So far, some theoretical investigations have been performed on the electrical transport properties of PbTe and derived materials [11–13]

There seems to be quite a few works, especially on quantum confinement:

PHYSICAL REVIEW B 70, 115334 (2004)
PHYSICAL REVIEW B 82, 115209 (2010)
PHYSICAL REVIEW B 82, 195102 (2010)
PHYSICAL REVIEW B 76, 155127 (2007)

The electron relaxation times scale with the vacancy/impurity levels. Phonon relaxation time scale with the inverse 4th power of frequency (energy) for defects, while the electron relaxation times scale with the Do your results have any implications for these studies, particularly with respect to the vacancy studies you performed?

The spectral energy density (SED) analysis is carried out to obtain the spectral relaxation time, mean free path and the contribution of individual phonon branches to the thermal conductivity in PbTe bulk.

Since the SED method does not have a validation, you should mention this when the technique is introduced. For example, Eq. (2) and (4) do not agree in the following:

PHYSICAL REVIEW B 84, 165418 (2011)

Where Eq. (2) here is your Eq. (7). Therefore, you should mention that Eq. (7) has not been validated.

So far only two interatomic potentials have been developed for PbTe [8, 14] and here we employ the two-body interatomic potentials for PbTe which can reasonably reproduce the mechanical and phonon properties of PbTe bulk crystal [14].

I think this statement is ok given that the conductivities agree reasonably well with experimental results, but a similar comment may be needed here about the validation of the SED method.

The electrostatic interactions in the system is accounted for by employing the Wolf method, which is shown to reproduce the full Ewald summation with an appropriate choice of parameter α [19].

Could you provide the value of this parameter that you used? It is quite useful when reproducing published results.

The corresponding MD domains are constructed by removing a designated amount of target atoms (either adjacent to each other or randomly distributed) from the domain of pristine PbTe bulk with 512 atoms.

Have you tested size convergence of your measurements on your defected systems?

Besides their effects on thermal transport, vacancies might have positive effects on electronic transport properties, for instance, by creating potential barriers to enhance Seebeck coefficient [27]. However, due to the fact that too large defect concentration may significantly deteriorate the transport of electronic carriers, an optimum concentration of vacancies for thermoelectrics may exist and should be verified in future work.

Ah, this answer my previous question. This seems like an interesting effect, do your predictions give any insight?

As suggested by Henry and Chen [30], we reoriented the simulation cells to align the direction of interest with the longest edge of a rectangular domain. In doing this, domains composed of 16 × 4 × 4, 16 × 6 × 4, and 8 × 6 × 3 cells are constructed for [100],[110],[111] directions, allowing 17, 17, and 13 k points between Γ and BZ boundary. Again, the cells used for each domain are different according to the reorientation.

Has a validation of the technique been performed? Presumbaly this allows one to achieve higher resolution of the Brioullin zone along the longer dimension direction. Inconsistent prediction have been observed for this technique, see:

A. J. H. McGaughey and J. Li, "Molecular dynamics prediction of the thermal resistance of solid-solid interfaces in superlattices," ASME paper IMECE2006-13590, presented at 2006 ASME IMECE, November 2006, Chicago, IL.

I believe the manuscript is well written and makes a good contribution.