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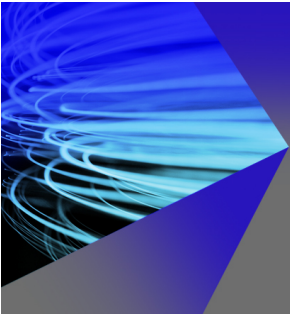
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Thermal conductivity limits of MoS₂ and MoSe₂: Revisiting high-order anharmonic lattice dynamics with machine learning potentials

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Tuğbey Kocabaş,¹  Murat Keçeli,²  Tanju Gürel,³  Milorad V. Milošević,^{4,5}  and Cem Sevik^{4,a)} 

AFFILIATIONS

¹Department of Advanced Technologies, Eskisehir Technical University, 26555 Eskisehir, Turkey

²Computational Science Division, Argonne National Laboratory, Lemont, Illinois 60517, USA

³Department of Physics, Tekirdağ Namik Kemal University, Tekirdağ, TR 59030, Turkey

⁴COMMIT, Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium

⁵Stavropoulos Center for Complex Quantum Matter, Department of Physics and Astronomy, University of Notre Dame, Notre Dame, Indiana 46556, USA

^{a)}Author to whom correspondence should be addressed: cem.sevik@uantwerpen.be

ABSTRACT

Group-VI transition metal dichalcogenides (TMDs), MoS₂ and MoSe₂, have emerged as prototypical low-dimensional systems with distinctive phononic and electronic properties, making them attractive for applications in nanoelectronics, optoelectronics, and thermoelectrics. However, their reported lattice thermal conductivities (κ) remain highly inconsistent, with experimental values and theoretical predictions differing by more than an order of magnitude. These discrepancies stem from uncertainties in measurement techniques, variations in computational protocols, and ambiguities in the treatment of higher-order anharmonic processes. In this study, we critically review these inconsistencies, first by mapping the spread of experimental and modeling results, and then by identifying the methodological origins of divergence. To this end, we bridge first-principles calculations, molecular dynamics simulations, and state-of-the-art machine learning force fields (MLFFs), including recently developed foundation models. We train and benchmark GAP, MACE, NEP, and HIPHIVE against density functional theory and rigorously evaluate the impact of third- and fourth-order phonon scattering processes on κ . The computational efficiency of MLFFs enables us to extend convergence tests beyond conventional limits and to validate predictions through homogeneous nonequilibrium molecular dynamics as well. Our analysis demonstrates that, contrary to some recent claims, fully converged four-phonon processes contribute negligibly to the intrinsic thermal conductivity of both MoS₂ and MoSe₂. These findings not only refine the intrinsic transport limits of 2D TMDs but also establish MLFF-based approaches as a robust and scalable framework for predictive modeling of phonon-mediated thermal transport in low-dimensional materials.

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I. INTRODUCTION

Efficient thermal management has become a critical constraint in the design and operation of modern nanoelectronic, optoelectronic, and thermoelectric devices for energy conversion. As device dimensions continue to shrink and power densities increase, the ability of materials to dissipate heat effectively is essential to ensure optimal performance, stability, and long-term reliability. In this context, the lattice thermal conductivity (κ) has emerged as a key figure of merit for the selection and optimization of functional materials.^{1,2}

Among emerging low-dimensional systems, two-dimensional (2D) materials, particularly group-VI transition metal dichalcogenides (TMDs), such as molybdenum disulfide (MoS₂) and molybdenum

diselenide (MoSe₂), have attracted considerable attention due to their unique thermal, electronic, and optoelectronic properties.^{3–9} Significant experimental efforts have focused on quantifying their thermal conductivity using techniques such as Raman thermometry and optothermal methods.^{6,10} However, even for the prototypical case of monolayer MoS₂, experimental values of κ remain widely scattered. Reported room-temperature measurements range from 13 Wm^{−1}K^{−1}, based on early Raman studies on suspended flakes,¹¹ to 84 Wm^{−1}K^{−1}, using refined optical calibration techniques.⁶ Additional reports that account for anisotropic effects further extend the range from 24 to 100 Wm^{−1}K^{−1}.¹² Similar variability is observed for MoSe₂,¹⁰ albeit with consistently lower values, often attributed to its heavier chalcogen atom

and reduced phonon group velocities. The reported conductivities for MoSe₂ range from 20 (Ref. 10) to 59 Wm⁻¹K⁻¹.⁶

In addition to experimental studies, first-principles calculations have been widely used to predict the thermal conductivity of these materials.^{13,14} The combination of density functional theory (DFT) with the Peierls–Boltzmann transport equation (PBTE) has become the standard computational framework for such investigations. However, the resulting predictions exhibit substantial variation across the literature, largely due to methodological differences. Key contributing factors include the choice of exchange–correlation functional, supercell size, Brillouin zone sampling density, treatment of

anharmonic force constants, and convergence criteria. For monolayer MoS₂, DFT-BTE-based estimates of κ range from approximately 25 to more than 150 Wm⁻¹K⁻¹, depending on the computational parameters employed. Similarly, the theoretical predictions for MoSe₂ vary between 17 and 70 Wm⁻¹K⁻¹ (see Table I).

Complementary molecular dynamics (MD) simulations have also been applied to study the thermal transport in these materials.^{15–25} However, the variability in the reported results is often as large as or greater than that seen in first-principles studies. For monolayer MoS₂, room-temperature values of κ from MD simulations range from 1.35 Wm⁻¹K⁻¹ (Ref. 20) to 531 Wm⁻¹K⁻¹,²⁴ while values for MoSe₂

TABLE I. Room-temperature lattice thermal conductivity values of monolayer MoS₂ and MoSe₂ collected from the literature, based on first-principles, molecular dynamics, and experimental studies. All reported values have been rescaled according to the out-of-plane lattice constants used in this work: 6.15 Å for MoS₂ and 6.47 Å for MoSe₂. Italicized values indicate that the original source did not provide an explicit out-of-plane lattice constant.

First-principles			
MoS ₂		MoSe ₂	
Method	κ (Wm ⁻¹ K ⁻¹)	Method	κ (Wm ⁻¹ K ⁻¹)
DFT-BTE ⁵⁸	151.36	DFT-BTE ⁵⁹	54.13
DFT-BTE ⁶⁰	135.20	DFT-BTE ⁶¹	~ 70
DFT-BTE ⁶²	130.20	DFT-BTE ⁶³	~ 60
DFT-BTE ⁶⁴	130.00	DFT-BTE ⁶⁵	54
DFT-BTE ⁶⁵	103.00	DFT-BTE ⁶⁶	46.2
DFT-BTE ⁶⁷	81.42	DFT-DFPT-Slack Model ⁶⁸	17.6
DFT-BTE ⁵⁹	89.56		
DFT-DFPT-NEGF ⁶⁹	24.52		
DFT-BTE (3 ^{ph} , 3 ^{ph} +4 ^{ph}) ²⁷	133.5, 27.7		
DFT-BTE ⁶⁶	82.2		
DFT-BTE ⁶³	~ 75		
DFT-DFPT-Slack Model ⁶⁸	33.6		
DFT-DFPT-Umklapp Model ⁷⁰	29.2		
<i>Molecular Dynamics</i>			
REBO-LJ-HNEMD ²⁴	123.66	SW-NEMD ²⁵	24.80
(SW13, SW13E, SW16)-HNEMD ²⁴	535.85, 203.98, 290.65	SW-EMD-Green-Kubo ¹⁹	40.19
TB-(EMD-NEMD) ²⁰	0.97, 1.22	SW-NEMD-(AC, ZZ) ²¹	17.76, 18.93
SW-NEMD ²⁵	32.89	SW-NEMD-(AC, ZZ) ¹⁶	43.88, 41.63
SW-RNEMD-(AC, ZZ) ²³	32.95, 53.91	MLFF-NEP-HNEMD ¹⁷	77.73
SW-EMD-Green-Kubo ¹⁹	90.00	SW-SED ²²	29.18
SW-EMD-Green-Kubo ¹⁸	116.99		
SW-NEMD-(AC, ZZ) ¹⁶	101.39, 110.26		
SW-NEMD ¹⁵	19.95		
MLFF-NEP-HNEMD ¹⁷	161.62		
SW-SED ²²	89.4		
<i>Experimental</i>			
Raman (Heat Diff. Modeling) ³	36.46	Mech.Exf.-Raman (vacuum, air) ¹⁰	(20, 250)
Raman (Heat Diff. Modeling) ⁷¹	70.80	Mech.Exf.-Raman ⁶	59
CVD-RTD ⁷²	30		
Mech.Exf.-Raman ⁶	84		
CVD-Opt. Mod. ⁷³	19.8		
CVD-LHD ⁶⁰	13.3		
CVD-MJH ¹²	24–100		

span from 17.76 (Ref. 21) to $76.2 \text{ W m}^{-1} \text{ K}^{-1}$.¹⁷ These large discrepancies are primarily attributed to differences in the employed interatomic potentials, but other factors, including system size, boundary conditions, thermostat algorithms (e.g., Langevin or Nosé–Hoover), and averaging times, also play significant roles.

