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Tunable Topological Phonon for Next- generation Quantum Transduction

September 2025

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U.S. DEPARTMENT
of **ENERGY**

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Abstract

This project aims to understand the critical factors that determine transduction performance of topological phonons across an oxide perovskite/tungsten diselenide heterojunction. We will investigate mechanisms of their propagation and interfacial coupling using modeling and machine learning approaches. Methods include density functional theory, molecular dynamics, numerical transport simulations, and active learning for building up a training dataset for force field development.

Summary

In this work, we aim to understand the critical factors that determine the performance of topological phonon (TP) transduction, by revealing the mechanisms of their propagation and interfacial coupling through a combination of modeling and machine learning approaches. While TPs have been theorized and observed in isolated systems, their transport in heterostructures remains unexplored, where steep challenges lie in the complexity of coupled topological phenomena. Elucidation of dynamic TP behavior during their transport and interaction with external chemical and structural environments remains an active field of research. Our work will demonstrate the feasibility of directly representing TP and their topological transport using atomistic modeling, and set the foundation for establishing a generic model to predict the performance of quantum transducers for qubit co-design.

Acknowledgments

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Acronyms and Abbreviations

TP	Topological Phonon
MD	Molecular Dynamics
DFT	Density Functional Theory
WP	Wave Packet

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1.0 Introduction

The next generation of quantum systems call for revolutionary transduction. For example, quantum computers require scalability to realize their “quantum advantage”: the potential to solve complex problems in minutes instead of eons on classical systems. This necessitates distributed networks with interconnected components for processing and storage (Figure 1). The processing units – the only component realized today – are generally built upon superconducting qubits,¹ which provide fast gate operations but suffer from short coherence times; as such, they are not suitable for long-term storage or long-range operations. Hybrid quantum computing that interconnects different types of qubits, including spin qubits for long-lived quantum memory,² and optical qubits that facilitate long-range entanglement,³ is thus needed. However, despite promising theories on how individual types could work separately, efficiently coupling them together to create integrated networks remains unexplored. Phonons offer the best compromise between long-range transport and low decoherence, and provide a natural bridge between different qubit modalities due to their ability to couple to various quantum systems.⁴⁻⁶ However, they also suffer from decoherence caused by disorder and two-level system noise, and energy-loss from scattering. To address these challenges, we propose an emerging class of quasi-particles – the topological phonon (TP) as a solution that ensures robust, backscatter-free transport, protecting coherence during transduction.⁷

Our proposed research develops theories that enable robust, low-loss quantum transduction mechanisms, directly addressing DOE’s mission to advance quantum information science. Combining atomistic/numeric simulations and machine learning approaches, our work sets in motion the development of a generic model to predict the performance of quantum transducers, supporting goals under National Quantum Initiative (NQI) to establish next-generation quantum networks. Establishing the foundation for a new class of TP-based transducers—an innovation that could redefine quantum device architectures, as well as transforming our capability into the corresponding tool for qubit co-design, will enable us to address a broader range of sponsors’ needs.

