Topological nodal-link phonons, three-fold, Dirac and six-fold nodal-point phonons in the insulator SiO$_2$

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Abstract

By using first-principles calculations and symmetry analysis, we study the topologically nontrivial features of sextuple nodal-point phonons together with other kinds of topological phonons in realistic materials. The sextuple nodal-point phonons in all 230 space groups, enumerated in this paper, are localized at the boundaries of the three-dimensional Brillouin zone (BZ), and protected both by time-reversal symmetry ($T$) and little-group symmetries. Moreover, in a realistic material sample of insulator SiO$_2$, we find that the sextuple nodal-point phonons exist at the high-symmetry point $H$ of the first BZ, and generate four-fold surface states. Interestingly, owing to the special crystal symmetries in SiO$_2$, triple nodal-point phonons and Dirac phonons exist at the point $\Gamma$ and $P$, respectively, and exhibit exotic quadruple surface states. More than these, the topological phononic nodal links also appear around the point $\Gamma$, and exhibit drumhead like surface states in this material. Our theoretical work not only proposes an effective way to search for multi-fold topological phonons including Dirac phonons and sextuple nodal-point phonons, but also presents a realistic material sample to realize the coexistence of multiple nodal-point and nodal-link phonons.

1. Introduction

We well know that three different kinds of quasi-particles, i.e. Weyl, Dirac and Majorana fermions, are first predicted in high-energy physics while difficult to observe. The condensed-matter systems, hosting various types of quasi-particles excitations, provide the opportunities to discover these magic quasi-particles in realistic materials. Then the physical properties of these quasi-particles have been widely studied in solid-state materials in recent decades [1–12]. Following this idea, the researchers in the field of topology physics have proposed several novel quasi-particles exciting special topologically nontrivial features [13], such as three-fold excitations [13–16], four-fold Rarita–Schwinger Weyl fermions [17], six-fold excitations [13] and others. Moreover, thanking to the special crystal symmetries in SiO$_2$, triple nodal-point phonons and Dirac phonons exist at the point $\Gamma$ and $P$, respectively, and exhibit exotic quadruple surface states. More than these, the topological phononic nodal links also appear around the point $\Gamma$, and exhibit drumhead like surface states in this material. Our theoretical work not only proposes an effective way to search for multi-fold topological phonons including Dirac phonons and sextuple nodal-point phonons, but also presents a realistic material sample to realize the coexistence of multiple nodal-point and nodal-link phonons.
in a wide frequency region. These advantages are helpful to realize unusual carriers’ transport phenomena, such as quantized circular photogalvanic effect contributed by topological phonons [24]. Moreover, phononic surface states can be observed by using four-dimensional electron energy-loss spectroscopy technique [25]. Therefore, topological phonons have been developed to another hot topic in condensed-matter physics very recently [26–38]. Similar to topological fermions, topological phonons, mainly referring to the quantization of lattice vibrations protected by particular crystal symmetries, can be divided into Weyl phonons, Dirac phonons, nodal-line phonons and multi-fold nodal-point phonons. The former three classes of phonons have already been successfully observed in realistic materials, owing to the low degeneracies in phonon bands. For example, two-fold and three-fold nodal-point phonons are proposed to exist in CrI₃ [39] and the high-pressure CuCl [40], respectively. However, the multi-fold nodal-point phonons, such as four-fold (Dirac) [41] and six-fold nodal-point phonons, are still rarely reported in realistic materials, due to the essential conditions including high degeneracies in phonon bands and unique crystal symmetries, although the six-fold nodal-point phonons have been predicted in some material samples [42, 43]. Moreover, nodal-line phonons are protected both by time-reversal symmetry (T) and spatial-inversion symmetry (P), and as these symmetries are broken, the nodal-line phonons are usually open to form Weyl- or Dirac-type phonons, indicating that the symmetry protection conditions of nodal-line phonons and multi-fold nodal-point phonons are much different. As a result, a realistic material, exhibiting nodal-line phonons accompanied with multi-fold nodal-point phonons, has not been reported up to present. To develop the field of topological phonons, two questions arise naturally: (a) how do we find out effectively multi-fold nodal-point phonons, such as the six-fold nodal-point phonons, in all 230 space groups (SGs)? and (b) whether can we realize the coexistence of multi-fold nodal-point phonons and nodal-links phonons in a realistic material?

