Supplementary data

Theoretical Investigation of Lead Perovskite PbXO 3 (X=Ti, Zr and Hf) for Potential Thermoelectric Applications: Hybrid-DFT Approach

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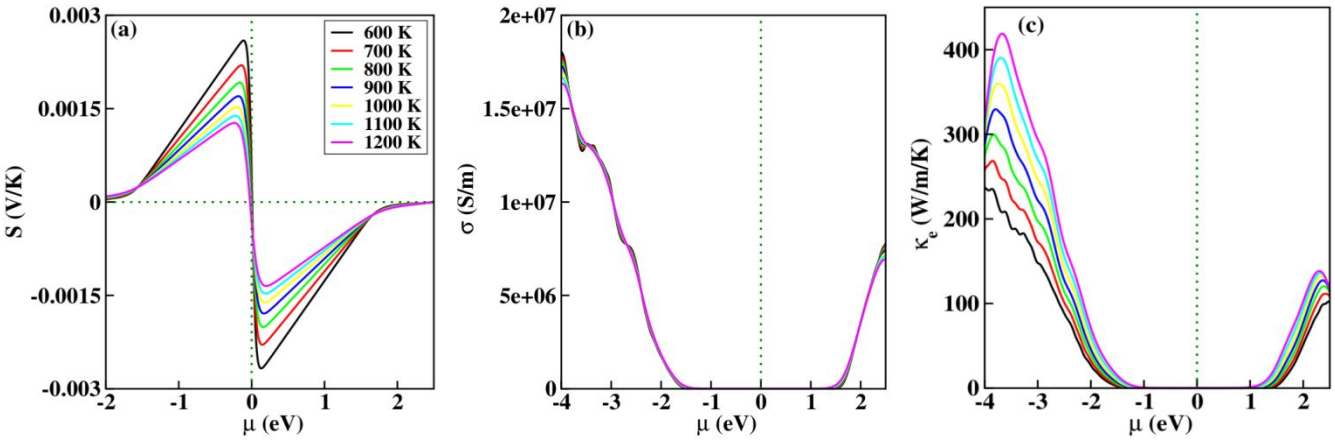

Fig. S1: Electron transport properties such as Seebeck coefficient (S), electronic conductivity ($\boldsymbol{\sigma}$) and electron thermal conductivity ($\boldsymbol{\kappa_e}$) for $PbTiO_3$ as a function of chemical potential generated from semiclassical Boltzmann transport theory (BoltzTrap) as implemented in CRYSTAL17-code.

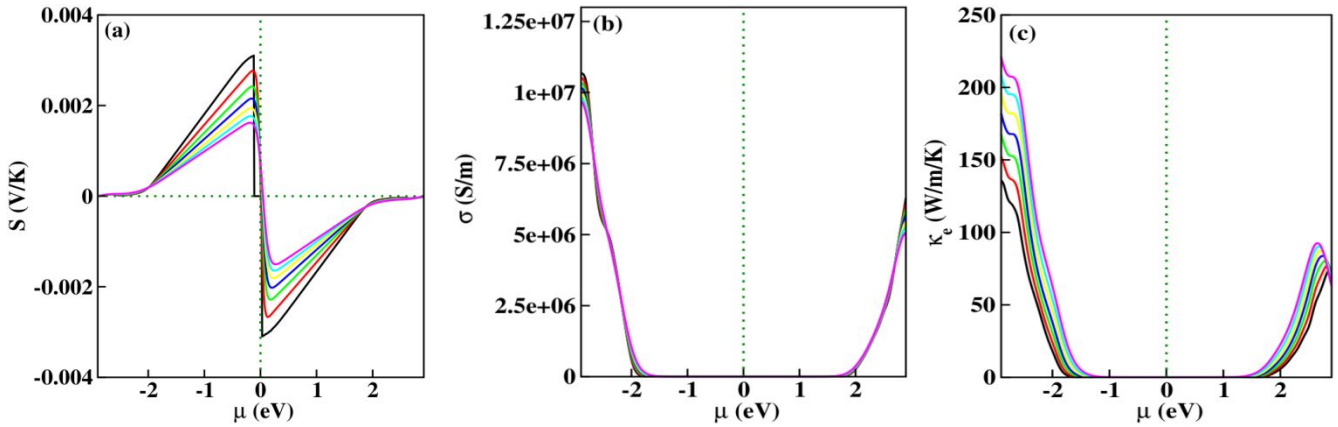

Fig. S2: Electron transport properties such as Seebeck coefficient (S), electronic conductivity (σ) and electron thermal conductivity (κ_e) for $PbZrO_3$ as a function of chemical potential generated from semiclassical Boltzmann transport theory (BoltzTrap) as implemented in CRYSTAL17-code.

