PbTe/PbSe Thermoelectric Nanocomposites: The Impact of Length Modulations on Lowering Thermal Conductivity

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Dedicated to Prof. Mercouri Kanatzidis on the Occasion of his 65th Birthday

PbTe and PbSe are among the most promising thermoelectric materials used in the mid-temperature (400–900 K) power generation range. In these materials the efficiency increase in thermoelectric performance is critically related to the lowering of lattice thermal conductivity ($\kappa_L$), without compromising the electronic power factor. By means of state-of-the-art equilibrium molecular dynamics (EMD), we investigate heat transport in several nanostructured PbTe/PbSe models as a function of material morphology. Layered composites show a reduction of the average $\kappa_L$ of about 35% with respect to the bulk. The insertion of PbSe nanoparticles into a PbTe matrix, or viceversa PbTe into PbSe reduces $\kappa_L$ by up to 45% while in more anisotropic nanocomposites the reduction exceeds PbSe/PbTe alloys. Layered composites show the lowest lattice thermal conductivity in the direction of layer stacking, for which an optimal thickness is identified. Along this line we provide a full account of the impact of alloying and (sub)nanostructuring on heat transport for this important class of materials. Particularly anisotropic nano-dot morphologies and layered (sub)nanocomposites emerge as a paradigm for outstanding thermoelectric materials.

Introduction

The increased energetic demand and climate changes due to fossil fuel combustion call for an integral effort towards a sustainable development. Heat harvesting from battery packs, fuel cell modules or photovoltaic cells have become central for increased efficiency in energy conversion. Finding high-performance thermoelectric materials capable of directly and reversibly convert heat to electrical energy is therefore a task of top priority. The efficient control of thermoelectric energy conversion processes relies on the ability to assemble materials with tailored thermal transport properties. The thermoelectric efficiency at a given temperature ($T$) is expressed by a dimensionless figure of merit $ZT = S^2\sigma T/\kappa$. Here $S$ is the Seebeck coefficient, $\sigma$ is the electrical conductivity, and $\kappa$ is the thermal conductivity, which in turn is the sum of lattice and electronic contributions $\kappa = \kappa_L + \kappa_e$. This expression suggests a large Seebeck coefficient and high electrical conductivity as requirements for good thermoelectric materials, besides a low thermal conductivity. Nonetheless, these conditions cannot be immediately translated into a design strategy, mainly due to the interdependence of the physical parameters giving the $ZT$ expression.

In binary lead chalcogenides thermal conductivity is dominated by the lattice contribution ($\kappa_L$), while the electronic part remains comparatively small. In this class of compounds phonon scattering is typically achieved by impurity modes or alloying, which effectively lower thermal conductivity. PbTe is a good thermoelectric material in the so-called intermediate temperature regime (500–900 K, $ZT$ (600 K) $\approx$ 0.9). Single-crystalline PbTe nanowires grown by chemical vapor transport show reduced thermal conductivity. The thermal conductance of 180 nm diameter, micrometer long PbTe nanowire is around 11 mW/K at 300 K, $\sim$10$^4$ times smaller than that of an equally thick layer of bulk PbTe. Different from bulk compounds, nanocomposites, endotaxial precipitates, mesoscale grain boundary engineering and heterogeneous multiphase materials are emerging paradigms for a broader scatter-
presence of Tl impurity levels in p-doped PbTe leads to a doubling of ZT (ZT \sim 1.5) at 773 K \[^1\].

In PbTe-based materials the good thermoelectric performance is largely due to the low lattice thermal conductivity. However, Te is not only rare in the Earth’s crust but also increasingly used in a number of other applications, such as steel metallurgy, solar cells, phase change materials for digital recording, and thermoelectric cooling devices based on Bi\_xTe\_y. Attractive Te-free alternatives to rock-salt PbTe are the congeneric PbSe and PbS, which have remarkably similar electronic and structural properties \[^{19,20}\]. Furthermore, even if PbSe-based materials usually have a lower figure of merit in the mid temperature range (around 500 K) compared to PbTe, in doped PbSe the Seebeck coefficient does not exhibit the usual “turn-over” at high temperature, but keeps increasing even at 1000 K, thus making it a good alternative to PbTe especially at higher temperatures, owing also to its higher melting point \[^{20}\].