In this work, by checking the symmetries of all 230 SGs, we exhaust the all sextuple (six-fold) nodal-point phonons existing in the three-dimensional (3D) Brillouin zone (BZ), and enumerate them at the high-symmetry points of the BZ in table 1, in which we find that the six-fold phonon bands tend to degenerate at high-symmetry points and every sextuple point stands for a sextuple nodal-point phonon. To confirm our findings, we study the phonon dispersions and the corresponding surface states in a realistic material, i.e. the insulator SiO₂ in SG 230. The first-principles calculations show that the sextuple nodal-point phonon exists at the high-symmetry point H in SiO₂. Interestingly, we find that two other kinds of multi-fold nodal-point phonons, i.e. triple nodal-point phonons and Dirac phonons, exist in this material (at the point Γ and P, respectively). More importantly, due to the special crystal symmetries in SiO₂, topological phononic nodal links also appear. Moreover, the Dirac phonons induced quadruple surface states and noncontractable surface arcs, the sextuple nodal-point phonons induced four surface states, and the topological nodal links induced drumhead-like surface states are all observed clearly in the (001) and (110) surfaces BZ of this material. To the best of our knowledge, the coexistence of drumhead-like phononic surface states and quadruple phononic surface states in the same material has not been reported previously. Our theoretical results not only put forward an effective way to search for the multi-fold nodal-point phonons such as Dirac phonons and sextuple nodal-point phonons in all 230 SGs, but also provide the first realistic material with the coexistence of triple nodal phonons, Dirac phonons, sextuple nodal-point phonons and topological phononic nodal links.

2. Symmetry analysis and calculations method

To search for the all sextuple nodal-point phonons in all 230 SGs, we should establish an effective way to obtain the topologically phononic states we need. To the end, we first calculate the little groups, the all single-valued possible irreducible representations (irreps) and the band degeneracies of all SGs [44, 45]. Then, based on the above numerical results, we continue to check the dimension of all possible irreps of 230 SGs in spinless systems, which helps us find out the six-dimensional (6D) irreps of little groups in the presence of T. Note that this searching covers all 230 SGs, and the lattice symmetries of materials should be located at high-symmetry points in the 3D BZ. Here a 6D irrep stands for a sextuple nodal-point phonon at the corresponding high-symmetry point. We screen out the six-fold points at high-symmetry points as listed in table 1.

To examine further the topological features of sextuple nodal-point phonons, we need to build the corresponding phononic k · p model. For convenience to perform our studies, we consider a six-band model at the point H in SG 230. The symmetries at this point include threefold screw symmetry $\{C_{3z} | \frac{1}{3} \frac{2}{3} \frac{0} \}$, twofold screw symmetries $\{C_{2z} | \frac{1}{3} \frac{2}{3} \}$ and $\{C_{2y} | \frac{0}{2} \frac{1}{2} \}$, glide symmetry $\{\sigma_{ad} | \frac{1}{0} \frac{0} \}$, T and P. Under the basis of $\Gamma_4$ irrep, the detailed matrix representations of above six symmetries are obtained as described in supplemental material, section A. Then, the k · p Hamiltonian $H^{kp}_{H}$ for the point H can be described below
Table 1. The complete list of the sextuple nodal points in 230 Space Groups (SGs). The first and the second columns indicate the SG number and symbol. The third column indicates the corresponding high-symmetry k point. The fourth and fifth columns show the little groups and the corresponding irreps. The sixth column shows the generators of the k point. To get more details for the little groups including their character tables, the definition of lattice vectors and others, one may refer to [44, 45].

