Topological phononic materials: Computation and data

Xing-Qiu Chen,¹,² Jiaxi Liu,¹ and Jiangxu Li¹

¹Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Science, Shenyang 110016, China
²Correspondence: xingqiu.chen@imr.ac.cn

Considering the current volume of materials data, it is impossible to investigate each compound by trial-and-error experiments involving labor-intensive efforts. The scientists in the Shenyang National Laboratory for Materials Science developed a home-made software, HT-PHONON, selecting over 5,000 topological phononic (TP) materials out of 13,000 materials within high-throughput computational materials design combined with a big data analysis. Furthermore, an online database for TP materials has been constructed, which is now freely open to the public community through the website www.phonon.synl.ac.cn. In this perspective, we review this platform and discuss exciting consequences of TP materials that are expected from manipulating the phonons, linking fundamental research to potential applications.

The topological phenomenon has been extensively studied in condensed matter physics and has attracted much attention in many different fields. Recently, topological phonons in crystalline materials have emerged as a new area of rapid development in both experiments and calculations. The phonon is the energy quantum of lattice vibrations and is one of the most common quasiparticles of collective excitations that make critical contributions to many physical properties, such as thermal conductivity, thermolectricity, superconductivity, etc. Prior to 2017, topological materials research mainly focused on electronic systems, including topological insulators, topological semimetals, and topological superconductors, which have driven the frontier of condensed matter physics and materials science for about two decades. However, related topological studies of phonons were scarce at that time. Similar to electrons, phonons can also be studied by theoretical theorems and topology concepts, giving impetus to the birth of TPs.²⁻⁵

In crystalline materials, TPs generally occur because of some specific vibrations of the atomic lattice within a terahertz frequency scale. Within the crystalline state, the topological characteristics are mostly related to symmetries. Naturally, TPs produce non-trivial topologically protected phonon surface or edged states. Both energy and signals can be directionally propagated along some specific topological modes, i.e., some lattice vibration modes. They are robust against interference and leakage. Along these channels provided by topological phonons, low-dissipation transmission can be realized, resulting in promising new properties and rich application prospects. For example, topological electronic insulators can conduct electricity on their outer edges, while their bulk is insulating. Similarly, it has been suggested that materials holding topological phonons should be used to achieve anomalous heat transfer.

Of course, scientists have been hunting for these real materials for a long time. Until recently, only a few materials have been suggested. Single-Weyl TPs have been predicted in non-centrosymmetric WC-type materials⁶ and double-Weyl TPs have been predicted and experimentally confirmed in FeSi-type materials.⁷ Coexisting single- and double-Weyl TPs have been suggested in SiO₂.⁸ In addition to these single-Weyl TPs, nodal-line (ring) TPs have also been theoretically demonstrated. In the famous BCS-type superconductor MgB₂, nodal-line Weyl TPs exist in its bulk-phonon dispersions,⁶ which cross the entire Brillouin zone (BZ), and in the most typical single-atom-thick 2D material, graphene, four types of Dirac TPs and a nodal-ring TP surrounding the BZ midpoint coexist.⁷

Given the fact that the phonon obeys the Bose-Einstein statistic without limitation of Fermi energy, TPs may exist much more universally in many materials other than topological electronic systems. Although some materials have been suggested, it would be a very urgent task to effectively clarify TPs among thousands of materials. However, it is not always easy, because obtaining the phonon dispersions for a crystalline material is difficult, no matter whether it is done by calculation or experiment. To calculate phonon dispersions, it is necessary to obtain accurate force constants through density functional perturbation theory or the finite displacement method, which, however, require extremely expensive calculations. Searching for TPs to classify them, to calculate the invariant of the phonon topology, is another kind of difficulty, because TPs have to be analyzed within the whole phonon spectrum, which is much heavier than electronic systems focusing only on the Fermi level. Furthermore, experimentally elucidating TPs always requires a state-of-the-art experiment, from the growth of a high-quality single crystal to the available time of the neutron diffraction beam or inelastic X-ray scattering technique to the illustration of topologically protected phonon surface states.

In this context, in combination with a big data analysis, we designed a high-throughput workflow and calculation package (code HT-PHONON) to enable automated phononic calculations and identification of TPs among materials, as shown in Figure 1. This process mainly consists of five steps: (1) the high-throughput first-principles calculations for structural optimization and force constants through available tools (i.e., VASP, QE, etc.); (2) the construction of the dynamic matrix to derive phonons at all lattice moments in the BZ; (3) the search for all possible phonon crossing points through the conjugate gradient algorithm; (4) the analysis of those points by calculating the topological invariants; and finally (5) the classification of materials through topological invariants.⁹ In addition, we developed a framework of data collections and constructed a Topological Phononic Materials Database (www.phonon.synl.ac.cn) including their structural details, phonon spectra, topological details, and computational methodologies. On the basis of this database, we launched a free and open website to display all crystal structures and phonon spectra with the marking of topological nodal points or nodal-line (ring) TPs, and BZs, combined with a set of tables for structural details, phonons, and topological data. It provides a flexible search engine, which is also friendly to various users.

