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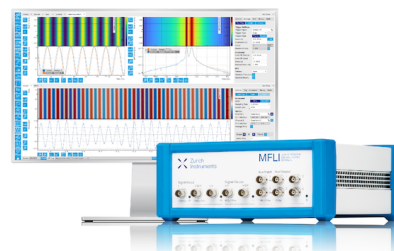
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Impact of classical statistics on thermal conductivity predictions of BAs and diamond using machine learning molecular dynamics

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ABSTRACT

Machine learning interatomic potentials (MLIPs) have greatly enhanced molecular dynamics (MD) simulations, achieving near-first-principles accuracy in thermal conductivity studies. In this work, we reveal that this accuracy, observed in BAs and diamond at sub-Debye temperatures, stems from an accidental error cancelation: classical statistics overestimates specific heat while underestimating phonon lifetimes, balancing out in thermal conductivity predictions. However, this balance is disrupted when isotopes are introduced, leading MLIP-based MD to significantly underpredict thermal conductivity compared to experiments and quantum statistics-based Boltzmann transport equation. This discrepancy arises not from classical statistics affecting phonon–isotope scattering rates but from its impact on the interplay between phonon–isotope and phonon–phonon scattering in the normal scattering-dominated BAs and diamond. This work underscores the limitations of MLIP-based MD for thermal conductivity studies at sub-Debye temperatures.

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The emergence of machine learning interatomic potentials (MLIPs) has significantly advanced molecular dynamics (MD) simulations.[1,2] By leveraging first-principles calculations as input, MLIPs are able to describe the interatomic interactions at a near-first-principles accuracy. This accuracy extends from the second-order to the third- and even fourth-order force constants.[3] Naturally, MLIP-based MD (MLMD) has emerged as a powerful method to simulate thermal transport in materials, achieving significantly higher accuracy in thermal conductivity prediction than empirical interatomic potentials.[4] For materials that are challenging to fit with empirical interatomic potentials, MLIPs are even more indispensable.

Surprisingly, it has been extensively shown that MLMD can predict the thermal conductivity accurately even at sub-Debye temperatures, when the classical statistics in MD deviate significantly from quantum statistics. For instance, for Si,[5] β-Ga$_2$O$_3$,[6] cubic BAs,[7] and diamond,[7] which have Debye temperatures of around 635,[8] 870,[9] 680,[10] and 2240 K,[11] respectively, the thermal conductivities predicted by MLMD using different MLIPs all closely match the experimental data at 300 K. Therefore, some work even suggested that quantum correction (QC) is unnecessary for predicting the thermal conductivities when using MLIPs.[6,7] However, this claim lacks a solid foundation.

The role of classical statistics in MLMD for predicting thermal conductivity at sub-Debye temperatures remains unclear.

In this Letter, we investigate the impact of statistics on thermal conductivity predictions in MLMD. BAs and diamond are selected for study for three reasons. (1) As the first and second highest thermal conductivity materials in nature, BAs and diamond hold great potential for next-generation electronics. (2) BAs and diamond have been extensively studied in the literature by using both DFT and MD, providing ample data for comparison. (3) With high Debye temperatures, BAs and diamond are ideal candidates for studying the effects of classical statistics at sub-Debye temperatures. Here, both pure and isotope-contained BAs and diamond are studied. The moment tensor potential (MTP)[12] is selected owing to its efficiency, reliability, and simplicity. Green–Kubo theory[13,14] is used to extract the thermal conductivity of materials based on the autocorrelation function of heat current from MD simulations. The size effect of Green–Kubo MD is minimal since it uses periodic boundary conditions, which allow long mean-free-path phonons (theoretically infinite long) to transport.[15,16] Phonon spectral energy density (SED)[17] analysis is performed based on MD trajectories to extract phonon scattering rates. For reference, Boltzmann transport equation (BTE) calculations are performed with three- and four-

phonon (3ph, 4ph) scattering rates obtained from density functional theory (DFT). Phonon–isotope scattering is calculated by using the Tamura formula based on Fermi's Gold rule. All the simulation details can be found in the supplementary material and our previous work.[18]

MTPs are trained for isotope-free and isotope-mixed BAs and diamond. The accuracy of MTPs is demonstrated by comparing the predicted forces and energies with DFT calculations as shown in Fig. 1 and supplementary material Figs. S1 and S2. The root mean square error (RMSE) of energies and forces for BAs are 0.144 meV/atom and 0.017 eV/Å, respectively, and 0.060 meV/atom and 0.010 eV/Å for diamond, respectively. The phonon dispersions calculated using MTP and DFT agree with each other, as shown in Figs. 1(c) and 1(f), demonstrating the accuracy of MTPs.