| SG No. | SG symbol | k point | Little groups | Irreps | Generators |
|--------|-----------|---------|---------------|--------|------------|
| 218    | P43n      | R       | G$_{48}$      | $\Gamma_1\Gamma_3$ | \{S$_{4d}^{\pm}[1 1 1]$, \{\sigma_d[1 2 3,}\} $\{C_{6h}[000]\}, T$ |
| 220    | I$\bar{4}$3c | H       | G$_{48}$      | $\Gamma_1\Gamma_3$ | \{S$_{4d}^{\pm}[1 1 1],\} \{$\sigma_d[1 2 3,}\} $\{C_{5h}[000]\}, T$ |
| 222    | Pn$\bar{3}$n | R       | G$_{48}$      | $\Gamma_4$ | \{C$_{2d}[010]$, \{C$_{2h}[000]\}, \{C_{2y}[000]\} \{C_2[000]\}, \{P[1 2 1]\}, T$ |
| 223    | Pm$\bar{3}$n | R       | G$_{48}$      | $\Gamma_4$ | \{C$_{2d}[010]$, \{C$_{2h}[000]\}, \{C_{2y}[000]\} \{C_2[000]\}, \{P[000]\}, T$ |
| 230    | Ia$\bar{3}$d | H       | G$_{48}$      | $\Gamma_4$ | \{C$_{2d}[0 1 1]\}, \{C_{2h}[0 1 1]\}, \{C_{2y}[0 1 1]\} \{C_2[000]\}, \{P[000]\}, T$ |

where $p$ and $q$ are constant coefficients. This matrix model demonstrates that the linear phononic dispersions exist at the point $H$. It should be stressed that this $k \cdot p$ model is also applicable at the point $R$ in SGs 222 and 223. As for the rest two SGs listed in table 1, the corresponding $k \cdot p$ models at the point $R$ in SG 218 and the point $H$ in SG 220 are also provided in supplemental material, section B.

Furthermore, the irreps of some other high-symmetry points and paths in the 3D BZ of SG 230 are listed in table 2. One can see that the high-symmetry point $\Gamma$ belongs to the little group $G_{48}$ and at this point, there exist four different irreps, i.e. $\Gamma_1\Gamma_2$ and $\Gamma_3$. Since these irreps are 3D, the band crossing at the point $\Gamma$ stands for a triple nodal-point phonon. Moreover, the point $P$ belongs to the little group $G_{48}$ and at this point, there are two 2D irreps, i.e. $\Gamma_1\Gamma_2$ and one 4D irrep, i.e. $\Gamma_3$, indicating that a quadruply degenerate nodal point, i.e. a Dirac phonon, exists at this point. To examine further the topological nature of Dirac phonons discovered here, we turn to derive its $k \cdot p$ model Hamiltonian. We know that the symmetries at the point $P$ include three-fold screw symmetry $\{C_{2d}[0 1 1]\}$, three two-fold screw symmetries $\{C_{2h}[0 1 1]\}$, $\{C_{2y}[0 1 1]\}$ and $\{S_{4d}^+[1 2 3]\}$. As for the detailed matrix representations of above four symmetries, one may refer to supplemental material, section C. Then, under the basis of $\Gamma_1\Gamma_2$ irreps, the $k \cdot p$ Hamiltonian $\mathcal{H}_{kp}^P$ for the point $P$ is described as

$$
\mathcal{H}_{kp}^P = \begin{bmatrix}
0 & -pk_x & -pk_y & -iqk_z & 0 & iqk_y \\
-pk_x & 0 & -pk_y & -iqk_z & -iqk_y & 0 \\
-pk_y & -pk_x & 0 & -iqk_z & -iqk_y & 0 \\
0 & iqk_y & 0 & iqk_x & -pk_z & 0 \\
0 & iqk_z & iqk_y & 0 & 0 & pk_y \\
-iqk_x & -iqk_z & 0 & pk_z & 0 & 0
\end{bmatrix},
$$

where $k_- = k_x - ik_y$ and $k_+ = k_x + ik_y$. According to this equation, one can conclude that the linear phononic dispersions appear at the point $P$. By using the similar symmetry analysis, we uncover further that the topological phononic nodal links also exist in the 3D BZ of SG 230. Note that the more details including the $k \cdot p$ model of topological phononic nodal links are provided in supplementary material, section D and meanwhile, the $k \cdot p$ model Hamiltonian of triple nodal-point phonons is given in supplementary material, section E.

