Phonons as bosons are different from electrons as fermions. Unlike interatomic electron hopping that can be either positive or negative and further tuned by spin-orbit coupling, interatomic force constant is positive, or the structure of atomic lattices would be dynamically unstable. Surprisingly, we found that topological phonon flat bands (FBs) can manifest either a positive or negative interatomic force constant that couples the FB-modes of opposite chirality, as exemplified by first-principles calculations of a 2D material of Kagome-BN. To reveal its physical origin, we establish a fundamental correspondence between a collective lattice-coupling (CLC) variable of two quasi-particle states (e.g., electronic states or phonon modes) of opposite parity in a periodic lattice with band topology. Topological semimetals arise with zero CLC at Dirac $k$-points protected by symmetry; while positive and negative CLC at these $k$-points gives rise to normal and topological insulators, respectively. Interestingly, topological FB corresponds to a zero CLC at all $k$-points, and multi-atom FB phonon mode can manifest effectively a negative interatomic force constant. The CLC-topology correspondence can also be generalized to high-order topological state. Our findings shed new light on our fundamental understanding of topology and provide a practical design principle for creating artificial bosonic topological states.

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In crystalline solids, quasiparticle transport is mediated by interatomic coupling constants in a periodic lattice, which can be different for fermionic electrons from bosonic phonons. Interatomic electron hopping of different valence orbitals can be either positive or negative; a negative hopping integral \((-t = t e^{i\pi})\) implies that the Bloch electrons acquire an additional phase of \(\pi\) as they hop over the periodic lattice. Also, the phase of electron hopping can be tuned by spin-orbit coupling (SOC), which is the key ingredient to open a nontrivial topological gap. In contrast, the interatomic force constant, coupling the atomic vibration modes, can only be positive; otherwise, the atomic structure would be dynamically unstable. This fundamental difference is evident from the observation that the sign of electron eigenvalues can be negative or positive, relative to the position of Fermi level, while all the phonon eigen frequencies must be positive, and the acoustic phonon mode has a zero frequency at the \(\Gamma\) point [the center of Brillouin zone (BZ)], accounting for translational motion of all atoms. Furthermore, phonon is spinless lacking SOC to tune the phase of force constant.

Let’s further illustrate the difference between interatomic electron hopping parameter and interatomic force constant, in the context of topological flat band (FB). We take Kagome lattice (Fig. 1(a)) as a prototypical example which is well-known to host FB [1-3]. A positive and negative electron hopping leads to a FB of opposite chirality sitting above and below the dispersive Dirac bands [4,5], respectively, as shown in Fig. 1(b) and 1(c). Now we examine a phononic Kagome lattice (Fig. 1(d)), where each lattice site is bonded with four nearest-neighbor (NN) sites. The z-mode phonon dynamical matrix is expressed in Eq. (1a) below (see methods in Section I in Supplementary Materials (SM) [6]):

\[
Du = k_f\begin{pmatrix}
0 & -1 - e^{\frac{i}{2}k_x} & -1 - e^{\frac{i}{2}k_x - \frac{i}{2}k_y} & -1 - e^{\frac{i}{2}k_x + \frac{i}{2}k_y} \\
-1 - e^{\frac{i}{2}k_x} & 4 & -1 - e^{-i k_x} & 4 \\
-1 - e^{\frac{i}{2}k_x + \frac{i}{2}k_y} & -1 - e^{i k_x} & 4 & -1 - e^{-i k_x} \\
-1 - e^{\frac{i}{2}k_x - \frac{i}{2}k_y} & 4 & -1 - e^{\frac{i}{2}k_x + \frac{i}{2}k_y} & 4
\end{pmatrix}\begin{pmatrix} u_A \\ u_B \\ u_C \\ u_A \end{pmatrix},
\]

