**Supplementary Material**

**Thermoelectric figure of merit and thermal conductivity of Type-I clathrate alloy nanowires**

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Clathrates of type-I have cubic structure with space group *Pmn*. The relaxed structure of cubic clathrates Ba8Cu6Si40 and Ba8Cu6Ge40 are obtained using VASP1 with PBE correlation functional2. Energy cut off was set to 300.0 eV and k-mesh was converged with k-points 4×4×4. The lattice constant of the cubic clathrates comes out to be 10.38 .

The phonon dispersion of the type-I clathrates Ba8Cu6Si40, Ba8Cu6Ge40 and diamond-Si structures have been calculated using PHONOPY3. The phonon band structure of Ba8Cu6Si40, Ba8Cu6Ge40 is shown in the Figure S1.

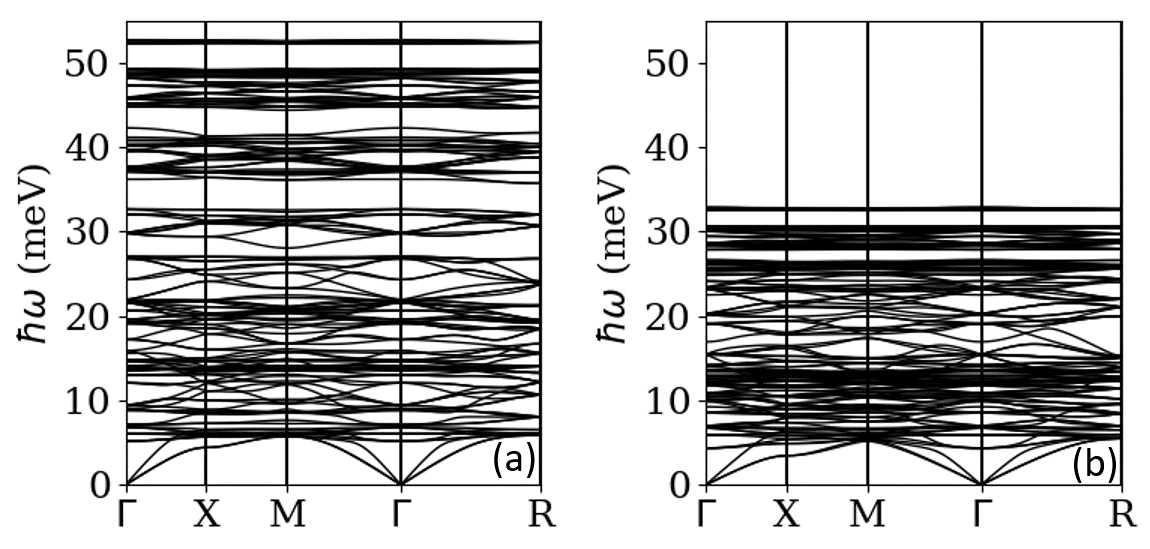


Figure S1. Phonon band structure along high symmetry direction for (a) Ba8Cu6Si40 and (b) Ba8Cu6Ge40.

The electronic transport coefficients were calculated using the Boltzmann transport equation coded in BoltzTraP software4. The data was fitted with the concentration of experimental alloy5. The concentration of Ba8Cu6Si40 and Ba8Cu6Ge40 was chosen to fit the data was 1.12×1021 cm-3 and 1.57×1021 cm-3 respectively. The relaxation time fitted with the experimental data4 was 1.8 ×10-15 s.