Based on the above symmetry analysis, the phonon dispersions of any realistic material sample in the SGs listed in table 1 should exhibit triple nodal-point phonons, Dirac phonons and sextuple nodal-point phonons at the corresponding high-symmetry points. To verify these findings, we turn to study systematically the phonon spectra of a realistic material sample, i.e. the insulator SiO$_2$ in SG 230, by using the first-principles calculations. The crystallographic data of SiO$_2$ are obtained from [46], and its primitive cell is illustrated in figure 1(a). The primitive cell of SiO$_2$ contains 36 atoms (12 Si and 24 O atoms) and belongs to body-centred cubic structure with Ia$\bar{3}$d. The corresponding 3D BZ is drawn in figure 1(b), where the blue and red square denotes the (001) and (110) surface BZ, respectively.
Table 2. The list of the irreps of some high-symmetry points and paths in SG 230. The first column indicates the high-symmetry points or paths in the 3D BZ. The second column indicates the little groups, and the third column shows the corresponding irreps. For more details, one may refer to [44, 45].

| High-symmetry points or paths | Little groups | Irreps                          |
|-------------------------------|---------------|---------------------------------|
| Γ                            | \(G_{38}^1\)  | \(\Gamma_4^+(3D); \Gamma_4^-(3D); \Gamma_3^+(3D)\); \(\Gamma_3^-(3D)\) |
| P                            | \(G_{36}^1\)  | \(\Gamma_1\Gamma_2(4D); \Gamma_3(4D)\) |
| Γ-H                          | \(G_{28}^1\)  | \(\Gamma_1(1D); \Gamma_2(1D); \Gamma_3(1D); \Gamma_4(1D); \Gamma_5(1D)\) |
| Γ-P                          | \(G_{36}^1\)  | \(\Gamma_5(2D)\)              |
| H-N                          | \(G_{28}^1\)  | \(\Gamma_5(2D)\)              |

Figure 1. Crystalline structure and phonon dispersions of the insulator SiO\(_2\) in SG 230. (a) Crystal structures of SiO\(_2\) in a primitive cell, where the blue (red) atoms stand for Si (O). (b) Bulk BZ of the insulator SiO\(_2\), and the (001) (blue square) and the (110) (red hexagon) surfaces BZ. (c) Phonon spectra along high-symmetry paths and the corresponding phononic density of states (DOSs) in SiO\(_2\). (d) Triple-fold nodal points (black point) from 16.0 to 18.0 THz at the point Γ. (e) Four-fold (red point) and the sextuple (green point) nodal points from 14.0 to 16.0 THz at the points P and H. (f) Four-fold Dirac point (red point) at the point P and the six-fold nodal point (green point) at H from 14.0 to 20.0 THz. (g) Six-fold nodal point (green point) at H, and topological phononic nodal links (blue point) along the Γ-H and N-Γ directions from 14.0 to 20.0 THz.

The phonon dispersions of SiO\(_2\) are calculated by the density functional theory using the Vienna \textit{ab initio} simulation package with the generalized gradient approximation in the form of a Perdew–Burke–Ernzerhof function for the exchange-correlation potential [47–49]. An accurate optimization of structural parameters is employed by minimizing the interionic forces less than 0.001 eV Å\(^{-1}\) and an energy cutoff at 500 eV. The 3D BZ is gridded with \(3 \times 3 \times 3\) \(k\) points. Then the phonon dispersions are gained using the density functional perturbation theory, implemented in the PHONOPY package [50, 51]. The force constants are calculated using a \(2 \times 2 \times 2\) supercell. To reveal the topologically nontrivial nature of phonons, we construct
the phononic Hamiltonian of the tight-binding (TB) model and the surface local density of states with the open-source software WANNIERTOOLS code [52] and surface Green’s functions [53]. The crystal structures are obtained from the Materials Project [46], and the irreps of phonon bands are computed by the program IR2TB on the phononic Hamiltonian of the TB model [54].