\(1a\)

\[
H\psi = t_{ppn}\begin{pmatrix}
0 & -1 - e^{\frac{i}{2}k_x} & -1 - e^{\frac{i}{2}k_x - \frac{i}{2}k_y} & -1 - e^{\frac{i}{2}k_x + \frac{i}{2}k_y} \\
-1 - e^{\frac{i}{2}k_x} & 0 & -1 - e^{-i k_x} & 0 \\
-1 - e^{\frac{i}{2}k_x + \frac{i}{2}k_y} & -1 - e^{i k_x} & 0 & -1 - e^{-i k_x} \\
-1 - e^{\frac{i}{2}k_x - \frac{i}{2}k_y} & 0 & -1 - e^{\frac{i}{2}k_x + \frac{i}{2}k_y} & 0
\end{pmatrix}\begin{pmatrix} \psi_A \\ \psi_B \\ \psi_C \\ \psi_A \end{pmatrix}.
\]

\(1b\)

In deriving Eq. (1a), without losing generality and for simplicity, we set atomic mass \(M_{A,B,C}=1\), lattice constant \(a = 1\) and interatomic force constant \(k_f=1\) (see Section I in SM [6]). The calculated phonon bands are shown in Fig. 1(e). One sees that there is a FB, similar to the
electronic FB (Fig. 1(b)). For comparison, we give the electronic tight-binding (TB) Hamiltonian $H$ for $p_z$-orbitals in a Kagome lattice in Eq. (1b). The two matrices are same except different diagonal elements, so that their eigen spectra appear similar, as shown in Fig. 1(b) and 1(e) for positive $t$ and $k^f$, and Fig. 1(c) and 1(f) for negative $t$ and $k^f$ (to be discussed below), respectively. This analogue shows that in principle propagation of $z$-mode vibrations can be qualitatively understood as hopping of electron $p_z$-states in a lattice.

However, there are two fundamental differences to be noticed. First, the diagonal elements of $H$ represent the atomic valence orbital on-site energies, which can be set positive or negative in accordance with eigenvalues relative to the Fermi energy. In contrast, the diagonal elements of $D$ represent the number of NN springs connecting to the atomic site, which must be a positive integer (4 in the present case), and the eigen frequency for the acoustic phonon frequency must tends to zero at $\Gamma$ point at the long-wavelength limit. Secondly, the atomic valence orbitals can have $s$, $p$, $d$ and $f$ symmetries whose NN hopping integrals [$t$ in Eq. (1b)] can be either positive or negative. Correspondingly, the position of electronic FB can be either above (Fig. 1(b)) or below (Fig. 1(c)) the Dirac bands for $+t$ or $-t$, respectively [4,5]. In contrast, the atomic vibrational modes have only $p$ symmetry and the interatomic force constant [$k^f$ in Eq. (1a), to be distinguished from momentum $k$ throughout] can only be positive. If one artificially assumed a negative $k^f$, one would get a phonon band structure as shown in Fig. 1(f), which has the FB below the Dirac bands, as expected from the analogy of electronic bands, but all the vibration frequencies would be negative (imaginary). This is apparently unphysical. It seems to indicate that in a Kagome lattice, phononic FB should always sit above the Dirac bands.

Surprisingly, we found that a phonon FB sits below the Dirac bands, i.e., manifesting a negative interatomic force constant, do exist in real materials such as Kagome-BN (Fig. 1(g)), as shown in Fig. 1(h) and 1(i). Kagome-BN was previously studied for its electronic Dirac bands and heavy fermion properties [7], while its phonon spectrum was also calculated which we reproduced here. In Fig. 1(h) (see Section I in SM [6] for details), there are two sets of Kagome phonon FBs sitting under Dirac bands in the optical branches between 25 and 50 THz. Hypothetically, one could fit them separately as if they arose from two Kagome lattices with one atom per lattice site (assuming the mass of atom is 1 atomic mass unit (amu)) as shown by dotted blue lines in Fig. 1(i). Then one would obtain an on-site single-atom mode frequency of 30.5 THz and 41.1 THz, respectively, with a negative interatomic force constant of $k^f = -2882$
$N/m$; however, the single-atom vibration modes cannot be coupled by a negative $k_f$. