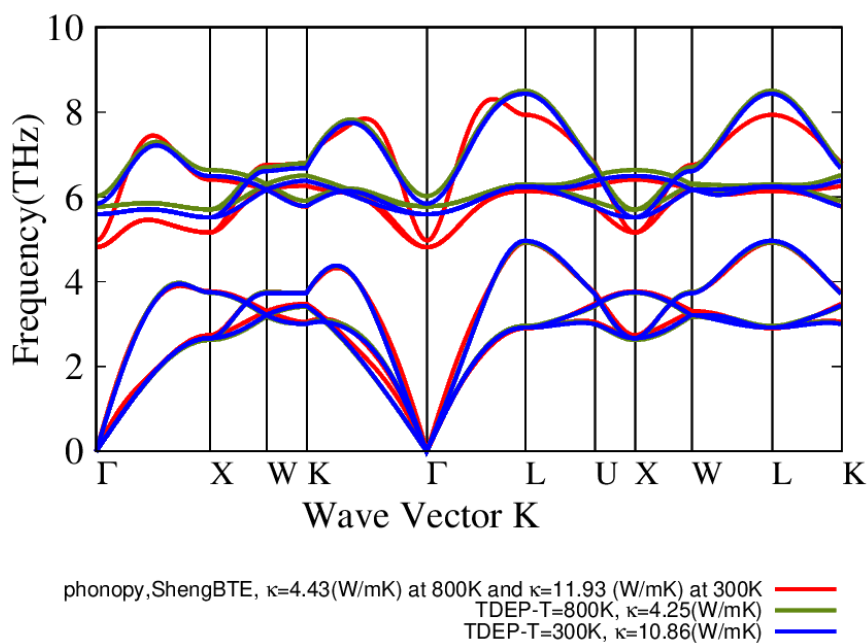


Supplementary information of
Anomalous mass dependence of phonon thermal transport in lanthanum monpnictides and its origin in the nature of chemical bonding

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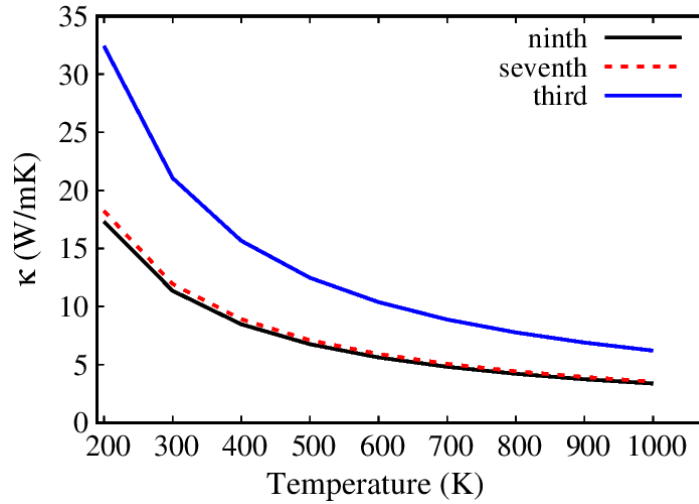
Here, we show convergence studies of the properties with respect to various parameters.

In Fig. S1 we show that including temperature dependence in the force constants does not affect much the phonon dispersion and the thermal conductivity.



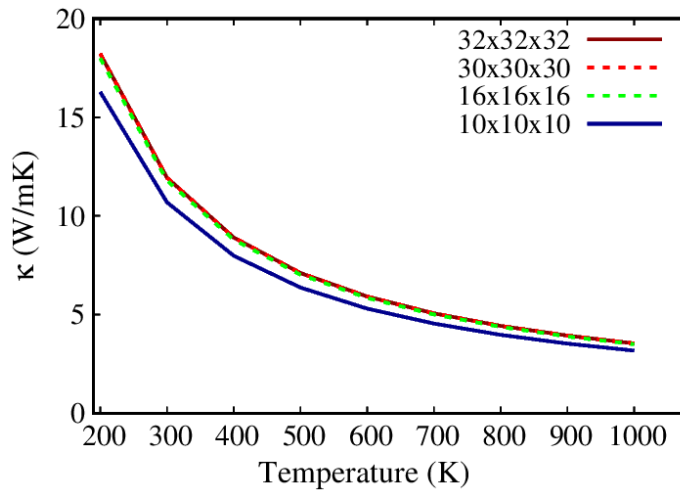
S1. Phonon dispersion curves for LaP are shown using Phonopy (red line) and the temperature-dependent effective potential (TDEP) at 300K (blue) and 800 K (gray). TDEP calculations at 300 and 800K show that the phonon dispersion is not much altered with temperature changes. Predicted thermal conductivities from TDEP and ShengBTE differ by 4% at 800K and by 9% at 300K.

In fig. S2, the convergence of the thermal conductivity with respect to the range of cubic force constants has been displayed.