3. Results and discussion

The phonon spectra and the corresponding phononic density of state (PDOS) of the insulator SiO$_2$ are calculated and shown in figure 1(c). One can see that as the frequency $f$ is increased from 15.0 to 22.0 THz (see the region colored by light red), the phonon spectra display lots of multi-fold band crossings at high-symmetry points. The related phonon bands with higher degeneracies show the following unique properties: Firstly, the three-fold degeneracy point appears at the point $\Gamma$ as highlighted by a black dot in figure 1(d), indicating the existence of triple nodal-point phonons in SiO$_2$. Along the high-symmetry path $\Gamma$–$\Sigma$–$\Gamma$, the triple nodal-point phonons can be divided into three single-fold bands while along the path $\Gamma$–$\Sigma$–$\Gamma$, into one double-fold band and one single-fold band. Secondly, the above double-fold bands tend to form a Dirac point at the point $\Sigma$, as denoted by the red dots in figure 1(e), indicating the appearance of Dirac phonons in this material. Thirdly, the double-fold bands cross with other two kinds of double-fold bands to form a six-fold nodal point at the high-symmetry point $H$, as highlighted by the green dot in figures 1(e) and (f), confirming the existence of sextuple nodal-point phonons in SG 230. Finally, as shown in figure 1(g), along the paths $H$–$\Gamma$ and $\Sigma$–$\Gamma$, there are two double-fold degenerate points, which are protected by $T$, $P$ and twofold screw symmetry $\{C_{2z}|0\frac{1}{2}\frac{1}{2}\}$, and tend to form a nodal ring in the $k_x - k_y$ plane, supporting the existence of topological phononic nodal link in the present insulator. Obviously, these particular features characterized by multi-fold degenerated points and bands are well consistent with the previous conclusions drawn from symmetry analysis.

To explore further the topological features of multi-fold nodal-point phonons and nodal-line phonons appearing in the insulator SiO$_2$, we plotted the spatial distributions of triple nodal-point phonons, Dirac phonons, sextuple nodal-point phonons and topological phononic nodal links in the first 3D BZ in figure 2(a). One can find that the triple nodal-point phonons (black dot) is located at the center of BZ, the Dirac phonons (red dots) at the corners shared by three planes, and the sextuple nodal-point phonons (green dots) at the corners shared by four planes. Moreover, three ideal nodal rings are perpendicular to intersect each other in the different planes and encircle around the point $\Gamma$ to form the well-defined topological phononic nodal links. To identify the topologically nontrivial nature of nodal rings, we calculated the corresponding Berry phase for a closed loop of the nodal ring as shown in figure 2(b) (for more calculation details, one may refer to supplemental material, section F). It is clearly shown that the Berry phase along the high-symmetry path $H$–$\Gamma$ gets a jump of $\pi$ across the nodal ring, verifying further of the topological nature of topological phononic nodal link. In addition, the 3D phonon spectra in the frequency region 16.0 THz $< f < 20.0$ THz are drawn in figures 2(c) and (d). As expected, triple nodal-point phonons, Dirac phonons, sextuple nodal-point phonons and a phononic nodal ring are observed clearly to coexist in the $k_x - k_y$ plane.

To explore further the topologically nontrivial features of multi-fold nodal-point phonons and the coexisting nodal-link phonons, we turn to examining the corresponding isofrequency surface contours and the surface states. As drawn in figure 1(b), the points $\Gamma$ and $H$ ($P$ and $N$) in the 3D BZ are projected on the points $\bar{\Gamma}(\bar{M})$ in the (001) surface BZ. In figure 3(a), we plotted the surface phonon dispersions on the (001) surface along the high-symmetry paths. At the first glance, we find that at the point $\bar{\Gamma}$, there are four surface arcs projected by sextuple nodal-point phonons as circled by the square box $S_1$ in figure 3(b) and the box $S_2$ in figure 3(c). Owing to the existence of three non-commuting glides symmetries $\{M_{2z}\frac{1}{2}\frac{1}{2}\}$, $\{M_{1z}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$ and $\{M_{2z}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$ in SG 230, the quadruple surface states [55–57] are formed on the (001) surface as shown in the square boxes $S_1$ and $S_2$ around the point $\bar{M}$. Moreover, in figures 3(d) and (e), we plotted the surface PDOS at two typical frequency values $f = 15.379$ and 20.778 THz chosen in the (001) surface BZ, as denoted by the white dotted lines in figure 3(a). It is noted that the sextuple nodal-point phonon-projected point $\bar{\Gamma}$ and the Dirac phonon-projected point $\bar{M}$ appear clearly in figures 3(d) and (e). To more clearly see the exotic surface states, we chose a square path $S_3$ around the point $\bar{M}$ in figure 3(e) to calculate the corresponding phononic surface states as drawn in figure 3(f). One can find that several quadruple surface states clearly appear in figure 3(c). More importantly, we find that the topological phononic nodal link-induced drumhead-like surface states and the Dirac phonon-induced quadruple surface states appear simultaneously along the $\bar{M}$–$\bar{\Gamma}$ direction as illustrated in figure 3(a) (see the square box $S_2$). It should be pointed out that it is first work to report the coexistence of the above two different phononic surface states in a material.

