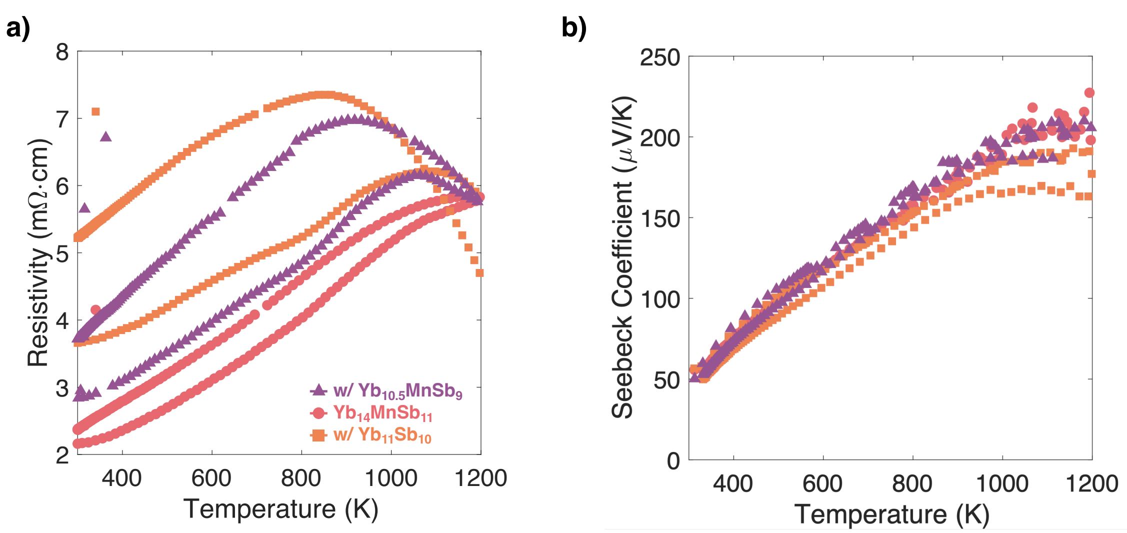

Figure S3: Transport curves both in heating and cooling for electrical resistivity (a) and Seebeck coefficient (b) measured at NASA JPL. The main text includes averaged curves (Figure 6a and b). While there is some hysteresis it is not significant and does not change the conclusions of the work.

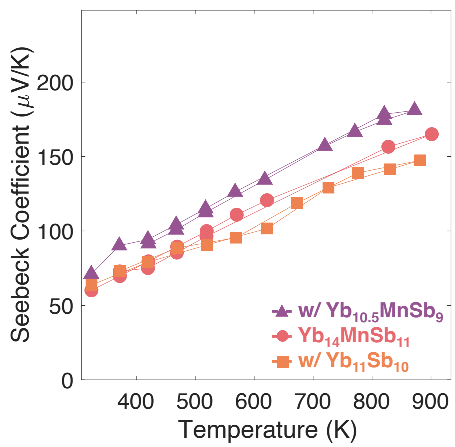

Figure S4: Complete data set in heating and cooling for Seebeck data shown as average points in the main text (Figure 6b). Very little hysteresis was observed.

References

(1) Jain, A.; Ong, S. P.; Hautier, G.; Chen, W.; Richards, W. D.; Dacek, S.; Cholia, S.; Gunter, D.; Skinner, D.; Ceder, G.; others Commentary: The Materials Project: A materials genome approach to accelerating materials innovation. *APL materials* **2013**, *1*.

(2) Jain, A.; Hautier, G.; Ong, S. P.; Moore, C. J.; Fischer, C. C.; Persson, K. A.; Ceder, G. Formation enthalpies by mixing GGA and GGA+U calculations. *Physical Review B—Condensed Matter and Materials Physics* **2011**, *84*, 045115.

(3) Borgsmiller, L.; Toriyama, M. Y.; Snyder, G. J. $Yb_{11}Sb_{10}$ and $Yb_{10}MnSb_9$ Small Change in Structure Leads to Profound Differences in Thermoelectric Properties Investigated Using Zintl Concepts. *Chemistry of Materials* **2024**,