Despite existing paradigms, a controlled design of thermoelectric materials remains an involved task. Atomistic simulations may represent the method of choice towards a deeper understanding of the thermoelectric phenomenon, as they provide the necessary resolution for elucidating the impact of defects, the role of interfaces, nanostructuring and morphology \[^{21}\]. Furthermore, calculations can provide benchmark values to assist the difficult experimental task of measuring thermal transport, in particular in nanoscale materials \[^{22,24}\]. In this work, we investigate the atomistic details of (sub) nanostructuring on lowering thermal conductivity in PbTe–PbSe mixed systems, using solid solutions (alloys) as reference systems. We use equilibrium molecular dynamics (EMD) simulations to compute the thermal conductivity of several PbSe/PbTe systems. The systems considered are PbTe–PbSe solid solutions of different composition (PbTe\_0.25Se\_0.75, PbTe\_0.5Se\_0.5, PbTe\_0.75Se\_0.25), PbTe/PbSe layered superlattices (Figure 1a) and PbSe (PbTe) spherical precipitates of variable diameter embedded in a PbTe (PbSe) matrix (Figure 1b). The latter comprises spherical inclusions of different size (Figure 1c) and dense nano-dot geometries (“eight-in-a-box”) (Figure 1d).

**Methods**

The realistic modeling of materials strongly benefits from the use of empirical interaction potentials of simple analytical form, which allow the simulation of much larger systems over longer time scales, compared to methods based on first principles. For binary semiconducting materials a simple interatomic potential was shown to very reliably account for structural and elastic properties, and to be very accurate even in the description of phase transitions \[^{25}\]. Nevertheless, the restricted number of available parameters limits this approach. Additionally, parameters adapted to binary compounds must be transferable to mixed system, which is rarely the case. To provide suitable potentials for heat transport calculations in PbSe/PbTe, transferable potentials for the binary compounds PbSe and PbTe were parameterized. The interaction between the atoms was described by a sum of Lennard-Jones (LJ) and Coulomb terms:

\[
U_i(r_{ij}) = U_{Coul}(r_{ij}) + U_{LJ} = \frac{q_i q_j}{4 \pi \epsilon_0 r_{ij}} + 4 \epsilon_{ij} \left[ \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^6 \right]
\]

Here \(r_{ij}\) is the distance between atoms \(i\) and \(j\); \(\epsilon_{ij}\) and \(\sigma_{ij}\) are the LJ parameters; \(q_i\) and \(q_j\) are partial charges on atoms \(i\) and \(j\); and \(\epsilon_{ij}\) is the dielectric constant of vacuum. Only LJ coefficients of pairwise equal atoms are fitted, as cross terms were obtained from Lorentz–Berthelot mixing rules. For PbSe, an existing set of parameters was taken from literature \[^{26}\]. Therein, four LJ coefficients and partial charges (5 parameters in total) were fitted to lattice parameter and elastic constants. In this work \(\epsilon_{ij}\) LJ coefficients were refitted using the GULP \[^{27}\] code, to additionally reproduce the thermal conductivity \(\kappa_{ij}\) of PbSe at room temperature (300 K) and its temperature dependence (300–1200 K) \[^{28}\]. To construct transferable parameter sets, \(\epsilon_{ij}\) and \(\sigma_{ij}\) of Te were fitted on PbTe lattice and elastic constants using Pb parameters from PbSe, again ensuring that the parameter reliably accounted for PbTe thermal conductivity as known from experiment \[^{29}\].

Calculated elastic and lattice constants for both PbTe and PbSe bulk are in good agreement with previous results \[^{30,31}\]. The values of \(\kappa_{ij}\), at 300 K are 1.98 ± 0.07 W/mK (PbSe) and 1.69 ± 0.08 W/mK (PbTe), in good agreement with DFT/BTE calculations \[^{32}\] and experiments \[^{33,34}\]. Moreover the predicted temperature dependence of \(\kappa_{ij}\) compares very well with available reference experimental data (Figure 2) \[^{30,31}\]. The \(\kappa_{ij}\) of solid solutions is also closely reproduced (Figure S1). Details of the potential parameters and fitting procedures can be found in the supporting information.