Next, we focus our attention on the phononic surface states in the (110) plane of SiO$_2$, which are also calculated as drawn in figure 4. As shown in figure 1(b), the high-symmetry points $\Gamma$ and $N$ ($P$ and $H$) in the
3D BZ are projected on the points $\tilde{\Gamma}$, $\tilde{P}$ and $\tilde{H}$ in the (110) plane. In figure 4(a), we plotted the phononic surface states in the frequency region from 14 to 22 THz. One can see that the Dirac phonon-induced double arcs surface states (highlighted by the square box $S_6$) and the sextuple nodal-point phonon-induced four-arcs surface states (highlighted by the square box $S_7$ in figure 4(b) and the box $S_9$ in figure 4(c)) appear clearly. More interestingly, the nodal link-induced drumhead like surface states appear in the square box $S_{10}$ and the Dirac phonon-induced quadruple surface states appear in the square box $S_8$ nearly at the same frequency values. These properties confirm further the topologically nontrivial features of Dirac phonons, sextuple nodal-point phonons and topological phononic nodal links discovered above. Moreover, it is interesting that the above two different kinds of phononic surface states, i.e. the Dirac phonons-induced quadruple surface states and the nodal link-induced drumhead like surface states, just coexist at the point $\tilde{P}$. In addition, the isofrequency surface contours at three different frequency values $f = 15.379$, 17.58 and 20.33 THz are shown in figures 4(d)–(f). We can see that some ideal surface arcs induced by Dirac phonons appear at the point $\tilde{P}$ in figure 4(e). Meanwhile, the sextuple nodal-point phonon-projected point $\tilde{H}$ and the Dirac phonon-projected point $\tilde{P}$ display clearly, indicating that at these frequency values of the corresponding surface BZ, Dirac phonons and sextuple nodal-point phonons can be detected easily in experiments, as shown in figures 4(d) and (f).
Figure 3. The (001) surface phonon dispersions and isofrequency surface contours of SiO$_2$. (a) Surface phonon dispersion in the (001) plane along the high-symmetry directions of SiO$_2$, QSS denotes quadruple surface states and DLSS denotes drumhead like surface states. (b) Enlarged view of $S_1$ from 15 to 16 THz, where FSS denotes four-fold surface states. (c) Enlarged view of $S_3$ and $S_5$ from 20.20 to 20.90 THz. (d) The isofrequency surface contours at $f = 15.379$ THz. (e) The isofrequency surface contours at $f = 20.778$ THz. (f) The surface phonon dispersion on the (001) surface along the paths of $S_6$ plotted in (e).

Figure 4. Surface phonon dispersions and isofrequency surface contours in the (110) plane of SiO$_2$. (a) Surface phonon dispersion on the (110) plane along the high-symmetry directions of SiO$_2$, where QSS denotes quadruple surface state and DLSS denotes drumhead like surface state. (b) Enlarged view of $S_7$ from 15.0 to 16.0 THz, where FSS denotes four-fold surface state. (c) Enlarged view of $S_9$ from 20.0 to 22.0 THz. (e), (f) Isofrequency surface contours at $f = 15.379, 17.58, 20.33$ THz, respectively.
4. Summary