The thermal conductivities of BAs and diamond calculated using MLMD are shown in Fig. 2. Without isotopes, the temperature-dependent thermal conductivities of both materials agree well with those calculated from DFT, being consistent with the literature.[7] However, when isotopes are present, while the DFT calculations agree excellently with experiment,[19–25] MLMD significantly underpredicts the thermal conductivity of both materials. For example, for isotopically pure BAs, DFT and MLMD yield 1500 and 1300 W/mK, respectively, closely matching experimental data (1500 W/mK).[22] For isotopically pure diamond, DFT and MLMD yield 3500 and 3400 W/mK, also aligning with experimental data (3300 W/mK).[23–25] However, for natural BAs, the MLMD result (760 W/mK) is significantly lower than both DFT (1300 W/mK) and experimental data (1300 W/mK). Similarly, for natural diamond, the MLMD result (1500 W/mK) is much lower than DFT (2300 W/mK) and experimental data (2400 W/mK).

To investigate why MLMD predicts thermal conductivities well without isotopes but inaccurately with isotopes, we look into phonon specific heat and lifetime. Figures 3(a) and 3(d) show $\kappa_{\mathrm{MLMD}}/\kappa_{\mathrm{DFT}}$, $c_{\mathrm{MLMD}}/c_{\mathrm{DFT}}$, and $\tau_{\mathrm{MLMD}}/\tau_{\mathrm{DFT}}$ for isotopically pure BAs and diamond, respectively, where κ is thermal conductivity, c is specific heat, and τ is phonon lifetime. Here, $\tau_{\mathrm{MLMD}}/\tau_{\mathrm{DFT}}$ is indirectly obtained by using $\tau_{\mathrm{MLMD}}/\tau_{\mathrm{DFT}} = \kappa_{\mathrm{MLMD}}/\kappa_{\mathrm{DFT}} \cdot c_{\mathrm{DFT}}/c_{\mathrm{MLMD}}$. It is seen that MLMD overestimates specific heat and underestimates phonon lifetimes significantly, especially at low temperatures. These two errors accidentally cancel each other out, resulting in an apparently accurate thermal conductivity prediction. The errors gradually shrink and disappear as temperature increases. Additionally, the error cancellation is material-dependent. For instance, it is more effective in diamond than in BAs.