To address these discrepancies, increasing attention has been given to the role of higher-order phonon scattering processes, specifically those beyond the standard three-phonon interactions typically included in DFT-based thermal transport calculations.^{26–39}

Recent studies have shown that four-phonon processes can significantly reduce predicted thermal conductivities,^{27–37} indicating that models limited to three-phonon interactions may systematically overestimate κ , particularly at elevated temperatures or in materials with strong anharmonicity. However, these calculations remain computationally challenging, as they demand large supercells and dense Brillouin zone sampling; consequently, the convergence and accuracy of reported fourth-order interactions are often uncertain.

In this work, we employ machine learning force fields (MLFFs) in conjunction with first-principles calculations and molecular dynamics simulations to advance the understanding of the fundamental limits in thermal transport of MoS_2 and MoSe_2 monolayers and address the aforementioned discrepancies. We systematically benchmark thermal conductivity predictions against density functional theory (DFT) by analyzing convergence with respect to both third- and fourth-order phonon scattering processes. Specifically, we assess the accuracy of four multi-layer perceptron (MLP) frameworks (GAP, MACE, NEP, and HIPHIVE) in modeling the thermal transport of these materials. Upon establishing strong agreement with DFT results, we leverage the computational efficiency of MLFFs to explore effects beyond conventional reach, including higher-order neighbor interactions and four-phonon scattering. Additionally, we validate thermal conductivity estimates via homogeneous nonequilibrium molecular dynamics (HNEMD) simulations. These high-accuracy simulations, unattainable with standard DFT methods, highlight the critical role of machine learning in scalable modeling of complex phonon processes in low-dimensional materials. Importantly, our results demonstrate that fully converged fourth-order scattering contributions are negligible, in contrast to some earlier reports, and thereby refine the intrinsic thermal transport limits of monolayer transition metal dichalcogenides.

II. COMPUTATIONAL DETAILS

Structural relaxations and force calculations were performed using DFT within the Perdew–Burke–Ernzerhof (PBE) formulation of the generalized gradient approximation (GGA)⁴⁰ as implemented in VASP.⁴¹ A plane wave basis set with an energy cutoff of 600 eV was used for all the calculations. Brillouin zone sampling was performed using a Γ -centered Monkhorst–Pack⁴² mesh of $24 \times 24 \times 1$ k -points. The electronic self-consistency loop was converged to an energy difference of 10^{-6} eV, while ionic relaxations were terminated when forces fell below 10^{-2} eV/Å. To eliminate spurious interactions between periodic images, a vacuum spacing of at least 20 Å was applied along the out-of-plane (z) direction.

Interatomic force constants (IFCs) up to fourth order were evaluated to accurately capture anharmonic lattice dynamics. The second- and third-order IFCs from DFT were obtained via the finite displacement approach using VASP in combination with the PHONOPY⁴³ and `thirdorder.py`⁴⁴ packages, respectively. For this purpose, an $8 \times 8 \times 1$ supercell and a $4 \times 4 \times 1$ Γ -centered k -point mesh were

adopted. To ensure high numerical accuracy in the force constants, the electronic minimization tolerance was tightened to 10^{-8} eV. The interaction range was extended up to the 18th nearest neighbors (NNs) for third-order IFCs.

Fourth-order IFCs were obtained exclusively from MLFFs since DFT calculations at this level are computationally prohibitive. For comparison, third-order IFC calculations with an 18-NN cutoff required 1144 force evaluations, whereas fourth-order IFC calculations with a 10-NN cutoff demanded nearly 35 000. This stark increase in computational cost illustrates the impracticality of DFT-based fourth-order calculations, which justifies the use of MLFFs for this purpose. Convergence of fourth-order displacements was examined for amplitudes between 0.01 and 0.05 Å, with 0.04 Å selected (see [supplementary material](#)). Similarly, interaction ranges were tested up to the 10th NN and convergence was achieved at the 6th NN, which was used in all subsequent calculations.

Training, validation, and test datasets for the MLFFs were generated using the *on-the-fly* learning scheme implemented in VASP.⁴⁵ To ensure representative sampling of relevant atomic configurations and phonon interactions, *ab initio* molecular dynamics (AIMD) simulations were performed on $8 \times 8 \times 1$ supercells containing 192 atoms for both MoS_2 and MoSe_2 . A vacuum spacing of approximately 20 Å was introduced along the out-of-plane direction, and periodic boundary conditions were applied in the in-plane directions. The simulations were carried out in the semi-isotropic NPT ensemble using the Langevin thermostat and barostat, allowing the in-plane lattice vectors to fluctuate while keeping the out-of-plane dimension fixed. Temperatures were gradually increased from 200 to 1500 K with a time step of 1.0–2.5 fs. The projector-augmented wave (PAW) method and the Perdew–Burke–Ernzerhof (PBE) exchange–correlation functional were employed with a plane wave energy cutoff of 600 eV. The Brillouin zone was sampled using a $4 \times 4 \times 1$ Monkhorst–Pack k -point mesh, and electronic self-consistency was achieved with an energy convergence threshold of 10^{-7} eV. For each material, 3000 configurations were used for training, while 250 structures were employed for validation and testing, respectively.

The MLFFs employed in this study include Gaussian Approximation Potentials (GAP),^{46,47} MACE,^{48,49} Neuroevolution Potential (NEP),⁵⁰ and HIPHIVE.⁵¹ For HIPHIVE, 200 DFT-generated training configurations were used for each of monolayer MoS_2 and MoSe_2 , employing the same computational parameters described above to ensure data consistency. During the fitting procedure, interaction cutoffs were set individually for n -body terms up to six-body interactions. For MoS_2 , the cutoffs for 2-, 3-, 4-, 5-, and 6-body interactions were 12.5, 12.5, 6.0, 4.5, and 3.0 Å, respectively, whereas for MoSe_2 , the corresponding values were 13.28, 13.28, 6.5, 5.0, and 3.0 Å. These cutoffs were selected based on convergence tests of the predicted force constants and phonon dispersion curves. The fitting parameters used for GAP, MACE, and NEP are provided in the [supplementary material](#), and the resulting potential files have been deposited in a public repository (Zenodo).

To ensure the reliability of higher-order IFC predictions, each MLFF was first validated by comparing its second-order IFC-derived phonon dispersion curves and third-order IFC-derived lattice thermal conductivity values with DFT results, which were used as reference. Once satisfactory agreement with the DFT benchmarks was achieved, the validated MLFFs were used to compute the fourth-order IFCs.

This strategy ensured that higher-order anharmonic effects were included in a physically consistent and computationally efficient manner.

Lattice thermal conductivity and related transport properties, including phonon lifetimes and Grüneisen parameters, were computed by iteratively solving the Peierls–Boltzmann transport equation (PBTE)⁵² using the standalone FOURPHONON package,⁵³ an extension of SHENGBTE⁵⁴ that supports both three- and four-phonon scattering processes. A dense q -mesh of $80 \times 80 \times 1$ was employed for convergence, and up to the 18th NN interactions were included in the three-phonon scattering calculations. For four-phonon scattering, the same q -grid was used, and the scattering rates were evaluated using the maximum likelihood estimation (MLE) method implemented in FOURPHONON. To ensure statistical accuracy, 100 000 sampling points were used for both the phase space estimation and the scattering rate integration. The effective layer thicknesses were taken as 6.15 and 6.47 Å for monolayer MoS₂ and MoSe₂, respectively.