By performing symmetry analysis in all 230 SGs, we uncover that another kind of unconventional nodal phonons, i.e. sextuple nodal-point phonons, exist in realistic materials, and present a complete list of sextuple nodal-point phonons in the high-symmetry $k$ points in table 1. According to the $k \cdot p$ model of sextuple nodal-point phonons, we uncover that the phonon dispersions of sextuple nodal-point phonons are linear along the all high-symmetry directions, which are similar with the previously known nodal points. Then, we chose a realistic material example, i.e. the insulator SiO$_2$ in SG 230, to understand their topologically nontrivial features. The first-principles calculations demonstrate that in SiO$_2$, the sextuple nodal-point phonons exist at the high-symmetry point $H$ between two frequency values 15.379 and 20.778 THz. Moreover, owing to the special structural symmetries in SG 230, other two kinds of nodal-point phonons including triple nodal-point phonons and Dirac phonons, and the topological phononic nodal links appear in the same material. More importantly, the nodal link-induced drumhead like surface states, the Dirac phonons-induced quadruple surface states and the sextuple nodal-point phonons-induced four surface arcs display clearly in the (001) and (110) surfaces BZ, confirming further the topologically nontrivial features of the multiple multi-fold degenerate phonons and the nodal-link phonons obtain here. It is noted that the coexistence of drumhead-like phononic surface states and the quadruple phononic surface states at the same frequency of the same material sample has not been reported previously. Our theoretical work not only proposes an effective way to search for multi-fold topological phonons such as sextuple nodal-point phonons in 230 SGs, but also presents the first realistic material sample to realize the coexistence of triple nodal-point phonons, Dirac phonons, sextuple nodal-point phonons and topological phononic nodal links.

Data availability statement

The data generated and/or analysed during the current study are not publicly available for legal/ethical reasons but are available from the corresponding author on reasonable request.