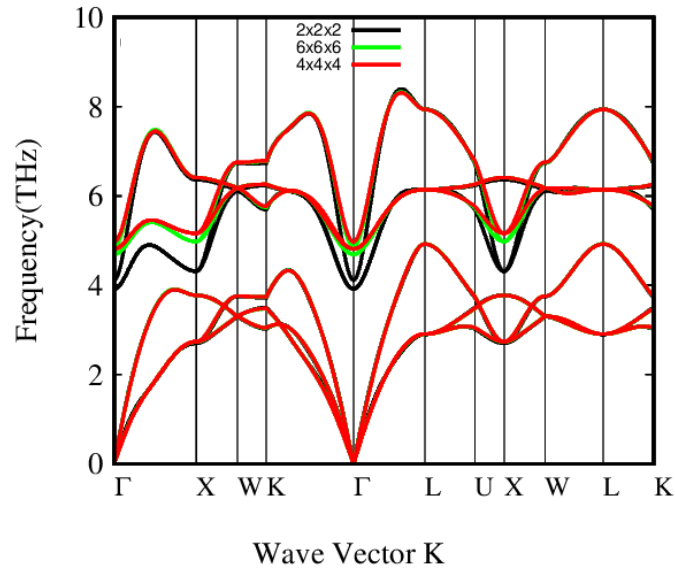
S2. Thermal conductivity as a function of the range of the cubic force constants versus temperature. It can be seen that the results are converged when up to 7th nearest neighbor shells are included. Including only up to third neighbors in cubic force constants produces a thermal conductivity that is twice larger.

In fig. S3, convergence of the thermal conductivity with respect to the size of mesh of kpoints has been displayed.



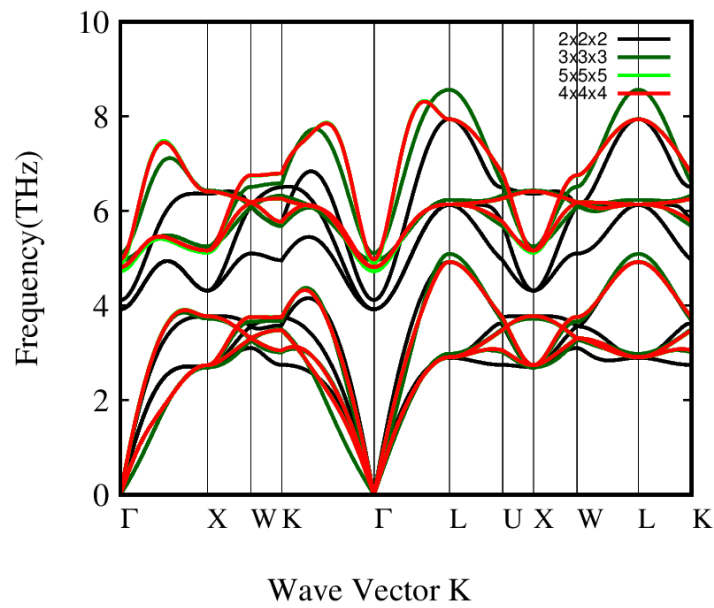
S3. Thermal conductivity as a function of the q-grid for solving the linearized phonon Boltzmann transport equation. The results seem converged for mesh sizes of 16 or above.

In fig. S4, convergence of the phonon dispersion with respect to the electronic kmesh size has been displayed.

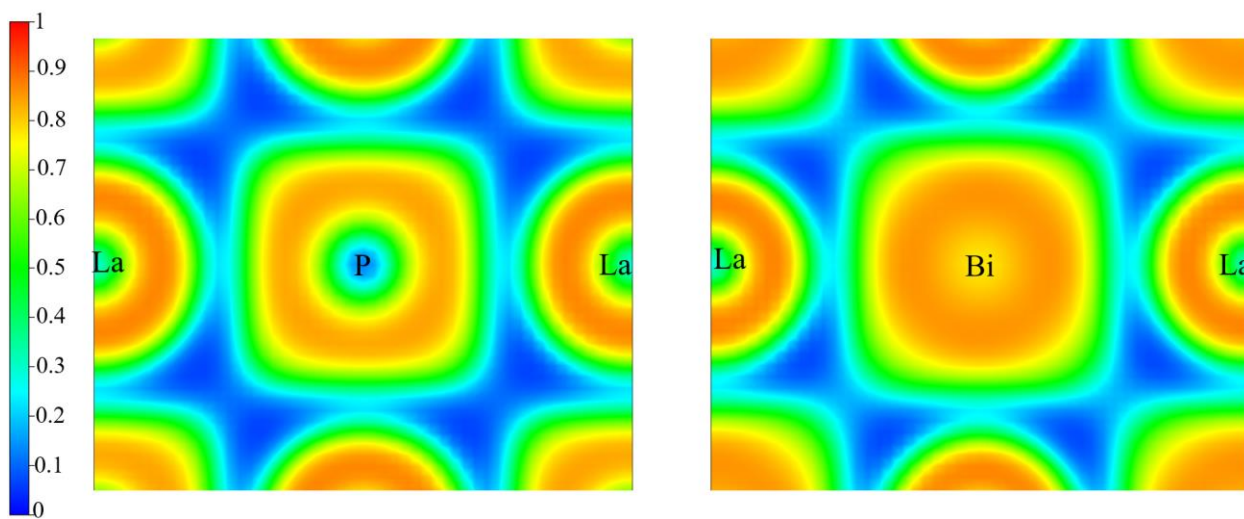


S4. Phonon dispersion curves as a function of k-points.

In fig. S5, convergence of the phonon dispersion with respect to the supercell size has been displayed.



S5. Phonon dispersion curves as a function of supercell size. A $4 \times 4 \times 4$ supercell produces converged results.



S6. Electron localization function (ELF) of LaP and LaBi. ELF values along the nearest neighbor bonds are almost the same (except at the end of the bond where atoms are different). Although LaP was shown to have a stronger metavalent character, its ELF can hardly be distinguished from that of LaBi.