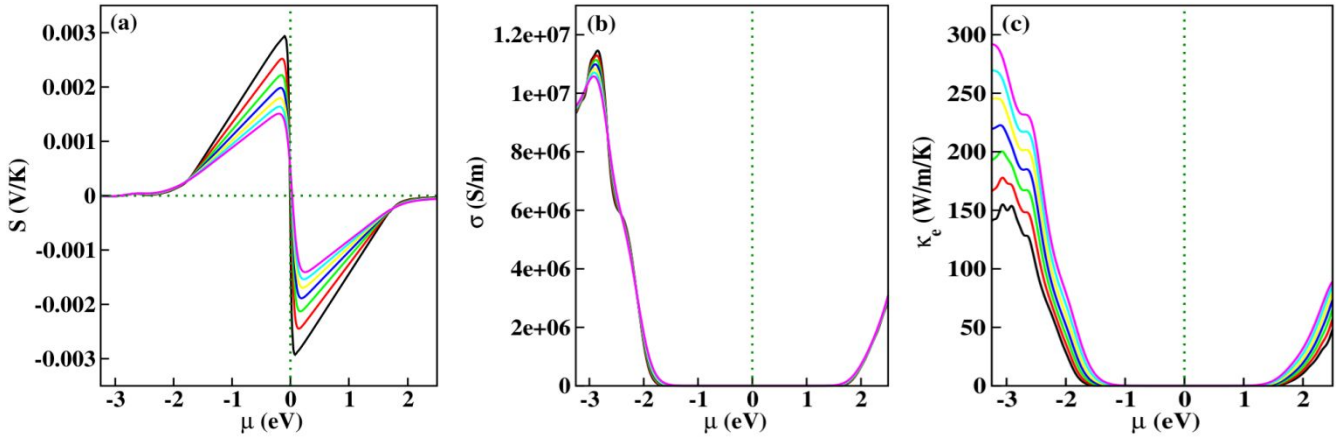

Fig. S3: Electron transport properties such as Seebeck coefficient (S), electronic conductivity (σ) and electron thermal conductivity (κ_e) for $PbHfO_3$ as a function of chemical potential generated from semiclassical Boltzmann transport theory (BoltzTrap) as implemented in CRYSTAL17-code.