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References

[1] Xu S-Y et al 2015 Science 349 613
[2] Lv B-Q et al 2015 Nat. Phys. 11 724
[3] Armitage N P, Mele E J and Vishwanath A 2018 Rev. Mod. Phys. 90 015001
[4] Lu L, Wang Z-Y, Ye D-X, Ran L-X, Fu L, Joannopoulos J D and Soljaci M 2015 Science 349 622
[5] Zhou S Y, Gweon G-H, Graf J, Fedorov A V, Spataru C D, Diehl R D, Kopelevich Y, Lee D-H, Louie S G and Lanzara A 2006 Nat. Phys. 2 595–9
[6] Kuroda K et al 2017 Nat. Mater. 16 1090–5
[7] Elliott S R and Franz M 2015 Rev. Mod. Phys. 87 137
[8] Young S M and Kane C L 2015 Phys. Rev. Lett. 115 126803
[9] Soluyanov A A, Gresch D, Wang Z, Wu Q, Troyer M, Dai X and Bernevig B A 2015 Nature 527 493–8
[10] Wieder B J, Kim Y, Rappe A M and Kane C L 2016 Phys. Rev. Lett. 116 186402
[11] Chang T-R et al 2017 Phys. Rev. Lett. 119 026401
[12] Kobayashi S and Sato M 2015 Phys. Rev. Lett. 115 187001
[13] Bradlyn B, Cano J, Wang Z, Vergniory M G, Felser C, Cava R J and Bernevig B A 2016 Science 353 aaf5037
[14] Tang P, Zhou Q and Zhang S-C 2017 Phys. Rev. Lett. 119 206402
[15] Chang G et al 2017 Phys. Rev. Lett. 119 206401
[16] Zhang T-T, Song Z-D, Alexandradinata A, Weng H-M, Fang C, Lu L and Fang Z 2018 Phys. Rev. Lett. 120 016401
[17] Harita W and Schwinger J 1941 Phys. Rev. 60 61
[18] Rao Z et al 2019 Nature 567 496
[19] Takane D et al 2019 Phys. Rev. Lett. 122 076402
[20] Sun Z-P et al 2020 Phys. Rev. B 101 155114
[21] Thirupathaiah S, Kushnirenko Y S, Kopevnik K, Piening B R, Buechner B, Aswartham S, van den Brink J, Borisenko S V and Fulga I C 2021 SciPost Phys. 10 L
[22] Nie S, Bernevig B A and Wang Z 2021 Phys. Rev. Res. 3 L012028
Zhang X et al 2020 Phys. Rev. B 102 035125
[23] de Juan F, Grushin A G, Morimoto T and More J E 2017 Nat. Commun. 8 15995
[24] Qi R et al 2021 Nature 599 399–403
[25] Liu Q-B, Qian Y, Fu H-H and Wang Z 2020 npj Comput. Mater. 6 95
[26] Liu Q-B, Wang Z and Fu H-H 2021 Phys. Rev. B 103 L161303
[27] Liu Q-B, Fu H-H, Xu G, Yu R and Wu R 2019 J. Phys. Chem. Lett. 10 4045
[28] Zhang L and Niu Q 2015 Phys. Rev. Lett. 115 115502
[29] Zhang T-T, Takahashi R, Fang C and Murakami S 2020 Phys. Rev. B 102 125148
[30] Xia B-W, Wang R, Chen Z-J, Zhao Y-J and Xu H 2019 Phys. Rev. Lett. 123 065501
[31] Liu Q-B, Fu H-H, Xu G, Yu R and Wu R 2019 J. Phys. Chem. Lett. 10 4045
[32] Zhang L-F, Ren J, Wang J-S and Li B-W 2010 Phys. Rev. Lett. 105 225901
[33] He C, Ni X, Ge H, Sun X-C, Chen Y-B, Lu M-H, Liu X-P and Chen Y-F 2016 Nat. Phys. 12 1124
[34] Prodan E and Prodan C 2019 Phys. Rev. Lett. 103 248101
[35] Liu Y, Chen X and Xu Y 2020 Adv. Funct. Mater. 30 1904784
[36] Li J, Xie Q, Liu J, Li R, Liu M, Wang L, Li D, Li Y and Chen X-Q 2020 Phys. Rev. B 101 024301
[37] Xie Q, Li J, Ullah S, Li R, Wang L, Li D, Li Y, Yunoki S and Chen X-Q 2019 Phys. Rev. B 99 174306
[38] Miao H, Zhang T-T, Wang L, Meyers D, Said A-H, Wang Y-L, Shi Y-G, Weng H-M, Fang Z and Dean M P M 2018 Phys. Rev. Lett. 121 035302
[39] Jin Y, Wang R and Xu H 2018 Nano Lett. 18 7755–60
[40] Liu Q-B, Fu H-H and Wu R 2021 Phys. Rev. B 104 045409
[41] Chen Z-J, Wang R, Xia B-W, Zheng B-B, Jin Y-J, Zhao Y and Xu H 2021 Phys. Rev. Lett. 126 185301
[42] Zhong M, Liu Y, Zhou F, Kuang M, Yang T, Wang X and Zhang G 2021 Phys. Rev. B 104 085118
[43] Xie C, Liu Y, Zhang Z, Zhou F, Yang T, Kuang M, Wang X and Zhang G 2021 Phys. Rev. B 104 045148
[44] Bradley C J and Cracknell A P 2009 The Mathematical Theory of Symmetry in Solids: Representation Theory for Point Groups and Space Groups (Oxford: Oxford University Press)
[45] Yu Z-M, Zhang Z, Liu G-B, Wu W, Li X-P, Zhang R-W, Yang S-A and Yao Y 2022 Sci. Bull. 67 375–80
[46] Hautier G, Fischer C, Ehrlacher V, Jain A and Ceder G 2011 Inorg. Chem. 50 656
[47] Kohn W and Sham L J 1964 Phys. Rev. B 136 A1133
[48] Blochl P E 1994 Phys. Rev. B 50 17953
[49] Perdew J P, Burke K and Ernzerhof M 1996 Phys. Rev. Lett. 77 3865
[50] Carreras A, Togo A and Tanaka I 2017 Comput. Phys. Commun. 221 221
[51] Togo A and Tanaka I 2015 Scr. Mater. 108 1
[52] Zhang Z, Zhang D-B, Sun T and Wentzcovitch R M 2019 Comput. Phys. Commun. 243 110
[53] Lopez Sancho M P, Lopez Sancho J M, Sancho J M L and Rubio J 1985 J. Phys. F: Met. Phys. 15 851
[54] Gao J-C, Wu Q-S, Persson C and Wang Z 2021 Comput. Phys. Commun. 261 107760
[55] Fang C, Lu L, Liu J and Fu L 2016 Nat. Phys. 12 936
[56] Cheng H, Sha Y, Liu R, Fang C and Lu L 2020 Phys. Rev. Lett. 124 104301
[57] Cai X, Ye L, Qiu C, Xiao M, Yu R, Ke M and Liu Z 2020 Light Sci. Appl. 9 38