HNEMD simulations were performed using the GPUMD^{55–57} package with NEP to evaluate the lattice thermal conductivity at the molecular dynamics level. For both materials, square simulation cells were constructed, each containing 37 440 atoms. The lattice constants were set to 330 Å for MoS₂ and 344 Å for MoSe₂. Periodic boundary conditions were applied in the plane, and all simulations used a time step of 1 fs. At each target temperature (300 and 600 K), the systems were equilibrated for 1 000 000 steps (1 ns) in the NVT ensemble using a Nosé–Hoover chain thermostat. Following equilibration, a small external driving force was applied to generate a homogeneous heat current, and the system was propagated for an additional 10 000 000 steps (10 ns) in the nonequilibrium production stage. An effective thickness of 6.15 Å for MoS₂ and 6.47 Å for MoSe₂ was used for volume normalization in the thermal conductivity calculations. For each material and each temperature, the thermal conductivity was determined by averaging the results of 50 independent simulations.

III. RESULTS AND DISCUSSION

Table I summarizes reported values of room-temperature lattice thermal conductivity for monolayer MoS₂ and MoSe₂, highlighting the significant discrepancies present in the literature. To allow a meaningful comparison with our results, we have rescaled the reported κ values using consistent out-of-plane lattice constant values, as specified in Sec. II. This scaling is essential because the out-of-plane lattice constant for two-dimensional materials is arbitrary and determines the final value of thermal conductivity in units of $\text{Wm}^{-1}\text{K}^{-1}$. Here, we particularly note that for entries presented in italic font, the original out-of-plane lattice constant values were not reported in the corresponding publication.

As shown in Table I, inconsistencies appear not only in first-principles calculations but also in molecular dynamics simulations and experimental measurements. For both materials, a reliable comparison with the experimental data remains challenging. While some variability in experimental values is expected due to difficulties in fabricating high-quality monolayers and accurately measuring thermal transport at the nanoscale, the divergence observed within results from the same theoretical approach is often attributable to differences in computational implementation. In the case of MD simulations, the results strongly depend on the quality of the employed interatomic potentials. Classical potentials, which are commonly used, often lack the fidelity required to reproduce first-principles results.

We leverage recent advances in machine learning force fields to overcome the limitations of both first-principles and classical MD approaches. Our results demonstrate that MLFFs enable high-accuracy modeling of lattice thermal transport in two-dimensional materials and allow for an efficient exploration of the intrinsic limits of thermal conductivity. Sections III A–III D present the framework we applied for this purpose, and the corresponding results in detail.

A. ML potentials

As a first step, we evaluated the accuracy of state-of-the-art machine learning force fields by comparing their predicted atomic forces with DFT-calculated reference values on an independent test dataset. The atomic forces obtained for each model (GAP, MACE, NEP, and HIPHIVE) are plotted against the DFT forces for monolayer MoS₂ and MoSe₂ in Fig. 1. Among these models, HIPHIVE achieves the lowest root mean square errors (RMSEs), with values consistently below 2 meV/Å in all Cartesian directions. This outcome is consistent with HIPHIVE's specialized design as a Python library dedicated to efficiently extracting high-order anharmonic force constants from first-principles data. However, we would like to note that while the dataset structure differs for HIPHIVE, it was generated using the same settings and the precision level with other models, enabling a fair comparison. GAP, MACE, and NEP were trained on the same DFT dataset, allowing a direct comparison of their generalization capabilities. GAP is based on a kernel regression framework that utilizes Smooth Overlap of Atomic Positions (SOAP) descriptors to encode local atomic environments. MACE employs an equivariant message-passing neural network architecture designed to capture the geometric and symmetry properties of atomistic systems. NEP, which can be used within the GPUMD package, uses symmetry-preserving neural networks optimized for GPU-accelerated simulations. Despite differences in their internal architectures, all three models yield consistent results compared to DFT reference forces. MACE and GAP produce lower RMSEs in the range of 2–6 meV/Å, while NEP shows higher values, around 17 meV/Å. However, NEP delivers physically meaningful results, as further demonstrated by its accurate reproduction of both the phonon dispersions and the lattice thermal conductivity over a broad temperature range (details are presented below). These findings demonstrate that NEP captures the key characteristics of interatomic interactions relevant to thermal transport.

B. Thermal transport properties: PBTE solution via DFT and MLFFs

The predictive performance of the GAP, MACE, NEP, and HIPHIVE potentials was evaluated by comparing their calculated lattice thermal conductivity values with DFT results for monolayer MoS₂ and MoSe₂ over the temperature range of 200–800 K. The comparison is illustrated in Fig. 2, which includes both the calculated conductivity values and the relative errors with respect to DFT. It is important to note that the thermal conductivity values were not predicted directly by the potentials themselves. Instead, atomic forces obtained from each potential were used to construct the second- and the third-order force constants, which were then employed in the iterative solution of the Peierls–Boltzmann transport equation.

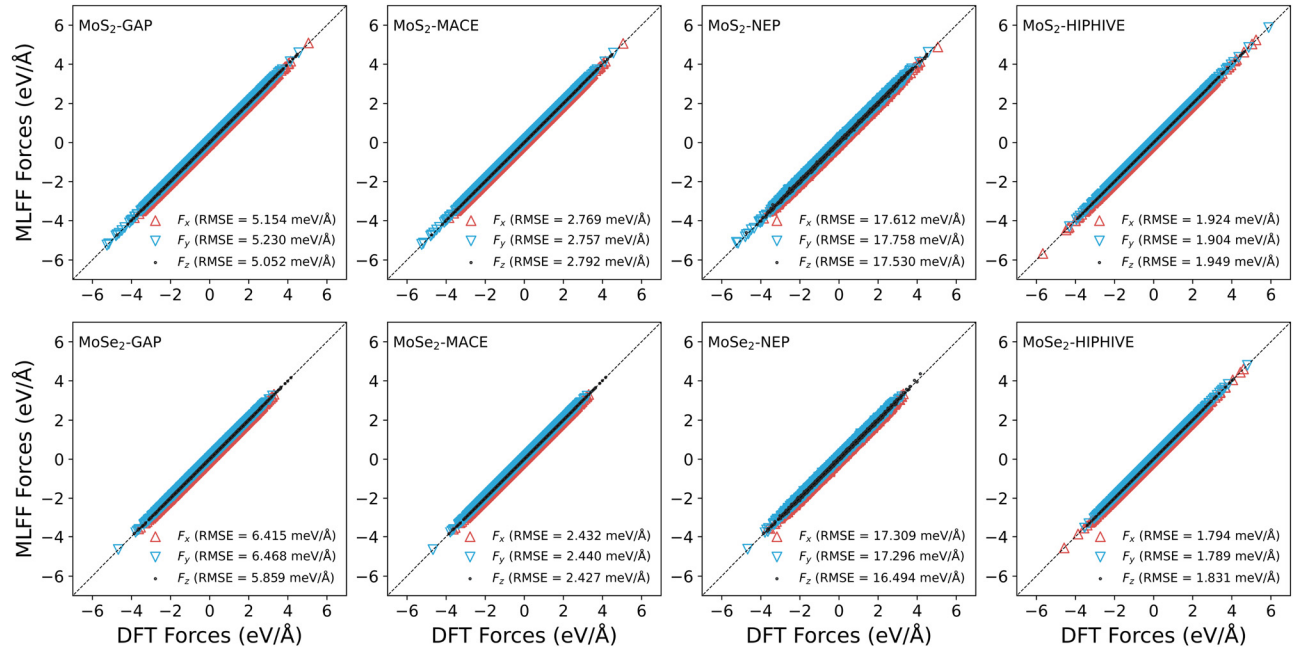


FIG. 1. Comparison of MLFF-predicted atomic forces with DFT reference values for monolayer MoS₂ and MoSe₂ on an independent test set.

