

Is Cu_3SbSe_3 a promising thermoelectric material?

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Figures S1-S3 demonstrate the electrical resistivity, Seebeck coefficient, power factor and thermal conductivity measured first (black squares) and second (red circles) times for samples Q-A-HP, MA-HP and MA-HP-A, respectively.

It is seen that for Q-A-HP (with the highest phase purity) and MA-HP-A, the data repeatability is satisfactory, suggesting good thermal stability of the two kinds of samples that have been subjected to an annealing process. For them, the combined or the average data from both measurements were adopted in the manuscript.

For MA-HP, however, after a measurement up to 650 K, severe reduction in density from 6.12 to 4.93 g/cm³ occurred, causing a great decrease in thermal conductivity. It is interesting to note that the value of thermal conductivity of MA-HP by the second measurement is similar to that of MA-HP-A. It is also seen that the upturn of electrical resistivity around 450 K associated with the phase transition appeared in the second measurement, but did not occur in the first one. In fact, a cycle of measurement to high temperatures can be regarded as an annealing process. As a result, for MA-HP, we only used the data of the first measurement.

It seems safe to argue that samples' thermal stability can be maintained with a proper annealing treatment. Nonetheless, for Cu_3SbSe_3 good thermal stability is not expected at high temperatures for a long time. This is partly evidenced by the low density of the annealed samples.

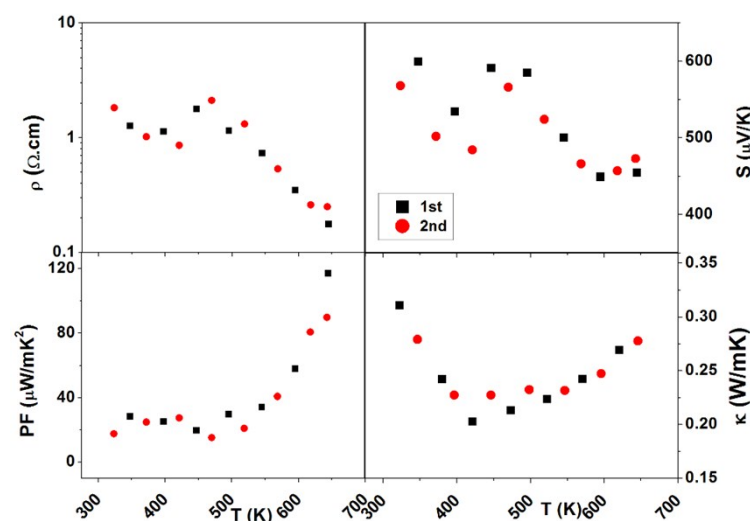


Fig. S1 Repeated measurements of thermoelectric transport properties of Q-A-HP

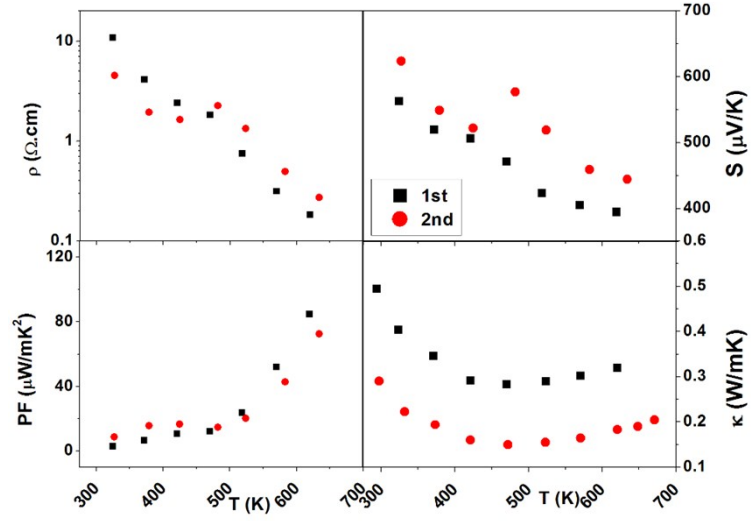


Fig. S2 Repeated measurements of thermoelectric transport properties of MA-HP

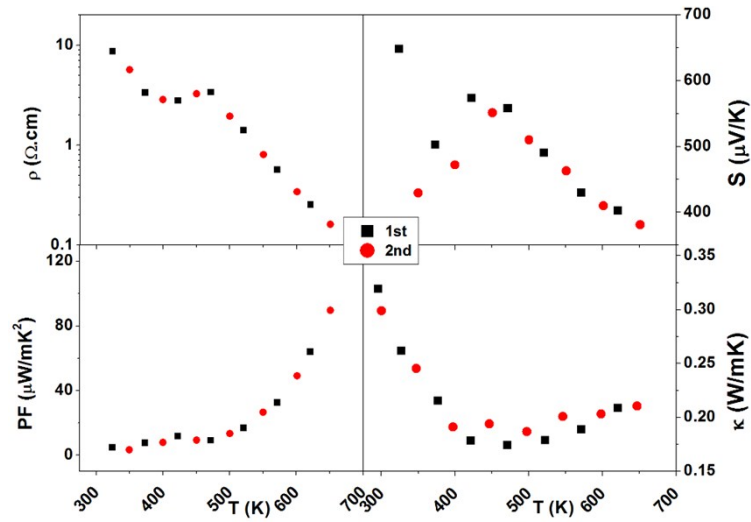


Fig. S3 Repeated measurements of thermoelectric transport properties of MA-HP-A