The lattice thermal conductivity \(\kappa_{ij}\), was calculated using the Green-Kubo (GK) relation based on the fluctuation-dissipation theorem \[^{35}\]:

\[
\kappa_{ij} = \frac{1}{k_b V T} \int_0^\infty \langle J(t) \cdot J(0) \rangle \frac{3}{3} dt
\]

where \(k_b\) is the Boltzmann constant, \(V\) is the volume of the system, \(T\) is the temperature and \(\langle J(t) \cdot J(0) \rangle / 3\) is the heat current autocorrelation function averaged over three directions. The heat current vector for a pair potential is defined as:

\[
J = \sum_i N_i \varepsilon_i \mathbf{v}_i + \frac{1}{2} \sum_{i>j}^N (\sigma_{ij} \cdot \mathbf{v}_i)
\]

where \(\varepsilon_i\) and \(\mathbf{v}_i\) are the site energy and velocity associated with atom \(i\), respectively. The 3x3 tensor \(\sigma_i\) denotes the atomic virial stress.

**Results**

Different kinds of convergence tests have been performed. The truncation time \(\tau_{ij}\) chosen to evaluate the integral in the Green-Kubo relation in Eq. 2 was tested on a reference system,
Figure 1. (a) Layered structure of PbTe (in blue) and PbSe (in red) in their rock-salt modification. Layers are (from, left to right) 25, 12.5 and 6.25 Å thick. (b) Intercalated PbTe(Se) spheres in a PbSe(Te) matrix. Sphere radii are, from left to right 5, 10, 15 and 20 Å, respectively. (c) 25 Å and 15 Å radius spheres and (d) "eighth-in-a-box" spheres of 15 Å radius.

Figure 2. Predicted lattice thermal conductivity of bulk PbSe (a) and PbTe (b) in comparison with experimental counterpart values.\cite{30,31}
the solid-solution composition PbSe_{0.50}Te_{0.50} with 4096 atoms in the cell, considered in this work (see Figure S2 in the Supporting Information). After \( t_{\text{eq}} = 40 \) ps the values calculated for \( \kappa_z \) converged. Size-dependence effects were investigated as well. This is necessary as the small size of the simulation box may affect the computed value of the thermal conductivity. For semiconductors this is of relevance as low frequency phonons may have long mean free paths, which provide a significant contribution to \( \kappa_z \).

Supercells containing up to \( \sim 10^4 \) atoms, i.e. \( 4 \times 4 \times 4 \) replicas of the original nanostructured systems (\( \sim 10^3 \) atoms), were considered. The values calculated from supercells are equal within standard deviations (Figure S3), while linear regression lines are parallel in the size range considered, meaning that relative values of thermal conductivity for the different geometries may be already acceptable for small cells (4096), while in larger cells (\( \sim 10^4 \)) size effects become negligible. Top performing nanocomposites were therefore evaluated in a large simulation box containing 10648 atoms, as this size represents a viable compromise between size effect impact and computational efficiency (results are shown in Table 1). Nonetheless, systematic calculations in a small cell of 4096 atoms were used to identify trends towards best candidates, as it is summarized in Table S3. Accordingly, at 400 K the \( \kappa_z/\kappa_x \) ratio reaches 0.51 and at higher temperature it is close to 1, since increased anharmonic three-phonon scattering takes over phonon scattering at the interfaces. Nonetheless \( \kappa_z \) remains below the values of the PbTe_{0.50}Se_{0.50} alloy by as much as \( \sim 25\% \) (Figure S4a–c). In contrast with nano inclusion compounds \( \kappa_z \) is not a monotonic function of the superlattice spacing. The observed trends of \( \kappa_z \) as a function of size and dimensionality in PbTe and PbSe systems show analogies with Si/Ge superlattices. The best alloy as temperature is increased (Figure S4a–c). In both cases, for \( \sim 1 \) nm lattice spacing 2D geometries provide a more efficient reduction of \( \kappa_z \), but even lower thermal conductivity can be achieved using larger nano-dots. Similarly to Si/Ge systems the crossover of \( \kappa_z \) between 2D and 0D nanostructures occurs beyond \( 3 \) nm.