In addition to the phonon lifetime ratio ($\tau_{\mathrm{MLMD}}/\tau_{\mathrm{DFT}}$) that is derived indirectly from thermal conductivity and specific heat, the mode-dependent τ_{MLMD} and τ_{DFT} are directly extracted and compared with each other, as shown in Figs. 3(b) and 3(e). Indeed, MLMD significantly underestimates the lifetime compared to DFT, supporting the error-cancelation claim and the observation in Figs. 3(a) and 3(d). Furthermore, it is seen that the phonon lifetime underestimation in MLMD is more prominent for lower frequency phonons. This is surprising since classical statistics deviate from quantum statistics relatively smaller for lower frequency phonons than for higher frequency phonons. We hypothesize that these lower frequency phonons, despite having smaller statistics-induced errors, may scatter significantly with higher frequency phonons, which have larger statistics-induced errors. This can also be seen by replacing the quantum phonon population (n_{Q}) in the 3,4-phonon scattering formalism with the classical population (n_{C}), as shown in Figs. 3(b) and 3(e). However, it is noted that
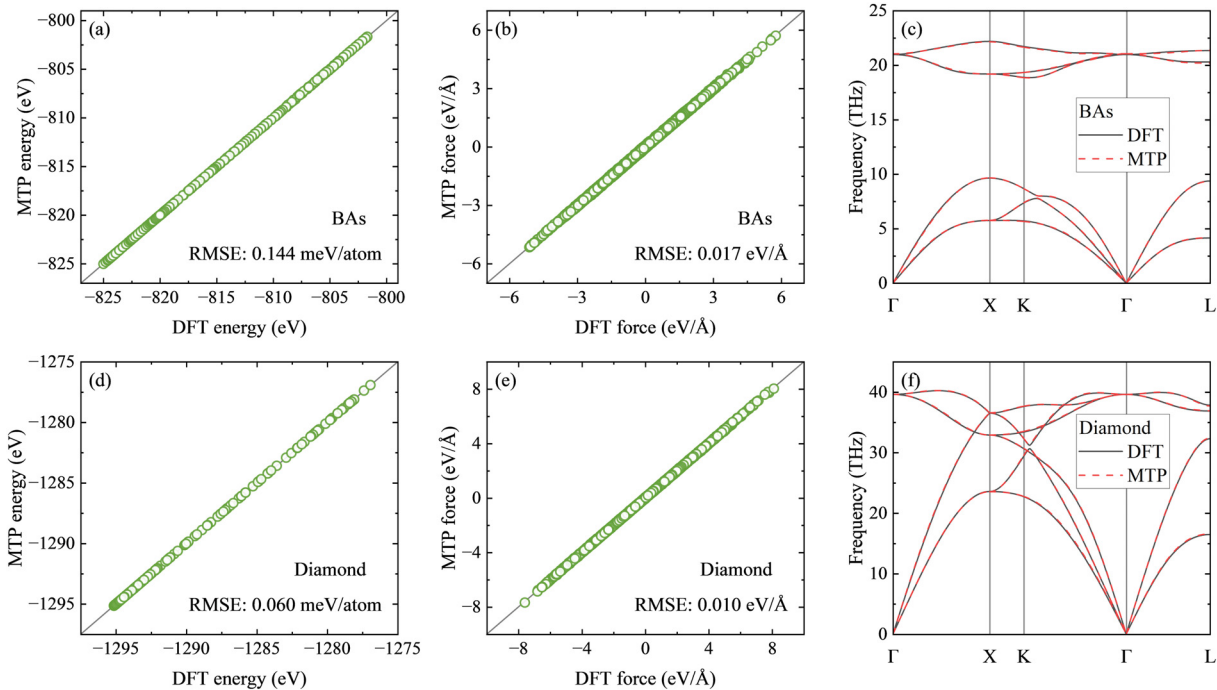
FIG. 1. Validation of MTP machine learning potentials for (a)–(c) BAs and (d)–(f) diamond. (a) and (d) Comparison between energies calculated from MTP and DFT. (b) and (e) Comparison of forces. (c) and (f) Comparison of phonon dispersions.
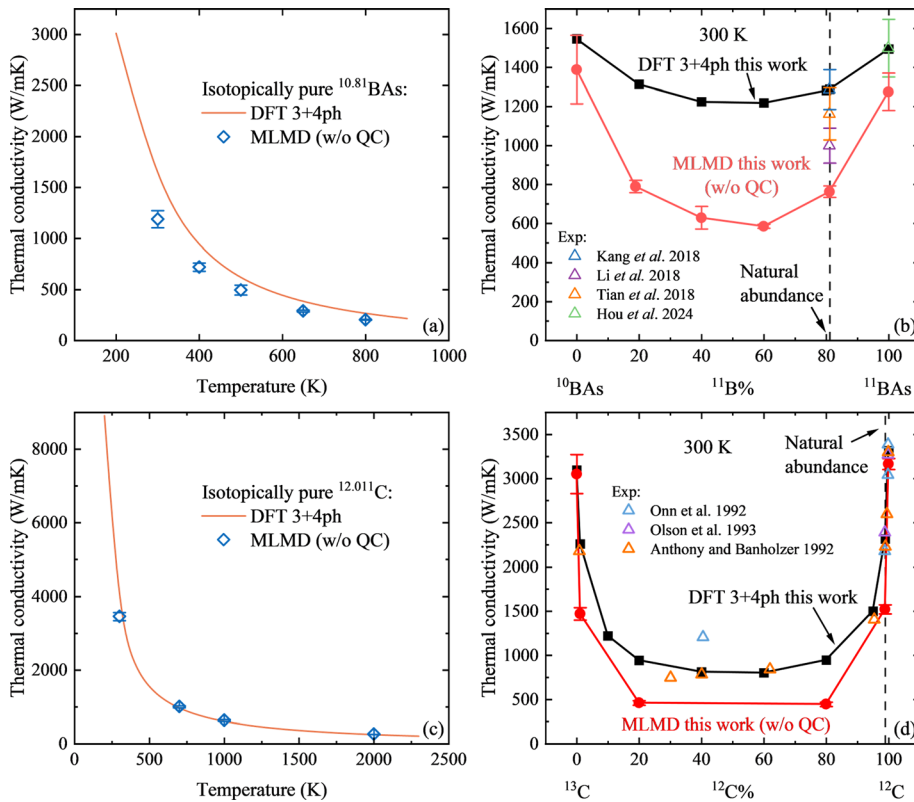
FIG. 2. (a) Temperature-dependent thermal conductivity of isotope-free BAs calculated by using DFT (3 + 4ph) and MLMD (without quantum correction). (b) Isotope concentration-dependent room-temperature thermal conductivity of BAs calculated by DFT (3 + 4ph) and MLMD (without quantum correction) compared to experimental data. (c) and (d) The same as (a) and (b) but for diamond. References of experimental data in (b): Kang et al.,[21] Li et al.,[19] Tian et al.,[20] Hou et al.,[22] and in (c): Anthony and Banholzer,[23] Onn et al.,[24] and Olson et al.[25]