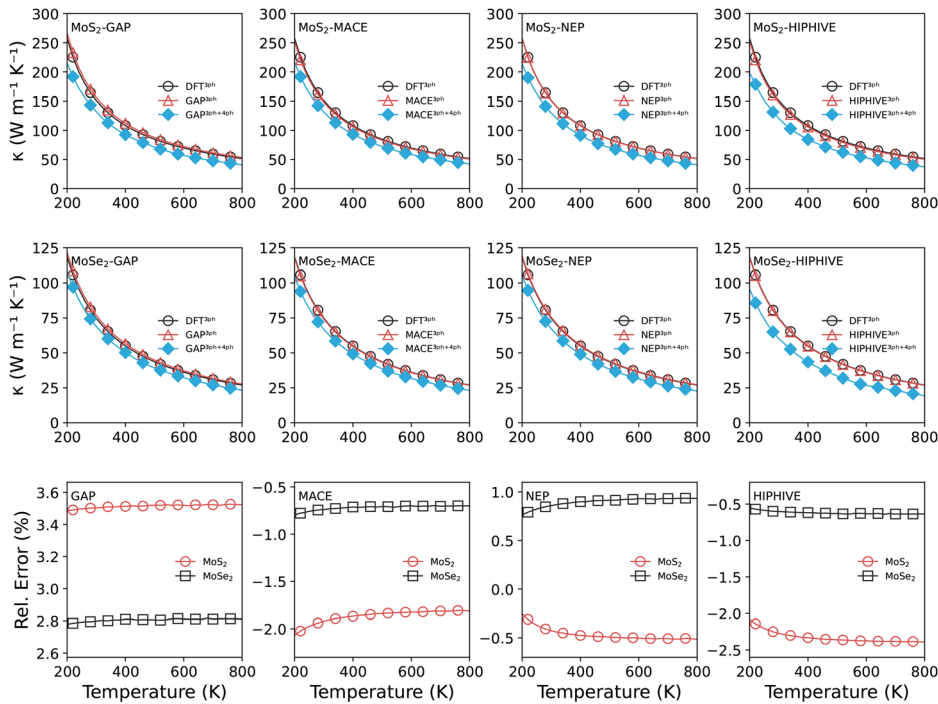


FIG. 2. Lattice thermal conductivity of MoS₂ and MoSe₂ as a function of temperature (200–800 K), calculated considering (i) three-phonon interactions up to the 13th nearest neighbors, and (ii) combined three-phonon (13th nearest neighbors) and four-phonon (6th nearest neighbors) interactions. The bottom panels show the relative errors of MLFF-predicted three-phonon thermal conductivities with respect to DFT values for both materials.

In all comparative κ calculations presented in Fig. 2, phonon interactions were considered up to the 13th NN shell, and the atomic displacement magnitude in the finite displacement method was set to 0.03 Å for both second- and third-order force constant evaluations. All

computations were performed using a $8 \times 8 \times 1$ supercell containing 192 atoms. For the combined three-phonon and four-phonon ($3^{\text{ph}}+4^{\text{ph}}$) scattering processes, convergence tests—performed as strongly recommended in Ref. 74—resulted in the use of a 0.04 Å

displacement and a 6th NN cutoff. In this comparison, three-phonon scattering processes were considered consistently across all models and the DFT reference.

For MoS₂, NEP yields the closest agreement with DFT, with relative errors $(100[\kappa_{MLFF} - \kappa_{DFT}]/\kappa_{DFT})$ remaining below 0.6% across the entire temperature range, as seen in the bottom row of Fig. 2. GAP shows the largest deviations, with errors up to 3.5%, followed by HIPHIVE with deviations reaching 2.4%. MACE also performs well, though its deviations can rise to about 2.1%. For MoSe₂, the overall trend is similar: NEP and HIPHIVE both remain within 1% relative error, while MACE shows modest deviations under 0.8%. GAP again presents the largest differences, up to about 2.8%. These comparisons indicate that all models produce reliable predictions of thermal conductivity, with NEP consistently showing the best agreement with DFT. The somewhat larger deviations for GAP, and to a lesser extent HIPHIVE and MACE, highlight subtle differences in force-matching accuracy. Such variations underscore the importance of careful potential selection when quantitative precision in monolayer thermal transport is required.

For the 3rd-order calculations, the 13th NN cutoff was selected based on a systematic convergence analysis of κ as a function of the NN range; see Fig. 3. Subsequently, this value was adopted as a reference point for the previous comparison of κ in different interatomic potentials. However, the level of fluctuations beyond the 13th NN is not the same for different approaches, as illustrated in Fig. 3. The more pronounced fluctuations observed in MLFFs' predictions arise from both physical and numerical factors. Physically, κ depends on the IFCs, and truncating interactions at different distances alters the included phonon-phonon scattering pathways. Numerically, MLFFs are data-driven models that interpolate atomic forces based on training data distributions. As the interaction cutoff increases, models must extrapolate to less-represented atomic environments, which can

introduce instability or increased error, particularly when long-range interactions are weak but non-negligible. In contrast, DFT provides forces derived from a self-consistent quantum-mechanical formalism, which is inherently less sensitive to such extrapolation and better captures the behavior of interaction decay. The force prediction RMSEs presented in Fig. 1 and the further analysis presented below confirm that the MLFFs remain accurate within the trained range. The moderate fluctuation in κ is not due to overfitting or extrapolation errors, as evidenced by consistent performance of the test set and strong agreement with DFT throughout the temperature range.

To ensure consistent and accurate thermal conductivity predictions using the solution of PBTE, we find it more appropriate to average the values over a small range extending slightly beyond the DFT convergence threshold. Specifically, the values of κ at 300 and 600 K averaged over the 13th–18th NNs' range are summarized in Table II (columns labeled 3^{ph}), together with the relative errors referenced to DFT. This procedure yields room-temperature κ values of 153 Wm^{−1}K^{−1} for monolayer MoS₂ and 74 Wm^{−1}K^{−1} for monolayer MoSe₂. Relative errors of less than 5% for GAP, MACE, and NEP demonstrate that trained MLFFs achieve first-principles-level accuracy in predicting lattice thermal conductivity.

These well-converged and carefully benchmarked results lie in the upper bound of the values reported in the first-principles literature: 81–151 Wm^{−1}K^{−1} for MoS₂ and 18–75 Wm^{−1}K^{−1} for MoSe₂, determining the reference point that can be obtained by using a similar first-principles framework. Notably, the calculated κ values for both materials exceed most experimental reports, as summarized in Table I. The generally lower experimental values arise from several factors, including the inherent challenges of accurately measuring thermal conductivity in two-dimensional systems and, more critically, the unavoidable presence of structural imperfections. Even low concentrations of point defects, grain boundaries, or interactions with supporting substrates can introduce substantial phonon scattering, leading to significant reductions in the observed thermal conductivity.^{75–78}

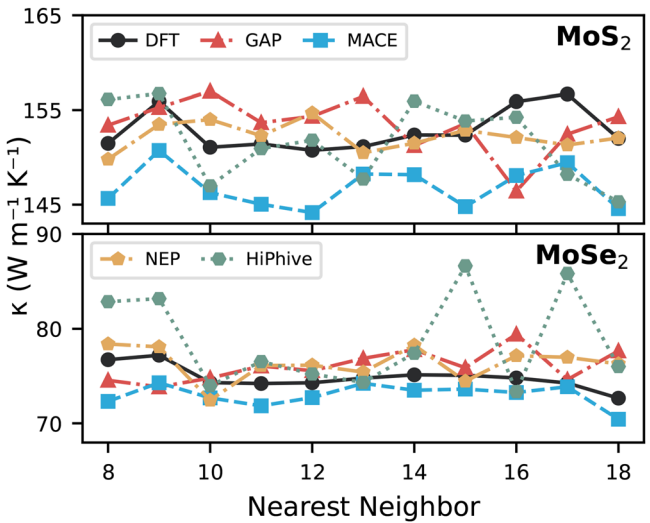


FIG. 3. Lattice thermal conductivity (κ) of monolayer MoS₂ and MoSe₂ at room temperature as a function of the nearest-neighbor cutoff used in the third-order force constant calculations. Results are shown for DFT and machine-learned force fields (GAP, MACE, NEP, and HIPHIVE), including only three-phonon (3^{ph}) scattering contributions.

TABLE II. Lattice thermal conductivity values (Wm^{−1}K^{−1}) of monolayer MoS₂ and MoSe₂ at 300 and 600 K, calculated using the optimized MLFFs. Results labeled 3^{ph} are obtained from PBTE, including only three-phonon scattering, with κ values averaged over the 13th–18th nearest-neighbor (NN) range to ensure convergence with DFT. The 4^{ph} results include both three- and four-phonon processes, where three-phonon contributions are obtained for the 13th NN, and four-phonon contributions are averaged over the 6th, 8th, and 10th NN ranges.