Currently, we have applied this code and database to more than 13,000 materials and, interestingly, among these, 5,014 TP materials have been identified in terms of calculated force constants (partly from our 3,000 materials calculated in-house in our laboratory and partly from publicly available force constants at Kyoto University in Japan¹⁰). As demonstrated in Li et al.,¹⁰ our results demonstrate the wide occurrence of TPs in nature, the evolution of TPs and their correlation, and several new types of TPs. For example, hourglass nodal net TPs protected by non-symmorphic symmetry in TeO₂, clean and single-type-I Weyl TPs between acoustic and optical branches in half-Heusler LiCaAs, nodal-ring and straight-line coexisting TPs in centrosymmetric Zintl...
phase ScZn, and triple and quadruple coexisting Weyl TPs in the non-centrosymmetric superconductor AuBe. This database has provided a rich platform to search for more interesting TP materials.

Significantly, thousands of TPs exist, and exciting consequences can be expected by manipulating the phonons linking fundamental research to potential applications. On the one hand, we expect that many phenomena related to the elementary bosons can be studied based on our database of TP materials and can be modulated by pseudo-spins and pseudo-spin-orbit couplings from crystal symmetry and pseudo-angular moments for the possible occurrence of various phonon-related quantum Hall effects, quantum anomalous Hall effects, and quantum spin Hall effects, in analogy to topological electronic systems. Breaking time-reversal symmetry will produce phonon states with non-zero Chern numbers, that is, the phonon Hall effect. It has a unidirectional non-scattered phonon boundary mode. The one-way edge states are ideal channels to realize dissipationless phonon wave guides and can be also utilized for the construction of ideal phonon diodes in a multiterminal system. By breaking spatial inversion symmetry, valleys with non-zero Berry curvature exist, which can be used as a new quantum degree of freedom for regulating phonon transport. It would result in a valley phonon Hall effect. The valley polarized boundary states with valley-momentum locking have many potential applications as phonon valley filters, phononic antennas, and negative refractive index materials. If these two symmetries are simultaneously broken, it would be expected to generate topological phase transitions, thereby deriving rich TP quantum states.

On the other hand, for phonon-related applications, we expect that TPs would be possible for advanced thermoelectric functions, excellent topological superconductivity, and novel phonon devices for anomalous heat transport and unidirectional phonon waveguides due to topologically protected states that are immune to backscattering. In particular, it needs to be emphasized that both TPs and topological electrons can coexist in the same material, because topological properties are usually correlated with crystal symmetry. Their mutual interactions between topological electrons and TPs would be a highly interesting direction deserving further studies. Currently, almost no related work focuses on this aspect. Gapless TP modes would be possible to provide more scattering channels in the three-phonon-phonon scattering process, so as to decrease the mean free path and to suppress the lattice thermal conductivity. Electronic densities of state at the Fermi level usually increase to a certain degree, due to the occurrence of topological

Figure 1. Topological phononic materials from high-throughput calculations to the database Top: high-throughput computational package HT-PHONON for topological analysis and phononic spectra derived from force constants. Bottom: the framework of the database of TP materials and various TPs and their shapes.
electronic nodal-line (ring) states. This would be, somehow, beneficial to the increase in Seebeck coefficient. In combination with gapless TPs, both topological electrons and TPs thus provide a promising space for the optimization of the figure of merit (zT) of thermoelectric materials. In addition, from the viewpoint of chemistry, catalysis may also profit from TPs in combination with a topological electronic system.10

REFERENCES
1. Prodan, E., and Prodan, C. (2009). Topological phonon modes and their role in dynamic instability of microtubules. Phys. Rev. Lett. 103, 248101.
2. Liu, Y., Chen, X., and Xu, Y. (2020). Topological phononics: from fundamental models to real materials. Adv. Funct. Mater. 30, 1904784.
3. Li, J.X., Xie, Q., Ullah, S., et al. (2018). Coexistent three-component and two-component Weyl phonons in TiS, ZrSe, and HfTe. Phys. Rev. B. 97, 054305.
4. Zhang, T.T., Song, Z., Alexandradinata, A., et al. (2018). Double-Weyl phonons in transition-metal monosilicides. Phys. Rev. Lett. 120, 016401.
5. Wang, R., Xia, B., Chen, Z., et al. (2020). Symmetry-protected topological triangular Weyl complex. Phys. Rev. Lett. 124, 105303.
6. Li, J.X., Xie, Q., Liu, J., et al. (2020). Phononic Weyl nodal straight lines in MgB2. Phys. Rev. B. 101, 024301.
7. Li, J.X., Wang, L., Liu, J., et al. (2020). Topological phonons in graphene. Phys. Rev. B. 101, 081403.
8. Li, J.X., Liu, J., Baronett, S.A., et al. (2021). Computation and data driven discovery of topological phononic materials. Nat. Commun. 12, 1204.
9. Atushi, T. (2018). Phonon database at kyoto university. http://phonondb.mtl.kyoto-u.ac.jp/.
10. Li, J.X., Ma, H., Xie, Q., et al. (2018). Topological quantum catalyst: Dirac nodal line states and a potential electrocatalyst of hydrogen evolution in the TiSi family. Sci. China Mater. 61, 23.

ACKNOWLEDGMENTS
We are grateful for support from the National Natural Science Fundation for Outstanding Young Scholars (Grant No. 51725103).

DECLARATION OF INTERESTS
The authors declare no competing interests.