replacing n_Q with n_C in phonon scattering formalism is not a scientific way to obtain phonon lifetime under classical statistics. This is because the phonon scattering formalism is derived based on n_Q. Without n_Q, the phonon scattering formalism is not valid anymore.[26–30] Actually, since n_C is larger than n_Q by 0.5 at the classical limit, replacing n_Q with $n_C - 0.5$ in the phonon scattering formalism can yield better thermal conductivity than using n_C (see the supplementary material Fig. S3).

To eliminate the errors caused by classical statistics, quantum corrections, if possible, need to be done on both specific heat and phonon scattering rate. The discussion of quantum corrections has a long history. In early years, QC was done by correcting the temperature, via equating the total energies of classical and quantum systems,[31–33] i.e., $\sum E_C n_C = \sum E_Q n_Q$. While many early studies used this QC method, it was demonstrated to be unreasonable by Turney and McGaughey in 2009[27] no matter the zero-point energy is considered or not. They used anharmonic lattice dynamics with Stillinger–Weber potential to self-consistently demonstrate this by replacing the n_Q with n_C-1/2. They also found that both specific heat and lifetime were affected by the statistics, and thus QC should be performed on both. In addition, QC should be applied on a mode level instead of a system level. Despite the discovery of Turney and McGaughey, QC has been primarily applied to specific heat only.[34–39] On the one hand, QC to lifetime is difficult and remains unfeasible, while that to specific heat is simple. On the other hand, it is found that the QC to lifetime is only important for crystalline materials.[26,34,35,40] QC to specific heat is sufficient for strongly disordered systems where phonon–phonon