Although at room temperature alloys are competitive or even better than both systems with nano-inclusions and superlattices, the value of \( \kappa_z \) of bulk PbSe and PbTe and of nanostructured materials rapidly approaches the one of the best alloy as temperature is increased (Figure S4a–c). The lattice thermal conductivity of layered superlattices is strongly anisotropic at room temperature, as \( \kappa_z \) is markedly lower than \( \kappa_x \) (\( \kappa_z/\kappa_x \approx 0.5 \)). This anisotropy rapidly disappears as a function of temperature. Already at 400 K the \( \kappa_z/\kappa_x \) ratio reaches 0.51 and at higher temperature it is close to 1, since increased anharmonic three-phonon scattering takes over phonon scattering at the interfaces. Nonetheless \( \kappa_z \) remains below the values of the PbTe_{0.50}Se_{0.50} alloy by as much as \( \sim 25\% \) (Figure S4a–c). In contrast with nano inclusion compounds \( \kappa_z \) is not a monotonic function of the superlattice spacing. The observed trends of \( \kappa_z \) as a function of size and dimensionality in PbTe and PbSe systems show analogies with Si/Ge superlattices. In both cases, for \( \sim 1 \) nm lattice spacing 2D geometries provide a more efficient reduction of \( \kappa_z \), but even lower thermal conductivity can be achieved using larger nano-dots. Similarly to Si/Ge systems the crossover of \( \kappa_z \) between 2D and 0D nanostructures occurs beyond \( 3 \) nm.

The \( \kappa_z \) of samples with smaller nano-dots (radius from 0.5 to 1 nm) is of the order of that of bulk PbTe and PbSe, whereas a significant reduction of \( \kappa_z \) is obtained from larger nano-inclusions (1.5 or 2 nm, Table S3). The effect of enlarging the sphere diameter is more prominent in the case of PbTe spheres into a PbSe matrix than vice versa. A trend of lattice thermal

### Table 1. Average lattice thermal conductivity (300 K) computed for PbTe(PbSe) spheres into PbSe(PbTe) matrices, alloy (50/50 Te/Se) and 12.5 Å thick layered structure for systems containing 10468 atoms in the simulation box. Values are in units of W/mK. For sphere inclusions, the sphere-sphere distance is indicated. The distance \( d \) between two spheres is defined in Figure 3b.

<table>
<thead>
<tr>
<th>Sphere (Te in Se)</th>
<th>300 K</th>
<th>Distance ( d ) (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 Å radius</td>
<td>2.07 ± 0.06</td>
<td>55</td>
</tr>
<tr>
<td>15 Å radius</td>
<td>1.88 ± 0.09</td>
<td>45</td>
</tr>
<tr>
<td>20 Å radius</td>
<td>1.65 ± 0.05</td>
<td>38</td>
</tr>
<tr>
<td>25 Å radius</td>
<td>1.25 ± 0.06</td>
<td>24</td>
</tr>
<tr>
<td>30 Å radius</td>
<td>1.16 ± 0.03</td>
<td>13</td>
</tr>
<tr>
<td>“eight-in-a-box” 15 Å radius</td>
<td>1.04 ± 0.05</td>
<td>9</td>
</tr>
<tr>
<td>“different size”, 15 Å and 25 Å</td>
<td>1.45 ± 0.09</td>
<td></td>
</tr>
<tr>
<td>Sphere (Se in Te)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10 Å radius</td>
<td>2.94 ± 0.22</td>
<td>55</td>
</tr>
<tr>
<td>15 Å radius</td>
<td>2.47 ± 0.12</td>
<td>45</td>
</tr>
<tr>
<td>20 Å radius</td>
<td>2.21 ± 0.13</td>
<td>38</td>
</tr>
<tr>
<td>25 Å radius</td>
<td>1.75 ± 0.09</td>
<td>24</td>
</tr>
<tr>
<td>30 Å radius</td>
<td>1.33 ± 0.08</td>
<td>13</td>
</tr>
<tr>
<td>“eight-in-a-box” 15 Å radius</td>
<td>1.13 ± 0.08</td>
<td>9</td>
</tr>
<tr>
<td>“different size”, 15 Å and 25 Å</td>
<td>1.59 ± 0.06</td>
<td></td>
</tr>
<tr>
<td>Alloy</td>
<td></td>
<td></td>
</tr>
<tr>
<td>50%/50% Te/Se</td>
<td>1.06 ± 0.03</td>
<td></td>
</tr>
<tr>
<td>Layered, 12.5 Å</td>
<td></td>
<td></td>
</tr>
<tr>
<td>x</td>
<td>1.44 ± 0.07</td>
<td></td>
</tr>
<tr>
<td>y</td>
<td>1.47 ± 0.13</td>
<td></td>
</tr>
<tr>
<td>z</td>
<td>0.74 ± 0.03</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>1.22 ± 0.06</td>
<td></td>
</tr>
</tbody>
</table>
conductivity reduction as a function of size of embedded spheres is thus emerging (Figure S5). However, since cells of 4096 atoms limit the maximal host sphere radius to 2 nm, the investigation was extended to the larger cell of 10648 atoms. The trend of \( \kappa_L \) for sphere radii between 1 nm and 3 nm for different system sizes (4096 vs 10648) are compared in Figure S5. Enlarging sphere sizes has a reduced impact on lowering lattice thermal conductivity. The spacing between spheres is rather the relevant parameter here. Table 1 summarizes values of \( \kappa_L \) at ambient temperature (300 K) for large cell systems (10648): single sphere inclusions, two spheres with different size (Figure 1c) and “eight-in-a-box” PbSe(Te) nanocomposites in PbTe(Se) matrices (Figure 1d) are compared to the best-performing PbSe_{0.50}Te_{0.50} alloy with the same size. Narrowing the distance between nano-dots (as shown in Figure 3b) causes lattice thermal conductivity to decrease. With reference to Figure 3a, the trend of \( \kappa_L \) reduction as a function of size eventually yields a value of \( \kappa_L \) smaller than the best 50% solid solution, underpinning the relevance of the (sub)nano-regime for devices.