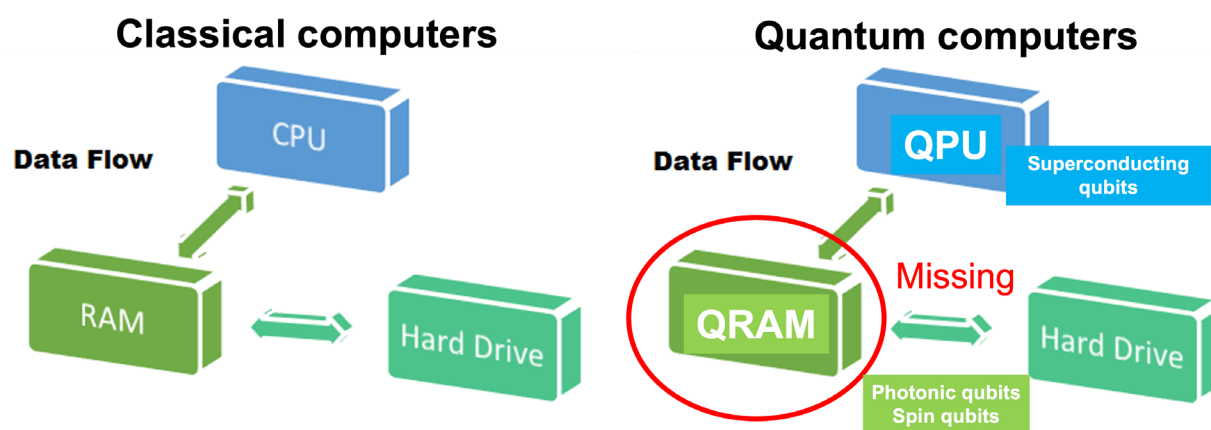


Figure 1. Compared to classical computers, current quantum computers lack essential components (such as quantum random access memory, or QRAM) distributed networks to realize scalability. The coupling among different types of qubits that is necessary for realizing the quantum network, is also missing.

2.0 Research Design and Methodology

Among the many types of TPs, we focus on the Weyl and chiral phonons for their topology-protected directionality and robustness against disturbance. Their strong coupling to electrons and spins also enables electron-phonon-spin conversions. We propose to investigate the TP transport across an oxide perovskite/WSe₂ heterojunction. Oxide perovskites (BaTiO₃, SrTiO₃ etc.) host Weyl phonons.⁸ They also possess potentially strong piezoelectric effects that make them excellent candidates for superconducting qubit-TP transducer interfaces.⁹ WSe₂ hosts chiral phonons and has been identified as a candidate for spin qubits,^{10, 11} and our choice can benefit from PNNL's major efforts in the syntheses and design of transition metal dichalcogenides.

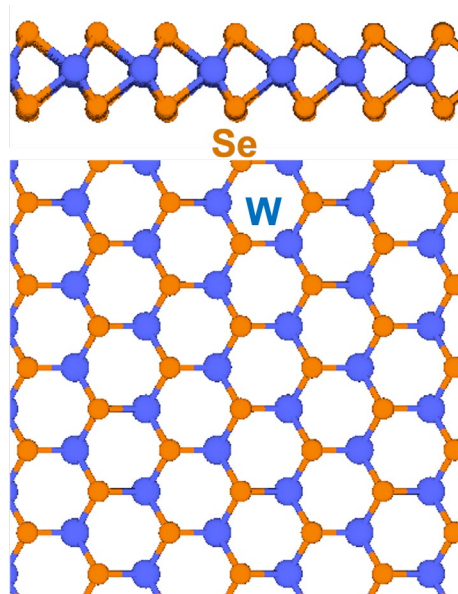


Figure 2. The side view and top view of 1H-WSe₂ monolayer. The threefold rotational symmetry is essential in ensuring the presence of chiral phonons.

To parameterize the governing equations for accurately representing the TP dynamics, we need to understand TP propagation and coupling across the heterostructures in the transducers, yet these TP behaviors are not well understood where steep challenges lie in the complexity of coupled topological phenomena at ultra-low temperatures. We plan to tackle this by directly representing the TP behavior in nanostructures with atomic-level inhomogeneities. Our parameterized *ab initio* wave packet (WP) approach based on molecular dynamics (MD),¹² developed under the Chemical Dynamics Initiative (CDI), is specifically designed for simulations in the millikelvin-temperature range. Still, challenges arise in the accurate representation of TP using stable atomic displacements; their behaviors at ultra-low temperatures are expected to be strongly influenced by lattice anharmonicity, which may not be captured by the existing classical force fields. As such, we propose to expand our WP approach to investigate TP transport.

- We will first identify chiral phonon modes in WSe₂ using density function theory (DFT) simulations. WP will be applied to demonstrate TP interfacial scattering and understand chiral phonon propagation in pristine and defected WSe₂.

All work will be done using the computation resources available at PNNL (The PNNL Institutional Computing program, or PIC).