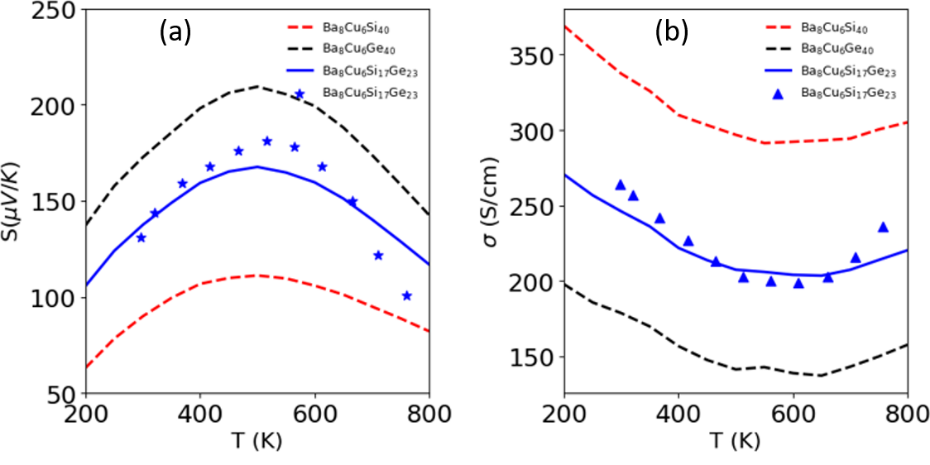


Figure S2. (a)Seebeck coefficient and (b)Electrical conductivity data for Ba8Cu6Si40, Ba8Cu6Ge40 and Ba8Cu6Si17Ge23

The calculation of Seebeck coefficient and electrical conductivity for Ba8Cu6Si40, Ba8Cu6Ge40 and Ba8Cu6Si17Ge23 is shown in Figure S2. The data is sufficiently matching with the experimental data for alloy5. The calculation of Seebeck coefficient and electrical conductivity for alloy is done using virtual crystal approximation as done in Ref.6.\

The figure of merit for the alloy is calculated according to the formula as used in Ref.6,

(1)

where x is the fractional concentration of the pure compound A and rest is of the other pure compound B. In the numerator, the and are power factors for compound A and B respectively. The denominator is total thermal conductivity of clathrate alloy comprising of phonon and electron part as = + . The value of figure of merit for bulk and nanometer size is shown in the Figure S3. The value of figure of merit for bulk clathrate alloy is around 0.17 at temperature ~400K with total thermal conductivity 1.18 W/m-K.

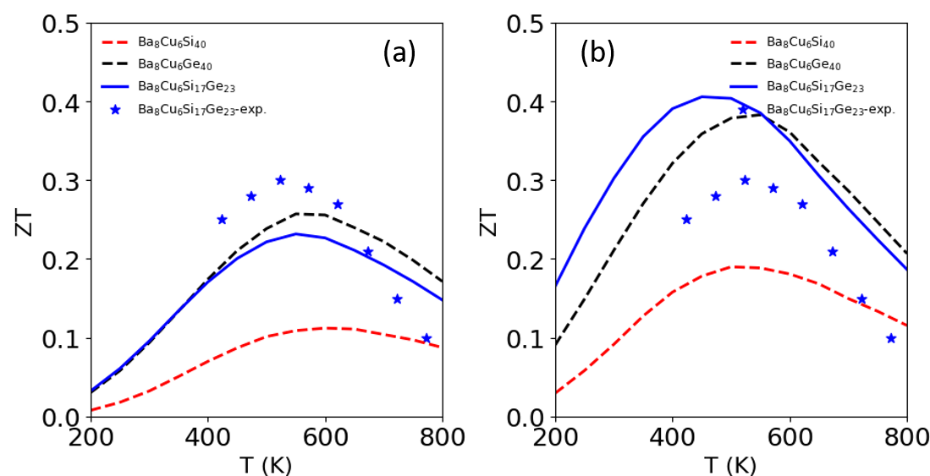


Figure S3. Figure of merit (ZT) with temperature for Ba8Cu6Si40, Ba8Cu6Ge40 and Ba8Cu6Si17Ge23 for (a)Bulk and (b)30nm

In the 30nm size, the total thermal conductivity reduces to 0.51 W/m-K. This reduction in thermal conductivity increases the figure of merit to 0.39 at 400K. This increase in figure of merit is more than 50%.

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