Material	Method	300 K		600 K	
		3 ^{ph}	4 ^{ph}	3 ^{ph}	4 ^{ph}
MoS ₂	DFT (ref)	153 (ref)	...	71 (ref)	...
	GAP	152 [−0.65%]	140	70 [−1.41%]	61
	MACE	147 [−3.92%]	139	68 [−4.23%]	60
	NEP	152 [−0.65%]	138	70 [−1.41%]	59
	HIPHIVE	151 [−1.31%]	127	70 [−1.41%]	53
MoSe ₂	DFT (ref)	74 (ref)	...	36 (ref)	...
	GAP	77 [+4.05%]	72	37 [+2.78%]	33
	MACE	73 [−1.35%]	70	35 [−2.78%]	33
	NEP	76 [+2.70%]	70	37 [+2.78%]	32
	HIPHIVE	79 [+6.76%]	63	38 [+5.56%]	28

On the other hand, first-principles predictions that consider only third-order phonon–phonon scattering processes may significantly overestimate the lattice thermal conductivity. Several studies have shown that the inclusion of four-phonon scattering can lead to substantial reductions in the predicted κ values. Notable examples include decreases from 3383 to 810 W m^{−1} K^{−1} in graphene,³⁴ 1303 to 180 W m^{−1} K^{−1} in monolayer *h*-BN,³⁰ 3322 to 1721 W m^{−1} K^{−1} in BAs,³⁵ 181 to 51 W m^{−1} K^{−1} in AlSb,³⁵ 421 to 210 W m^{−1} K^{−1} in BS,²⁸ 332 to 57 W m^{−1} K^{−1} in BSe,²⁸ and 109.25 to 11.67 W m^{−1} K^{−1} in Penta-NiN₂.³² For monolayer MoS₂, the material of interest in this work, Chaudhuri *et al.* reported a reduction from 133.5 to 27.7 W m^{−1} K^{−1} upon accounting for four-phonon interactions.²⁷

Motivated by these findings, we systematically examine the impact of fourth-order phonon–phonon scattering processes on the lattice thermal conductivity of the studied materials. Our approach combines an iterative solution of the Peierls–Boltzmann transport equation (PBTE) for three-phonon interactions with the relaxation time approximation (RTA) for four-phonon scattering, as implemented in FOURPHONON code. To enable accurate and computationally efficient evaluation of higher-order force constants, we employ MLFFs, which allow us to include extended interaction ranges—up to the 10th nearest neighbor—encompassing approximately 35 000 distinct fourth-order atomic displacements. In contrast, conventional first-principles methods are severely constrained by computational cost, often limiting the interaction range and potentially leading to unconverged or inconsistent predictions of κ . As in the three-phonon case, the final conductivity values were averaged over the 6th, 8th, and 10th NN cutoffs to ensure convergence and robustness (see Fig. S12 in the [supplementary material](#)).

As shown in Fig. 2, inclusion of four-phonon scattering yields a moderate reduction of less than 20% in the lattice thermal conductivity. At room temperature, the final values obtained after accounting for fourth-order phonon interactions are about 140 and 70 W m^{−1} K^{−1} for MoS₂ and MoSe₂, respectively. The corresponding reductions at 300 and 600 K are summarized in Table II (columns labeled 4^{ph}) for all MLFFs considered. Although this reduction is consistently observed across models, it is significantly less pronounced than the drastic suppression reported in earlier DFT-based studies (e.g., from 133.5 to 27.7 W m^{−1} K^{−1} in Ref. 27). These results highlight the importance of employing highly accurate MLFFs to obtain converged higher-order phonon scattering rates, thereby ensuring reliable and physically meaningful predictions of lattice thermal conductivity.

To elucidate the role of anharmonic phonon scattering further, we systematically analyzed phonon lifetimes in monolayer MoS₂ and MoSe₂ at *T* = 300 K arising from both three-phonon and four-phonon interactions. Separate figures are provided to illustrate the individual scattering channels: splitting and combination processes for the three-phonon interactions, and splitting, combination, and redistribution processes for the four-phonon interactions. These lifetimes were computed via forces obtained from both DFT and MLFFs. As shown in Fig. S2, 3^{ph} lifetimes in MoS₂ reach up to 250 ps in the low-frequency acoustic regime (<3 THz) and decrease steadily with increasing frequency. In contrast, optical phonons above ~8 THz exhibit significantly shorter lifetimes, on the order of 5–30 ps, due to the increased scattering phase space. These trends are robust across all the employed models.

The 4^{ph} lifetimes are notably longer, with acoustic modes reaching up to 7500 ps and optical branches generally exceeding 1000 ps. This disparity indicates that 4^{ph} scattering processes, despite their higher-order nature, act on longer timescales and contribute less to resistive scattering in the low-to-intermediate frequency range. MoSe₂ displays similar qualitative behavior (Figs. S4 and S8), though the lifetimes are uniformly shorter. In the 3^{ph} case, lifetimes do not exceed 200 ps, reflecting the reduced phonon group velocities due to the heavier selenium atoms. For 4^{ph} scattering in MoSe₂, lifetimes are also suppressed, typically remaining below 5000 ps, with especially short values (<1500 ps) for mid-to-high frequency optical modes. This suggests that quartic anharmonicity contributes more significantly to phonon scattering in MoSe₂ compared to MoS₂.

Overall, our results show that while 4^{ph} processes are characterized by much longer lifetimes than their 3^{ph} counterparts, their cumulative effect (particularly at elevated temperatures and for high-frequency optical modes) can still be substantial. The relative trends between MoS₂ and MoSe₂ align well with their experimentally and theoretically known thermal conductivities, highlighting the importance of including four-phonon interactions for an accurate and comprehensive description of intrinsic thermal transport. The three-phonon lifetimes predicted by all MLFFs (GAP, MACE, NEP, and HiPhive) are in excellent agreement with both the DFT results and with each other, while the four-phonon lifetimes—although not directly comparable to DFT—show mutually consistent trends across all MLFFs. Moreover, the consistent behavior observed across different MLFF frameworks underscores their capability to reliably capture both cubic and quartic anharmonic effects, provided that the models are sufficiently trained and converged.

As previously discussed, we employed an atomic displacement of 0.03 Å to compute the force constants used in both the phonon frequency and the phonon–phonon scattering rate calculations. While DFT-based forces are generally robust across a range of displacement magnitudes (typically between 0.005 and 0.04 Å) and yield consistent results, the accuracy of MLFFs in the finite displacement method (FDM) can be more sensitive to the chosen displacement. In particular, MLFFs tend to produce significant force prediction errors at very small displacement values.

To systematically assess this sensitivity, we performed third-order interatomic force constant (IFC) calculations for the considered monolayers using a range of displacement magnitudes (0.005, 0.01, 0.03, and 0.05 Å). In each case, the same displacement magnitude was employed for both second- and third-order IFC calculations to ensure consistency. As shown in Fig. 4, the phonon dispersion relations remain essentially unchanged across the tested displacements, exhibiting excellent agreement throughout the Brillouin zone for both materials. In contrast, the calculated κ values display a more pronounced dependence on displacement magnitude. For the smallest (0.005 Å) and largest (0.05 Å) displacements, the κ –*T* curves deviate noticeably, with the magnitude and direction of the variation depending on both the material and the employed MLFFs. These differences reflect the interplay between how each potential captures interatomic forces under very small or relatively large atomic perturbations in the finite-displacement framework, as well as intrinsic differences in the lattice dynamics of MoS₂ and MoSe₂—arising from their distinct atomic masses, bond strengths, and phonon spectra. By contrast, intermediate displacements of 0.01–0.03 Å yield nearly identical κ –*T* profiles for all