3.0 Results and discussion

3.1 Benchmarking interatomic potentials

The interatomic potential defines the law of physics in classical MD simulations; thus, a potential that accurately describes atomic interactions is essential for ensuring reliable simulation predictions. For phonon transport and heat transfer studies, the most important and fundamental benchmark is the phonon dynamical matrix. Therefore, when choosing from available potentials of Tersoff¹³ and Stillinger-Weber¹⁴ (SW) types from literatures, we calibrated their performance against the phonon dispersion, which represents the eigenvalues of the dynamical matrices. The dispersion relationship was calculated using the GULP package,¹⁵ and our results agree well with previous benchmarks against DFT predictions.¹⁴

To further benchmark the potential in practical MD simulations, we set up a single slab of 1H-WSe₂ containing 108×108 conventional unit cells (34,992 atoms) in a commensurate simulation cell with fixed boundary conditions (Figure 3). The simulations are conducted using the LAMMPS package.¹⁶ Both the Tersoff and SW potentials can preserve stable lattice structures that are almost geometrically identical to experimental measurements and DFT predictions. While the 2D slab largely remain stationary at temperatures lower than 100 K, there are significant “wobbling”—collective atomic movements forming long-wavelength phonons—across the slab at higher temperatures.

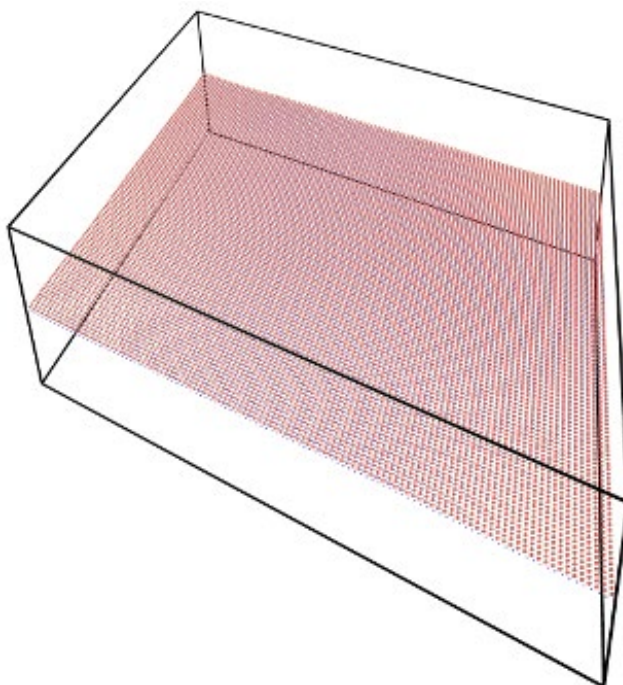


Figure 3. The side view and top view of 1H-WSe₂ monolayer. The threefold rotational symmetry is essential in ensuring the presence of chiral phonons.

In addition, we calculated the phonon density of states (PDOS), a higher-level physical quantity derived from phonon dispersion relations. Different from 3D materials, where the PDOS is largely independent of temperature, there is noticeable change in PDOS in monolayer 1H-WSe₂ at 100 and 300 K (Figure 3). This indicates that significant lattice distortion/relaxation occurs

when the temperature increases in addition to thermal expansion, which can be attributed to stronger atomic movements at elevated temperatures. There are also consistently a large amount of phonon states near zero Hz, which are attributed to the long-wavelength phonons (wobbling) which have low frequencies. Overall, both the Tersoff and SW potentials predict phonon dispersions and PDOS that match well with DFT predictions. The SW potential was eventually selected due to its higher computational efficiency (50% faster for ~35,000-atom simulations).