scattering is not dominant. Gu et al.[26] also mentioned in their review paper that QC should be applied to both specific heat and lifetime for crystals, but these two factors often cancel out each other, making the overall impact not strong, such as in graphene and silicon. However, the two factors were not canceled out in the 1D material, carbon nanotubes, as studied by Barbalinardo et al.[40] They limit $\hbar$ to zero to approach classical limit in solving the BTE, and a large gap is found between the thermal conductivity obtained using n_Q and n_C. Puligheddu et al.[28] found, using classical potentials, that the phonon lifetimes of MgO and PbTe obtained by replacing n_Q with n_C in BTE agree well with those obtained from MD with SED analysis, ending with the conclusion that phonon lifetime can be corrected by correcting the phonon population. This finding does not hold in the systems studied in this work (i.e., BAs and diamond), where we find that replacing n_Q with n_C in BTE results in unphysical results that cannot match with MD. In light of these efforts, here we explore several possible quantum correction methods for mode-level phonon lifetime, shown in Figs. 3(c) and 3(f). Based on the three-phonon scattering formalism, phonon scattering rate is generally proportional to phonon population at high temperatures. Therefore, the first trial to correct τ is to use n_C/n_Q, which, however, is found to not match with $\tau^{-1}_{\text{MLMD}}/\tau^{-1}_{\text{DFT}}$. Considering the three-phonon scattering contains $(1 + n)$ and $(1 + 2n)$ terms, the second trial is to use $(1 + n_C)/(1 + n_Q)$ and $(1 + 2n_C)/(1 + 2n_Q)$ for corrections, which are found to not match with $\tau^{-1}_{\text{MLMD}}/\tau^{-1}_{\text{DFT}}$ either. Other trials, like using E_C/E_Q and c_C/c_Q, all fail. It is found that τ is overpredicted by classical statistics more for lower frequency phonons, but all these corrections correct less lower
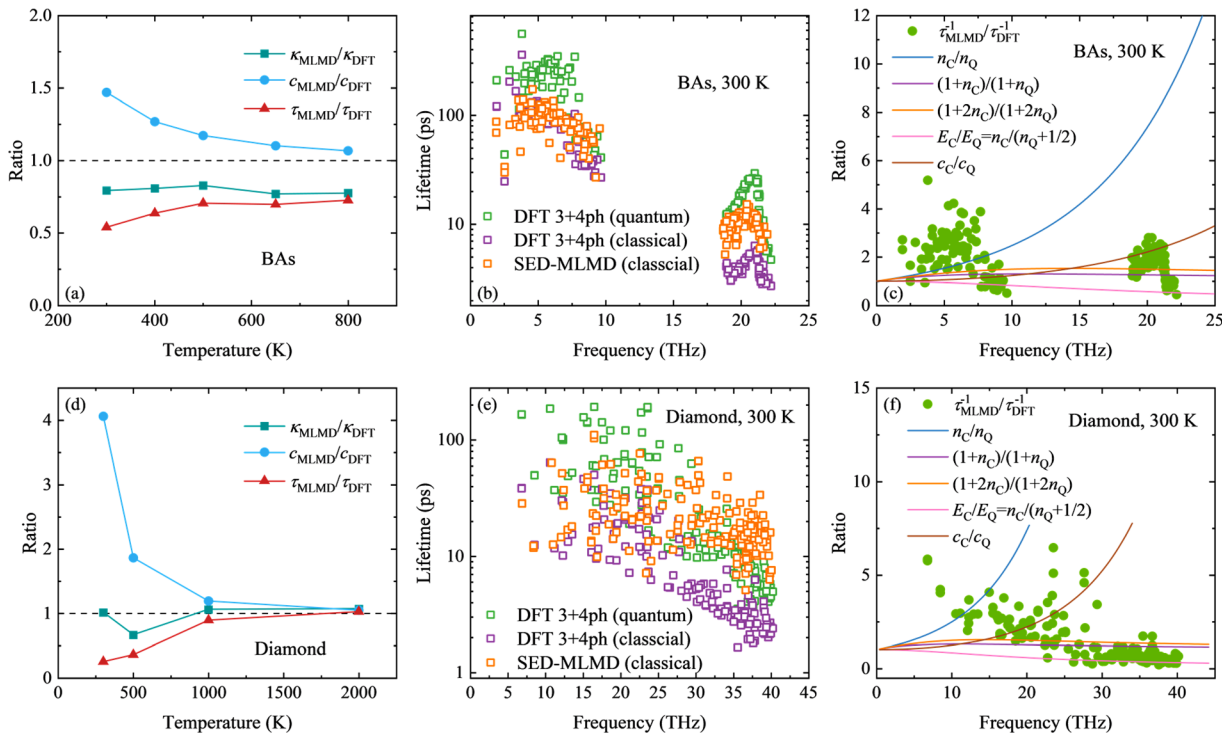
FIG. 3. Comparison between quantum and classical statistics-predicted thermal properties of (a)–(c) BAs and (b)–(d) diamond. (a) and (d) Ratios of thermal conductivity, total specific heat, and effective phonon lifetime obtained from MLMD and DFT as a function of temperature. (b) and (e) Mode-level phonon scattering rates at room temperature. (c) and (f) Possible quantum corrections for mode-level phonon scattering rates.

frequency phonons. These indicate that the quantum correction to phonon–phonon scattering rate is complex and is unlikely to be achieved in a straightforward manner.

