†Electronic Supplementary Information (ESI) available here:

Thermoelectric properties of Cu_3SbSe_3 with intrinsically ultralow lattice thermal conductivity

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This supporting information includes:

EDAX analysis
XPS analysis

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EDAX analysis

Figure S1 shows the EDXS of the chosen region which only exhibits the peaks corresponding to Cu, Se and Sb and shows a composition close to the stoichiometric value.

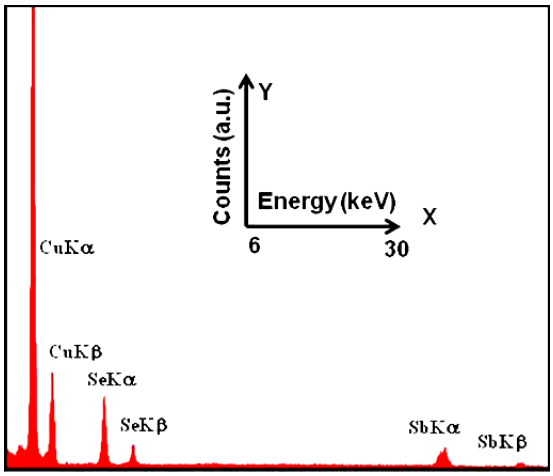

Fig. S1. EDXS pattern with X-axis: 6 to 30 keV, Y-axis: intensity (counts, arb. units).

X-ray photoelectron spectroscopy (XPS)

X-ray photoelectron spectroscopy (XPS) measurements were carried out in an ultra-high vacuum multi-probe surface analysis system with base pressure of 4 x 10^{-11} Torr. The chamber is equipped with an Omicron EA 125 electron energy analyzer and monochromatic Al K_α (1486.7 eV) X-ray source. Sample was mounted using conducting silver epoxy. All binding energies have been referenced to the Fermi edge of an Ar^+ sputtered clean polycrystalline Ag sample. Currently, XPS has been used to investigate the surface chemical composition of the Cu_3SbSe_3 sample and Fig. S2 shows the XPS survey spectrum of a clean Cu_3SbSe_3 surface over large binding energy range wherein the Tougard method was used to subtract background due to secondary electrons. All the features in survey spectra have been identified as indicated in the Fig. S2. Repeated *in-situ* mechanical scrapping of the sample resulted in contamination free surface as can be seen from the

absence of C (KVV) and O ($KL_{23}L_{23}$) Auger features. For clean surface, only Cu, Sb and Se related features are observed in the survey spectrum which confirms the purity of the sample and we have used Cu *3p*, Se *3d* and *Sb 4d* core levels to calculate the surface chemical composition. Area under the core levels were normalized with respective photoemission cross section, inelastic mean free path and analyzer transmission function. Surface chemical composition, determined using these normalized area ratios, was found to be very close to the actual stiochiometric value.

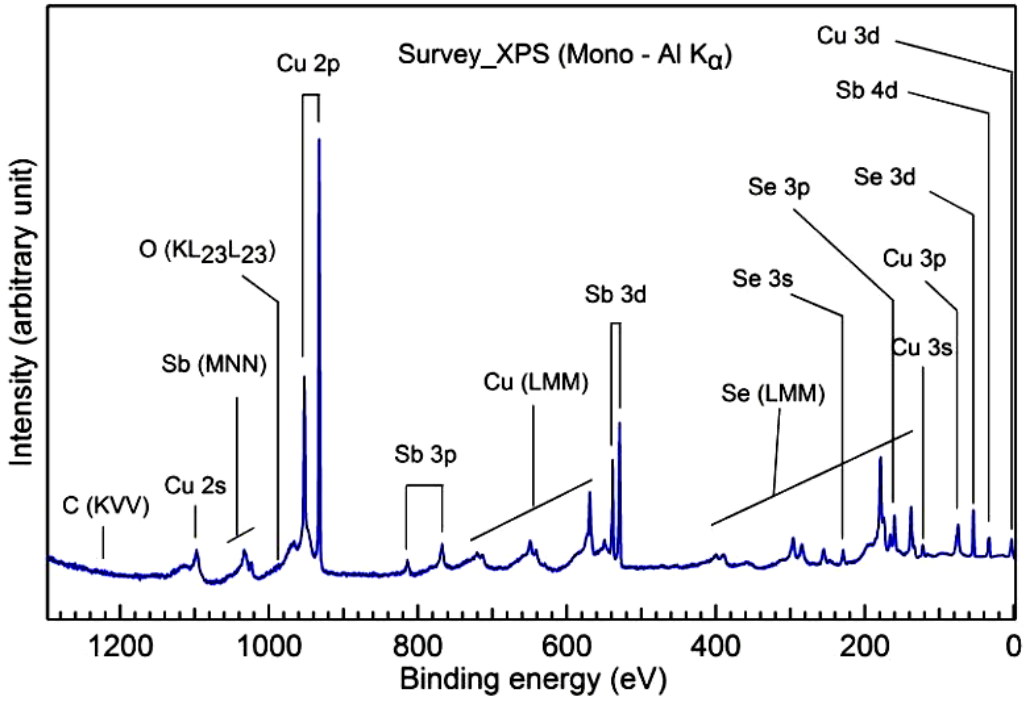

Fig. S2. X-ray photoemission spectrum over a wide binding energy range for clean surface of Cu_3SbSe_3. All the features in the spectrum are identified.