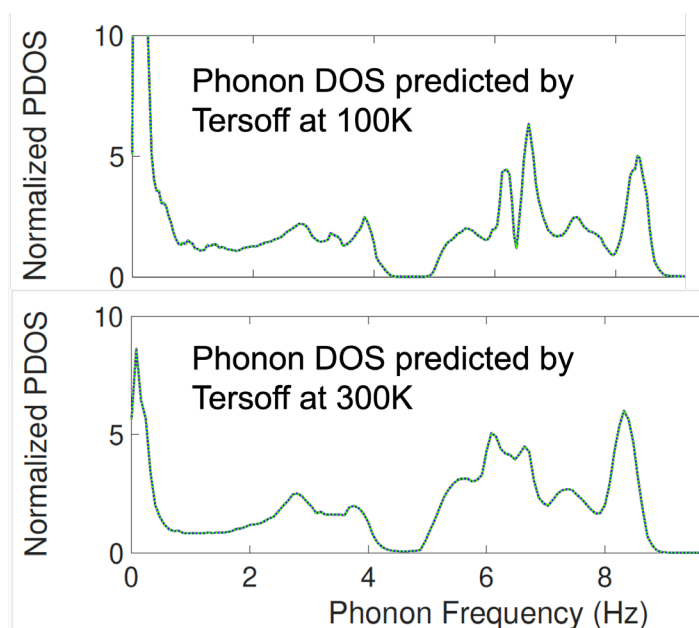


Figure 4. Comparison of PDOS predicted by Tersoff potential at 100 and 300 K, respectively. The noticeable difference at difference temperatures is a pronounced feature observed in 2D materials that is rarely present in 3D.

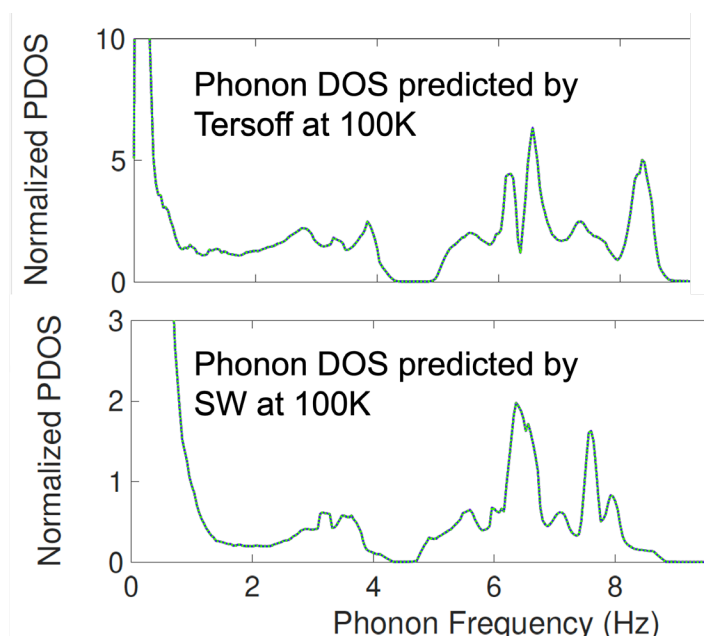


Figure 5. Comparison of PDOS predicted by Tersoff and SW potentials at 100 K show consistent profiles.

3.2 Calculating the Chiral Phonon Eigenvector

1H-WSe₂ monolayer hosts multiple chiral phonons.¹⁷ Only those with non-zero momentum, i.e. chiral phonons that can propagate are of interest, which can realize the function of transduction. We chose the chiral phonon at K point ([1/3, 1/3]) in the first-Brillouin zone—commonly referred to as the LO(K) chiral phonon¹⁸—as our case study (LO represents the “longitudinal optical” phonon branch).

The WP simulation requires the phonon eigenvector as inputs, which is used to calculate the initial atomic displacements and velocities that can correctly represent the phonon of interest. The eigenvector of LO(K) chiral phonon was calculated using GULP (Table 1), which yields two degenerate optical phonons at K with almost identical frequencies (6.39 and 6.57 THz). The eigenvectors take the form of atom-wise normalized unity vectors indicating the direction and amplitude of the atomic displacement. The complex form indicates the presence of a phase factor (the imaginary component) and represents circular movement of the atom. Both of the degenerate eigenvectors show zero movement in W atoms, where Se atoms move in circular motions around their equilibrium lattice points, consistent with previous studies. Note the two degenerate phonons have perpendicular eigenvectors with a phase shift of 90 degrees; thus, we conveniently designate them as LO and TO (transverse optical) branches. It is also noteworthy that while the chiral phonon is commonly referred to as LO(K), it is effectively a linear combination of the degenerate LO and TO phonons.