The “eight-in-a-box” spheres PbTe nanocomposites in a PbSe matrix represents the right balance between dot size and inter-dot distance. The resulting enhanced phonon scattering lowers lattice thermal conductivity to values smaller than the best alloy. Temperature dependence for these two systems has been investigated and is reported in SI, Figure S6. The decrease of \( \kappa_L \) in the alloy is close to monotonic, while nanostructured compounds display a rather step-like trend. In particular, at ambient and higher temperatures the inclusion of nano-dots is predicted to lower thermal conductivity to a larger extent than the best alloy compound.

**Discussion**

In order to understand the physics behind changes in thermal conductivity between our samples and bulk binary compounds, effective mean free paths of carriers as a function of frequency were computed. The size of larger systems of 10648 atoms per simulation box rapidly becomes too demanding with respect to memory allocation of the dynamical matrix. Therefore only 4096 atom systems were considered. We compared values for PbSe bulk (the case of PbTe shows qualitatively the same results with a shift at lower frequencies due to larger Te atomic mass, see SI, Figure S7) with the one obtained for the PbSe_{0.50}Te_{0.50} alloy, the largest PbTe sphere (20 Å of diameter) embedded in a PbSe matrix and the 12.5 Å thick layered structure.

The effective mean free path of mode \( i \) is given by \( \lambda_i = v^i_i \tau_i \) where effective group velocities \( v^i_i \) were obtained by diagonalizing the dynamical matrix of the system, and lifetimes \( \tau_i \) were computed by MD simulations from the normalized autocorrelation function of the energy (E) of each vibrational mode \( i \): \( \tau_i = \int_0^\infty (E_i(t) \cdot E_i(0))/E_i(0) \cdot E_i(t) \cdot dt \) (details of each calculation can be found in the Supporting Information, Figs. S8-S9). Figure 4 shows the impact of (sub)nanostructuring on thermal conductivity. From frequencies of \( \nu \approx 1 \) THz on, a significant average decreasing of the mean free path with respect to bulk PbSe is clearly visible. In the interval \( 1 \) THz \( \leq \nu \leq 3 \) THz, value reductions by a factor \( \sim 350 \) are found for the alloyed structure, \( \sim 310 \) for PbTe nanoparticles embedded in a PbSe matrix, while the layered structure outstands the previous ones by a factor as large as \( \lambda_{n} = \lambda_{a} \sim 40 \) along the stacking direction (\( \lambda_{n} = \lambda_{a} \sim 40 \)), in agreement with the trend of lattice thermal conductivity reduction shown in Table 1. The same analysis allows discriminating among layered nanocomposites. Comparing the mean free path for the 6.25 Å thick layered structure to the one with a thickness of 12.5 Å (Figure S10), the latter is distinguished by a markedly lower thermal conductivity across