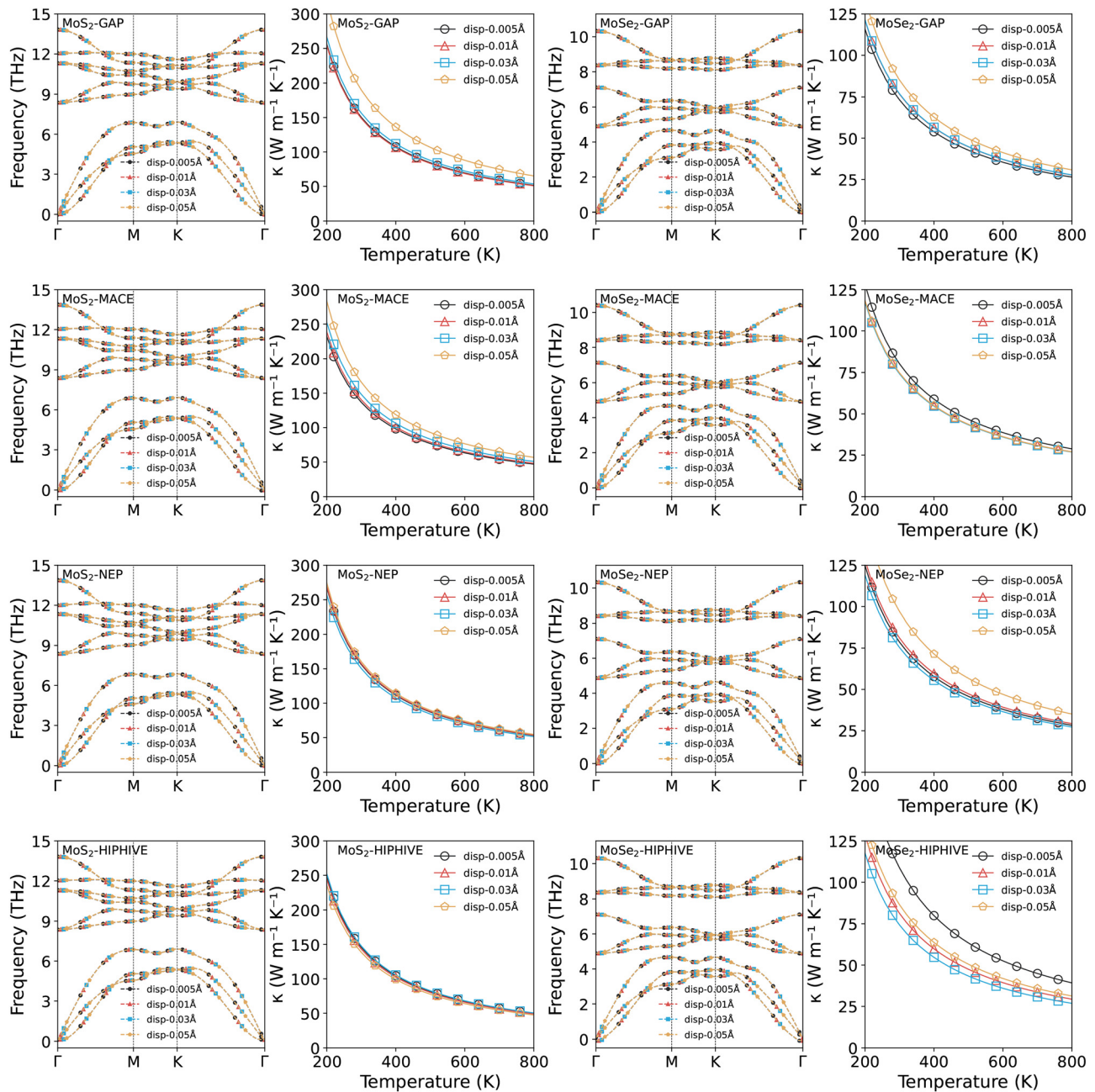


FIG. 4. Phonon dispersion relations and lattice thermal conductivity as a function of temperature for monolayer MoS₂ and MoSe₂, obtained using displacement amplitudes of 0.005, 0.01, 0.03, and 0.05 Å. Force constants are constructed up to the 13th nearest neighbors (NN).

tested models, indicating an optimal balance between numerical accuracy and the avoidance of artifacts associated with extreme displacement values. This optimal range is consistently observed for GAP, MACE, NEP, and HIPHIVE, suggesting that it is largely independent of the types of MLFF.

Compared to DFT reference thermal conductivities at 300 K (153 W m⁻¹ K⁻¹ for MoS₂ and 74 W m⁻¹ K⁻¹ for MoSe₂; see Table II),

displacements in the range of 0.01–0.03 Å yield κ values within 10% deviation for most MLFF models. This indicates that the 0.01–0.03 Å range offers an optimal trade-off between numerical stability and physical reliability. In contrast, displacements of 0.05 Å result in significantly larger deviations—exceeding 25% in some cases—notably for the MoS₂-GAP and MoSe₂-NEP models. These findings highlight the critical importance of displacement magnitude selection in

FDM-based workflows, particularly when evaluating third-order IFCs for phonon–phonon scattering and thermal transport calculations.

C. Thermal transport properties: HNEMD simulations

To further evaluate the reliability of the lattice thermal conductivity values obtained from PBTE solutions using DFT and MLFFs, we carried out homogeneous nonequilibrium molecular dynamics (HNEMD) simulations (see Ref. 56 for further details). This heat current-based dynamical evaluation yields κ_{total} values of 141 ± 7.6 and $61 \pm 4.9 \text{ W m}^{-1} \text{ K}^{-1}$ for MoS_2 at 300 and 600 K, respectively, and 72 ± 5.8 and $32 \pm 3.5 \text{ W m}^{-1} \text{ K}^{-1}$ for MoSe_2 at the same temperatures, as depicted in Fig. 5. The in-plane, κ_{xi} and out-of-plane, κ_{xo} phonon contribution to the total conductivity along the x -direction, κ_{Total} are

calculated separately within this approach. The time evolution profiles show that κ_{xi} dominates the total thermal conductivity, while κ_{xo} remains notably smaller in all cases. This behavior is physically expected because in-plane (LA/TA) phonons have higher group velocities due to the stiffness of covalent bonds in the plane, and their lifetimes are comparatively longer. In contrast, out-of-plane (ZA) phonons are softer modes with quadratic dispersion near the Γ point, resulting in lower group velocities and stronger anharmonic scattering, which together limit their contribution to heat transport.

These MD results serve as independent benchmarks for validating MLFF-based predictions. In particular, the fourth-order-corrected κ values from GAP ($140 \text{ W m}^{-1} \text{ K}^{-1}$), MACE ($138 \text{ W m}^{-1} \text{ K}^{-1}$), and NEP ($137 \text{ W m}^{-1} \text{ K}^{-1}$) are in excellent agreement with the HNEMD value of $141 \pm 7.6 \text{ W m}^{-1} \text{ K}^{-1}$ for MoS_2 at 300 K, deviating by less than

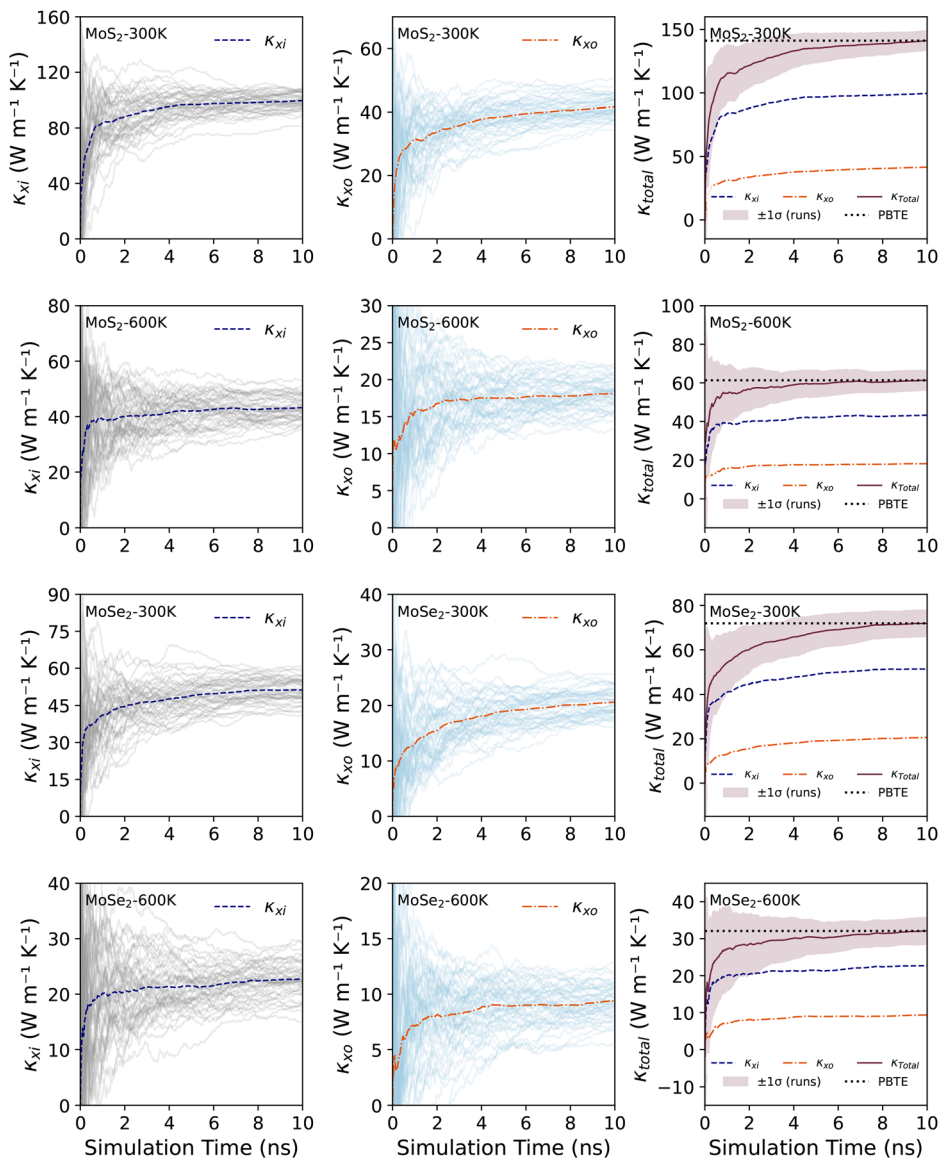


FIG. 5. Lattice thermal conductivity components (κ_{xi} , κ_{xo} , κ_{total}) of monolayer MoS_2 and MoSe_2 at 300 and 600 K, obtained from HNEMD simulations. Here, κ_{xi} and κ_{xo} represent the in-plane and out-of-plane phonon contributions along the x axis, respectively, while κ_{total} is their sum. The solid lines show averages over 50 independent runs, and the shaded areas indicate the corresponding $\pm 1\sigma$ statistical uncertainties.