Table 1. The eigenvectors of the two degenerate LO(K) and TO(K) phonons

Components of the eigenvector	LO	TO
W_x	0	0
W_y	0	0
W_z	0	0

Components of the eigenvector	LO	TO
Se _{1x}	-0.032-0.499i	0.054-0.497i
Se _{1y}	0.499-0.032i	-0.497i-0.054
Se _{1z}	0	0
Se _{2x}	-0.032-0.499i	-0.054+0.497i
Se _{2y}	0.499-0.032i	0.497+0.054i
Se _{2z}	0	0

3.3 Testing the WP simulation of the LO(K) chiral phonon

Atomic displacements were performed to the 108×108 slab 1H-WSe₂ according to the formalism described in our previous study.¹⁹ The excited phonon would then propagate according to its eigenvectors in the MD simulation. Snapshots of the phonon propagation, where the kinetic energy of the atoms is visualized to represent the wave packet, are shown in Figure 6. While initially excited as a single chiral phonon, it soon breaks down into its two degenerate components. The low decoherence is attributed to several possible factors: 1) the eigenvectors may not be accurate enough numerically; 2) the interatomic potential may not be accurate enough. Even a slight breakdown of the threefold rotation symmetry prevents the chiral phonon from forming properly; 3) as the wave packet has finite size, its frequency has a finite span too which contributes to its degeneration. Further study into enhancing the phonon coherent length is recommended.

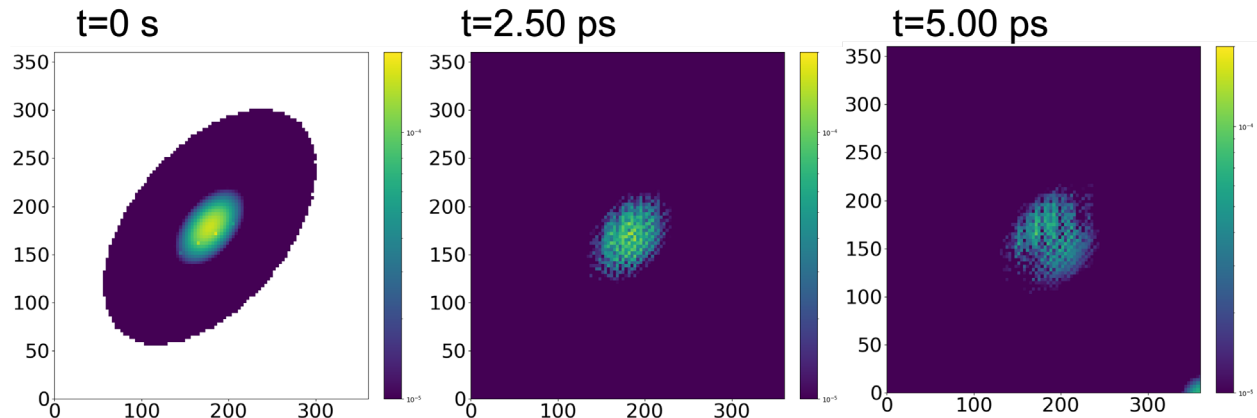


Figure 6. Propagation of the LO(K) chiral phonon in WP simulations. Initially a single phonon, it soon broke down into its two degenerate components.

4.0 Conclusion

We have successfully evaluated the feasibility of applying classical molecular dynamics in simulating chiral phonons. While the chiral phonon can be correctly excited in the crystal lattice, the coherent time is currently observed to be low. Further study into the underpinning mechanism and methods to enhance coherency is recommended.

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