**Figure 3.** (a) Lattice thermal conductivity dependence of PbTe(PbSe) and PbSe(PbTe) as a function of nano-dot distance \( d \) (b).
the layers. This in turn is due to a reduction of the mean free path of intermediate frequency modes, which suggests that a selective filtering on selected portions of the frequency range can be achieved as a function of morphological features of the composite. While the right scale of (sub)nanocompositing may be difficult to guess by trial and error, the computational approach of the present work is very precise in indicating a viable route for a systematic improvement of thermoelectric materials. While on the one hand our approach confirms the enhancement of the thermoelectric figure of merit for PbTe-PbSe solid solutions, it opens on the other hand a more promising and “intelligent” nanoengineering approach for the creation of specific geometries and interfaces. At room temperature, the insertion of PbTe(Se) nanoparticles into PbSe(Te) matrix causes a reduction of $k_L$ up to 45% with respect to the binary compound, while in layered nanocomposites the rather modest average reduction of about 35% for in-layer conduction is remarkably enhanced above 60% perpendicular to the layers. Furthermore, the study of lager systems suggests densely packed nano-dot as nanoengineering design targets. This qualifies nanocomposites with stong anisotropic features and dense packing as potentially outstanding thermoelectrics for renewable energy applications.

Our results indicate the overall decreasing of the thermal lattice conductivity in nanocomposites with respect to PbTe or PbSe to arise from a reduction of the mean free path of modes at selected frequency. PbTe-PbSe alloys are known to enhance thermoelectric efficiency because of phonon features, which are distinct from the binary phases. Our computational approach sheds light on a different strategy of thermal conductivity reduction, that is engineering at the (sub)nanometer scale. Along this line it is possible to obtain structures with potentially better phonon scattering properties. Experimentally,$^{42}$ $k_L$ resulted independent from layer thickness between 5 and 50 nm. Our calculations indicate that the threshold for an effect to set in has to be at shorter length values, also pinpointed by the indication of densely packed nano-dots spaced by less than a few nanometers. Considering group velocities, lifetimes and mean free path of low frequency vibrational modes of different layered structures, an optimal spacing between different species (alternating PbTe and PbSe layers) can be identified, which enhances anisotropy and reduces thermal conductivity along the layer stacking direction. Low values are also found if spherical PbTe nanoparticles are growth inside a PbSe matrix (or vice versa), as an alternative means to modulate material distribution and length sequences on the (sub)nano scale. Experimentally, ordered assemblies of nanocrystals can be obtained on a length scale compatible with these predictions.$^{43}$

Figure 4. Average mean free path of vibrational modes as a function of frequency for bulk PbSe sample (a), PbTe$_{0.50}$Se$_{0.50}$ alloy (b), 20 Å radius PbTe sphere in PbSe matrix (c) and directional mean free path for 12.5 Å thickness layer structure (4096 atoms in the simulation box) (d); colors (black, red, green) correspond to $x$, $y$ and $z$ directions.
Conclusions

This large-scale atomistic study of the priority material class of lead chalcogenides has provided a systematic investigation of size effects in PbSe/PbTe composites. By means of equilibrium MD calculations, lowest lattice thermal conductivity values were shown to be characteristic of a region between solid solutions (\(0^\circ\) nm) and nanostructured (~5 nm) materials. Length modulations in this region (i.e. between 0 and 5 nm) achieve efficient scattering of intermediate frequency modes. The precise reproduction of experimental curves and the precise evaluation of the temperature dependence of thermal conductivity as a function of morphological features provide guidance for the design of novel materials with improved properties. We expect our approach to be widely applicable for thermal transport evaluation, and for designing better thermoelectric materials.

Supporting Information

Details on transferable pair potential parameters for PbSe and PbTe, heat autocorrelation function, size validation, mean free paths for bulk, PbSe and PbTe, lifetimes and mean free paths for PbTe composites are provided as supplementary material.

Author Contributions

The manuscript was written through contributions of all authors. All authors have given approval to the final version of the manuscript.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords: Thermal transport · lead tellurides · lead selenides · nanomaterials · molecular dynamics · thermoelectrics


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