After understanding the isotope-free materials, we explore the reasons for the significant underestimation of thermal conductivity by MLMD when isotopes are present. Theoretically, the phonon–isotope scattering rate (τ_{ph-iso}^{-1}) should not depend on phonon population, based on the derivation of Tamura's formula using perturbation theory.[41] Numerically, this is verified by comparing the τ_{ph-iso}^{-1} calculated by Tamura's formula ($\tau_{ph-iso}^{-1} = \pi/2 \cdot \omega^2 g \cdot pDOS$) and $\tau_{ph-iso}^{-1} = \tau_{tot}^{-1} - \tau_{ph-ph}^{-1}$ obtained by SED analysis of MLMD, where ω is the phonon frequency, g factor is determined by isotope mass and concentration, pDOS is the projected density of state, and τ_{tot}^{-1} and τ_{ph-ph}^{-1} are the phonon linewidths in isotope-contained and isotope-free materials, respectively. As seen in Figs. 4(a) and 4(b), τ_{ph-iso}^{-1} obtained from the two methods agree with each other, supporting that τ_{ph-iso}^{-1} does not depend on phonon statistics. We note that some negative τ_{ph-iso}^{-1} data obtained by $\tau_{ph-iso}^{-1} = \tau_{tot}^{-1} - \tau_{ph-ph}^{-1}$ are due to the large uncertainty of SED analysis, especially when τ_{tot}^{-1} and τ_{ph-ph}^{-1} are very close. The τ_{ph-iso}^{-1} obtained by Tamura's formula using classical and quantum statistics also agree with each other for an artificial isotope abundance of BAs as shown in Fig. 4(c). Another evidence is temperature dependence. It is found that τ_{ph-iso}^{-1} does not depend on temperature in MLMD, indicating that τ_{ph-iso}^{-1} is invariant on phonon population.

Since τ_{ph}^{-1} is larger in MLMD than DFT, adding the same τ_{ph-iso}^{-1} is expected to generate smaller impact in MLMD, resulting in larger

thermal conductivity in MLMD than DFT. However, the fact is that MLMD shows smaller thermal conductivity than DFT for isotope-contained materials. A possible reason is that the isotopes do not only introduce phonon–isotope scattering but also change the original phonon–phonon scattering. This can be realized by the hydrodynamical behavior of phonons in BAs and diamond. In these two materials, the moment-conserved normal scattering dominates over the moment-unconserved Umklapp scattering, resulting in hydrodynamical movement of phonons.[29,42] Therefore, the single-mode relaxation time approximation (SMRTA) fails in describing thermal transport in BAs and diamond. The exact solution of BTE using iteration shows much higher thermal conductivity than SMRTA. Even though phonon statistics do not change τ_{ph-iso}^{-1} in SMRTA, it changes how normal scattering is coupled with Umklapp scattering in the iteration in solving BTE. As seen in Fig. 5, using classical statistics gives a much smaller increase in thermal conductivity after iteration than using quantum statistics. This is understandable since isotope scattering is preferable for high energy phonons and gives positive feedback to Umklapp scattering and increases the resistance. Consequently, the role of statistics becomes more complicated when a material is dominated by normal scattering processes.