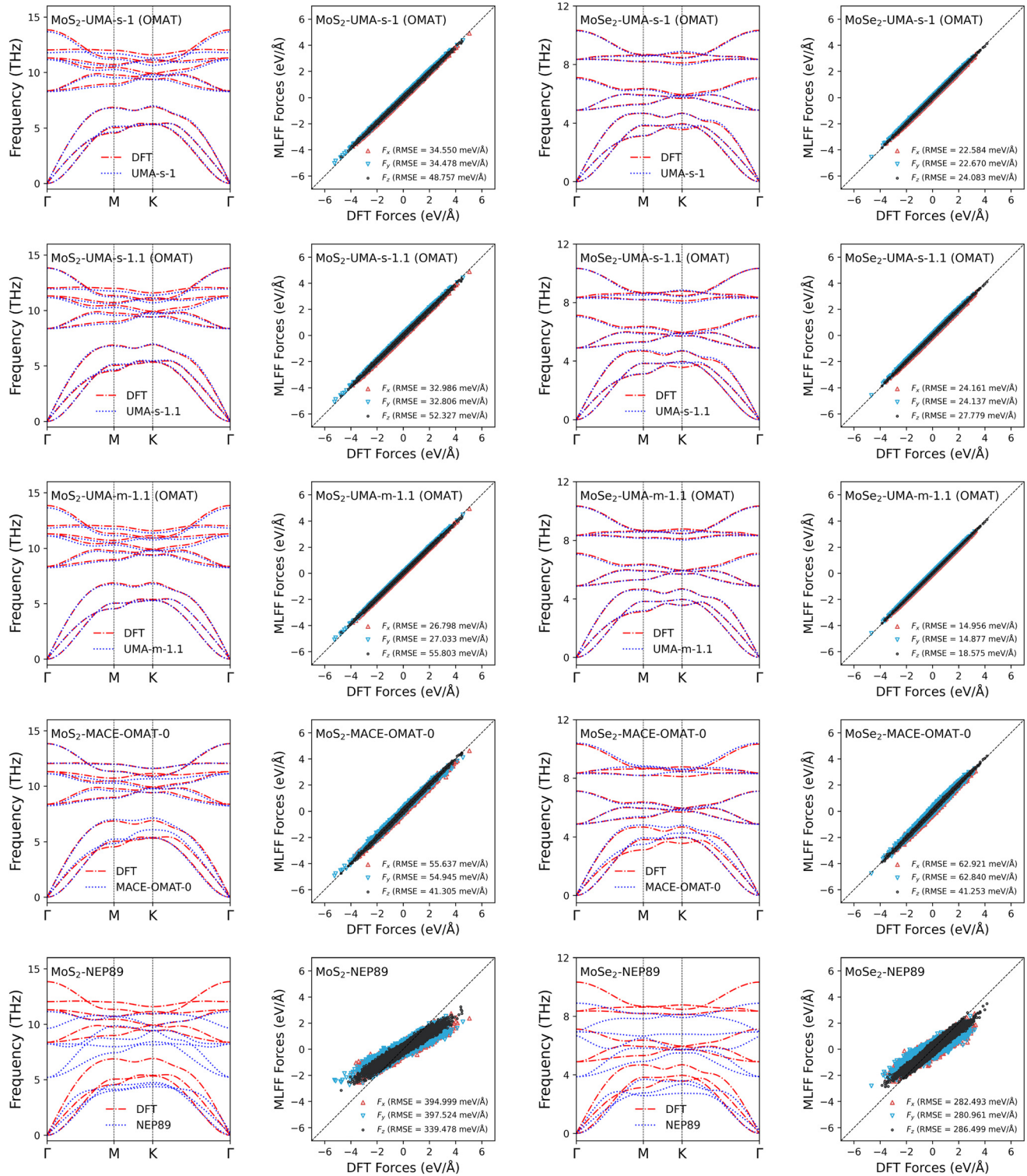


FIG. 6. Phonon dispersion relations and atomic force predictions for monolayer MoS_2 and MoSe_2 , evaluated using various universal MLFFs: UMA-s-1, UMA-s-1.1, UMA-m-1.1, MACE-OMAT-0, and NEP89. For each model, phonon spectra are compared with density functional theory (DFT) results, and the accuracy of predicted atomic forces is quantified by the root mean square error (RMSE) with respect to DFT values using independent test datasets.

3%. A similarly close match is observed for MoSe₂, where GAP (72 Wm⁻¹K⁻¹), MACE (70 Wm⁻¹K⁻¹), and NEP (70 Wm⁻¹K⁻¹) all reproduce the HNEMD value of 72 ± 5.8 Wm⁻¹K⁻¹ within the margin of statistical uncertainty. This high level of consistency reinforces the robustness of our MLFFs-based PBTE framework and further suggests that the dramatic κ reductions reported in some earlier monolayer MoS₂ studies after including fourth-order scattering are likely overestimated.

D. Universal potentials

The development of *universal interatomic potentials*, also referred to as pretrained foundation models, has recently emerged as a promising route toward transferable and data-efficient models for atomistic simulations across diverse material classes. Unlike traditional machine-learned force fields (MLFFs), which are trained for specific systems, these models are pretrained on large chemically diverse datasets and can be adapted via fine-tuning. Representative examples include MACE-OMAT-0,⁷⁹ UMA⁸⁰ developed by Meta AI, and NEP89.⁸¹ Their goal is to generalize atomic interactions and enable reliable predictions of energies, forces, and virials even in previously unseen systems.

We evaluated the transferability of these potentials in their released form, without any fine-tuning, by testing their ability to generate accurate interatomic force constants (FCs) for monolayer MoS₂ and MoSe₂. The harmonic properties were first examined through phonon dispersions derived from second-order FCs and force-parity plots benchmarked against DFT (see Fig. 6). UMA-s-1.1 and UMA-m-1.1 provided the closest agreement across the Brillouin zone, while MACE-OMAT-0 showed a modest high-frequency bias. NEP89 produced large force errors and distorted dispersions and was therefore excluded from transport calculations.

The anharmonic response was assessed by computing the lattice thermal conductivity at 300 and 600 K using Peierls–Boltzmann transport equation solutions with third- and fourth-order FCs. Consistent

with the trained MLFFs, the third-order force constants were averaged over neighbor cutoffs ranging from the 13th to the 18th shell, whereas the fourth-order force constants were calculated using a displacement amplitude of 0.04 Å and averaged over the 6th–10th shells. The corresponding results are summarized in Table III.

A closer inspection of the relative errors highlights clear trends in all evaluated models. For MoS₂, UMA-s-1.1 reproduces the three-phonon DFT value within +8.5%, while its four-phonon prediction differs from the HNEMD benchmark by less than 1%, indicating excellent agreement. UMA-m-1.1 also performs consistently well, with deviations within -1.3% (3^{ph}) and -7.1% (4^{ph}). By contrast, UMA-s-1 systematically underestimates κ , reaching errors up to -23% for the four-phonon case at 600 K, while MACE-OMAT-0 tends to overestimate, exceeding +12% in several cases. For MoSe₂, the variability is more pronounced: UMA-s-1.1 overpredicts three-phonon conductivities by nearly 40%, although its four-phonon values remain within +1.4% of HNEMD. UMA-m-1.1 maintains errors below 10%, whereas MACE-OMAT-0 underestimates four-phonon results by -14 to -16%. These patterns demonstrate that while certain universal potentials can reach near-DFT accuracy, model-to-model fluctuations on the order of 10%–20% remain common.