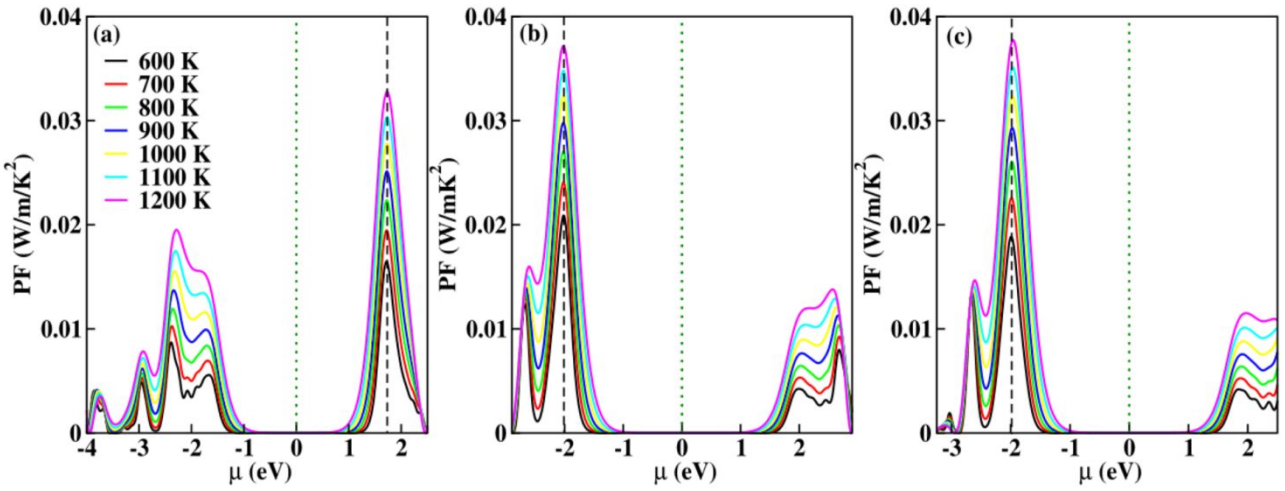

Fig. S4: Lattice part of thermal conductivity (κ_L) with respect to temperature (K) obtained from the extrapolation of experimental data presented by Tachibana *et al.* Calculated power factor (PF) (in W/m/K_2) with respect to chemical potential (μ) (in eV); (a) represents $PbTiO_3$, (b) represents PbZrO3 and (c) represents $PbHfO_3$. Here, the intersection point of black dotted line with the x-axis gives the optimum chemical potential for which the thermoelectric parameters are calculated as a function of temperature.

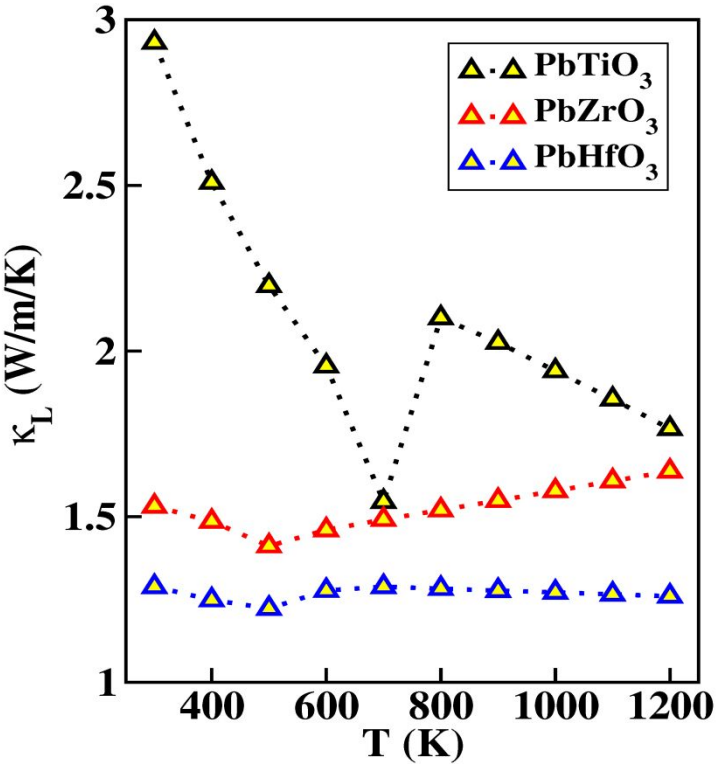

Fig. S5: Lattice part of thermal conductivity (κ_L) with respect to temperature (K) obtained from the extrapolation of experimental data presented by Tachibana *et al.*