In conclusion, we investigate the effects of phonon statistics on the thermal conductivity prediction of BAs and diamond using MLMD. We find that while MLMD, without any quantum correction, can well reproduce the thermal conductivity of isotopically pure BAs and diamond, it is an error-canceling effect: the classical statistics in MLMD overestimates specific heat and underestimates phonon
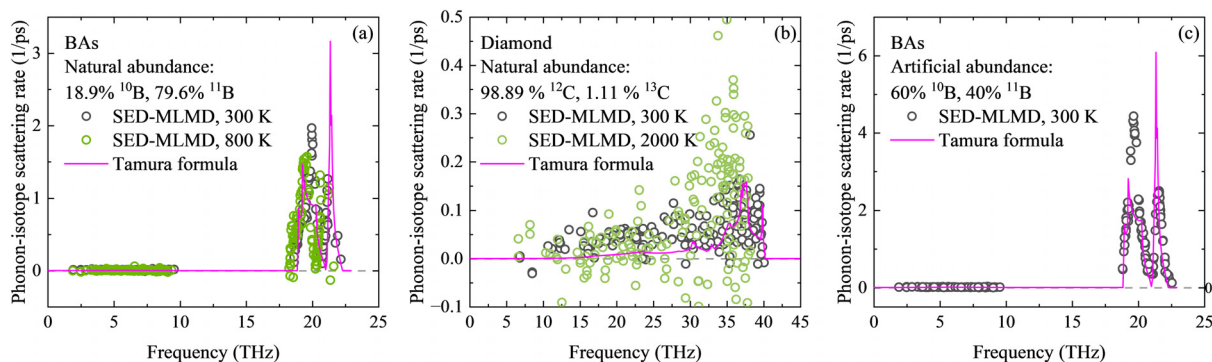
FIG. 4. Phonon–isotope scattering rates obtained from SED based on MLMD and Tamura formula for natural abundant (a) BAs, (b) diamond, and (c) BAs with artificial isotope abundance.
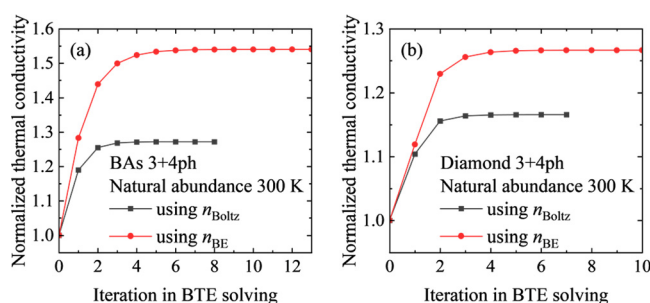
FIG. 5. Normalized thermal conductivity of isotopically mixed (a) BAs and (b) diamond with natural abundance obtained in ShengBTE at 300 K as a function of iteration step.

lifetime. This error-canceling effect is disrupted when isotopes are introduced, leading MLMD to significantly underpredict thermal conductivity compared to experiments and quantum statistics-based BTE. This discrepancy is not because classical statistics changes phonon–isotope scattering rates, but because the isotopes change phonon–phonon scattering mechanisms. Additionally, our results support the validity of the Tamura formula for phonon–isotope scattering. We hope this study provides a deeper understanding of thermal conductivity in MLMD simulations.

See the supplementary material for the following: Sec. S1: machine learning interatomic potential simulation details; Sec. S2: Green–Kubo molecular dynamics simulation details; Sec. S3: phonon spectral energy density analysis details; Sec. S4: first principles calculations; Figs. S1 and S2: validation of MTPs; and Fig. S3: temperature-dependent thermal conductivity of BAs and diamond obtained by solving Boltzmann transport equation using different statistics.

AUTHOR DECLARATIONS
Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Hao Zhou: Data curation (equal); Formal analysis (equal); Investigation (equal); Writing – original draft (equal). **Shuxiang Zhou:** Conceptualization (equal); Funding acquisition (equal); Resources (equal); Writing – review & editing (equal). **Zilong Hua:** Conceptualization (equal); Funding acquisition (equal); Writing – review & editing (equal). **Kaustubh Bawane:** Conceptualization (equal); Funding acquisition (equal); Writing – review & editing (equal). **Tianli Feng:** Conceptualization (equal); Formal analysis (equal); Funding acquisition (equal); Methodology (equal); Resources (equal); Supervision (equal); Writing – review & editing (equal).

DATA AVAILABILITY

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

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