Overall, UMA-s-1.1 and UMA-m-1.1 delivered harmonic and anharmonic transport properties competitive with task-specific MLFFs even without fine-tuning, but significant variability across models was observed. UMA-s-1 underestimated conductivities, MACE-OMAT-0 showed pronounced deviations, and NEP89 was excluded due to large force errors. Notably, all models except NEP89 reproduced the quadratic acoustic dispersion near the Γ point, capturing long-wavelength phonons and hence dynamical stability. Since acoustic modes are the main heat carriers in semiconductors, this accuracy is critical for reliable κ predictions. While universal models are not yet a substitute for custom MLFFs in high-precision studies, their performance in completely unseen systems highlights their potential as efficient starting points for fine-tuned applications.

TABLE III. Lattice thermal conductivity values (Wm⁻¹K⁻¹) of monolayer MoS₂ and MoSe₂ at 300 and 600 K, calculated using various universal potentials. Results labeled 3^{ph} are obtained from PBTE, including only three-phonon scattering, with κ values averaged over the 13th–18th nearest-neighbor (NN) range to ensure convergence with DFT. The 4^{ph} results include both three- and four-phonon processes, where three-phonon contributions are obtained for the 13th NN, and four-phonon contributions are averaged over the 6th, 8th, and 10th NN ranges.

Material	Method	300 K		600 K	
		3 ^{ph}	4 ^{ph}	3 ^{ph}	4 ^{ph}
MoS ₂	DFT (ref)	153 (ref)	...	71 (ref)	...
	HNEMD (ref)	...	141 ± 7.6 (ref)	...	61 ± 4.9 (ref)
	UMA-s-1	143 [-6.54%]	114 [-19.15%]	66 [-7.04%]	47 [-22.95%]
	UMA-s-1.1	166 [+8.50%]	140 [-0.71%]	77 [+8.45%]	56 [-8.20%]
	UMA-m-1.1	151 [-1.31%]	131 [-7.09%]	70 [-1.41%]	54 [-11.48%]
	MACE-OMAT-0	174 [+13.73%]	158 [+12.06%]	80 [+12.68%]	67 [+9.84%]
MoSe ₂	DFT (ref)	74 (ref)	...	36 (ref)	...
	HNEMD (ref)	...	72 ± 5.8 (ref)	...	32 ± 3.5 (ref)
	UMA-s-1	75 [+1.35%]	61 [-15.28%]	39 [+8.33%]	25 [-21.88%]
	UMA-s-1.1	103 [+39.19%]	73 [+1.39%]	49 [+36.11%]	30 [-6.25%]
	UMA-m-1.1	80 [+8.11%]	66 [-8.33%]	39 [+8.33%]	28 [-12.50%]
	MACE-OMAT-0	70 [-5.41%]	62 [-13.89%]	34 [-5.56%]	27 [-15.62%]

TABLE IV. Average computation times for evaluating atomic forces using different methods. MLFF timings are averaged over 100 structures.

Method	Comp. time	Hardware
GAP	1.45 s	CPU via ASE
MACE-GPU	0.37 s	1 × A100 GPU
MACE-CPU	4.96 s	CPU via ASE
NEP	0.05 s	CPU via ASE
HIPHIVE	0.93 s	CPU via ASE
DFT	90 min	4 × A100 GPUs

IV. COMPUTATIONAL TIMES

Since high-order anharmonic calculations are computationally demanding, the practical value of MLFFs and universal potentials depends not only on accuracy but also on computational efficiency. Table IV reports the average time required to compute atomic forces for the considered methods.

All MLFFs achieve speedups of several orders of magnitude compared to DFT, reducing the force evaluation time from hours to milliseconds. Among them, GPU-accelerated MACE delivers the highest performance overall, while NEP offers the lowest latency on CPUs, making it particularly attractive for large-scale MD. GAP and HIPHIVE provide balanced accuracy–efficiency tradeoffs with stable throughput, and CPU-based MACE remains competitive despite being slower. By contrast, DFT is prohibitively expensive, requiring ~90 min per structure, even on multiple GPUs.

These efficiency gains are not merely technical: they make it feasible to include extended neighbor cutoffs and fourth-order IFCs in PBTE calculations, and they also enable long-time molecular dynamics simulations that are beyond the reach of first-principles methods. In practice, the ability to choose between GPU-accelerated and CPU-based MLFFs provides flexibility depending on the available resources and the scale of the targeted problem, ranging from high-throughput screening to detailed transport modeling.

V. CONCLUSIONS

The characterization of thermal transport in TMDs, and low-dimensional materials more broadly, has been persistently hampered by large discrepancies between the calculated and the measured lattice thermal conductivities. In this work, we combined state-of-the-art MLFFs with high-accuracy *ab initio* calculations to resolve these long-standing inconsistencies. Our systematic evaluation, which integrates MLFFs with both the PBTE and molecular dynamics simulations, demonstrates that this approach provides a reliable and computationally efficient reference for reconciling conflicting findings in the literature. All the tested MLFFs (GAP, MACE, NEP, and HIPHIVE) successfully capture the essential physics of lattice thermal transport. Notably, the NEP model achieves good fidelity to first-principles benchmarks while simultaneously delivering an order-of-magnitude improvement in simulation speed when compared with the other tested alternatives. This powerful combination of accuracy and efficiency marks a significant step forward, enabling predictive and high-throughput studies of thermal transport that were previously intractable.

Beyond benchmarking, our analysis clarifies the role of higher-order phonon–phonon interactions. We found that quartic anharmonicity introduces only moderate corrections, in contrast to earlier predictions of drastic reductions, yielding intrinsic conductivity limits of MoS₂ and MoSe₂ at approximately 140 and 70 Wm^{−1}K^{−1}, respectively. This refinement highlights the need for convergence-tested methodologies and illustrates the value of MLFFs in extending the accuracy of first-principles calculations to regimes that were previously inaccessible.

Looking ahead, MLFFs emerge not only as efficient substitutes for density functional theory in quantitative transport studies but also as enabling tools for broader applications. The encouraging performance of transferable universal potentials points toward a pathway for general-purpose force fields that can accelerate high-throughput exploration while retaining physical fidelity. Such advances set the stage for the solution of more complex thermal transport problems in two-dimensional systems, including the critical influence of defects, interfaces, and nanoscale heterogeneity.

SUPPLEMENTARY MATERIAL

See the [supplementary material](#) for additional tables and figures supporting the main findings. Tables S1–S3 summarize the training and model-specific hyperparameters of the machine-learned force fields (GAP, MACE, and NEP). Table S4 lists the real-space cutoff distances corresponding to successive nearest-neighbor interactions in MoS₂ and MoSe₂, which were used as NN-based cutoff values in the three-phonon lattice thermal conductivity calculations. Figures S1–S9 present phonon dispersions and frequency-dependent three- and four-phonon lifetimes for monolayer MoS₂ and MoSe₂, highlighting the consistency between the DFT and MLFF predictions. Figures S10–S13 show the convergence behavior of the lattice thermal conductivity with respect to the interaction cutoff and displacement amplitude, while Fig. S14 compares the DFT and ML-predicted forces for the displaced supercells employed in constructing the third-order interatomic force constants.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Tugbey Kocabas: Conceptualization (lead); Data curation (equal); Formal analysis (equal); Investigation (equal); Methodology

(equal); Project administration (lead); Supervision (equal); Validation (equal); Visualization (equal); Writing – original draft (lead); Writing – review & editing (equal). **Murat Keçeli:** Conceptualization (lead); Data curation (equal); Formal analysis (equal); Investigation (equal); Methodology (equal); Project administration (lead); Supervision (equal); Validation (equal); Writing – original draft (equal); Writing – review & editing (equal). **Tanju Gürel:** Data curation (equal); Formal analysis (equal); Investigation (equal); Methodology (equal); Validation (equal); Writing – original draft (equal); Writing – review & editing (equal). **Milorad V. Milošević:** Data curation (equal); Formal analysis (equal); Investigation (equal); Methodology (equal); Writing – original draft (equal); Writing – review & editing (equal). **Cem Sevik:** Conceptualization (lead); Data curation (equal); Formal analysis (equal); Investigation (equal); Methodology (equal); Project administration (lead); Validation (equal); Visualization (equal); Writing – original draft (lead); Writing – review & editing (equal).

DATA AVAILABILITY

The MLFFs and the training test and validation data that support the findings of this study are openly available in Zenodo at <https://doi.org/10.5281/zenodo.17911641> (Ref. 82). Also, any additional data that support the findings of this study are available from the corresponding author upon reasonable request.

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