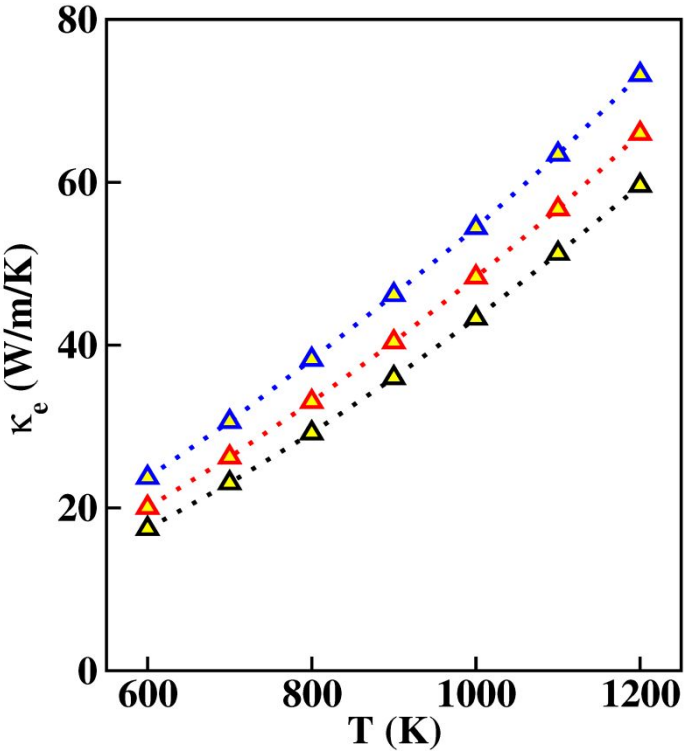

Fig. S6: Electronic part of thermal conductivity (κ_e) with respect to temperature (K) obtained at the optimum chemical potential.

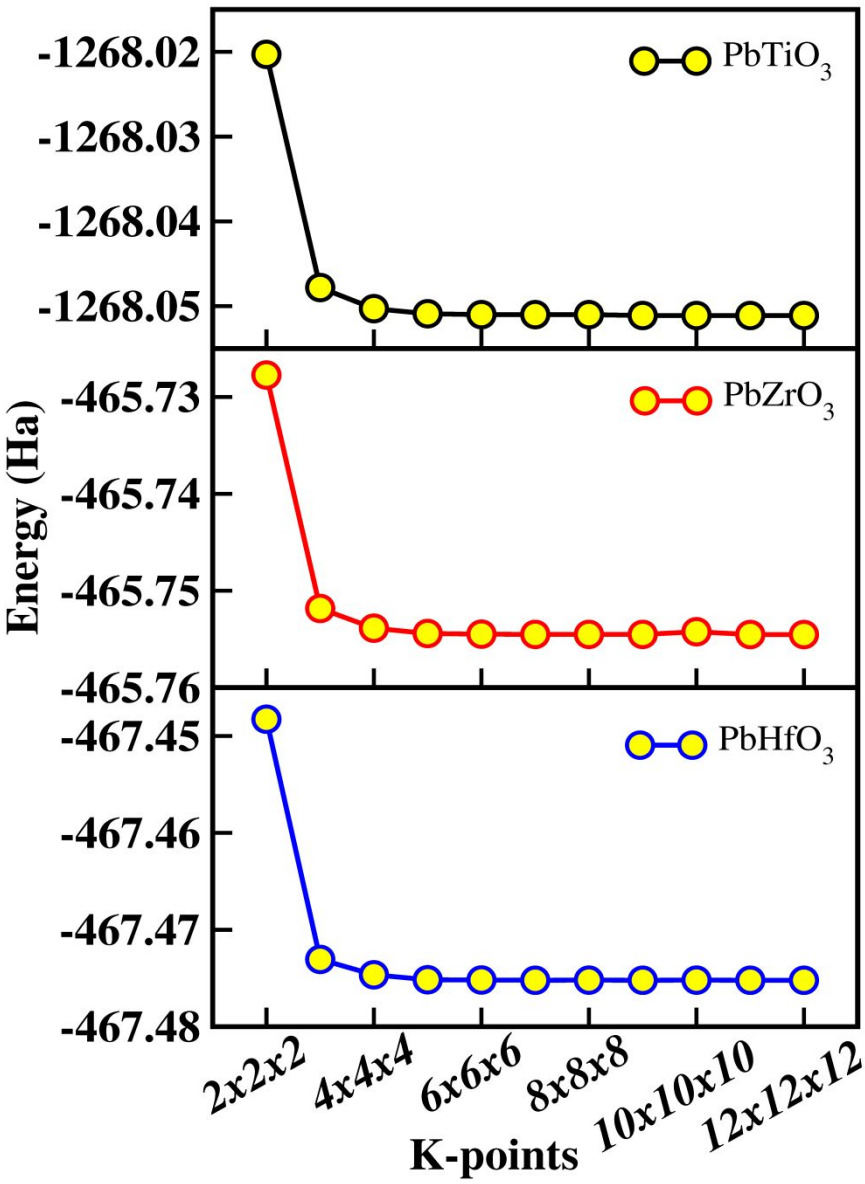

Fig. S7: Graphical representation for convergence results of k-mesh for all the investiagated materials.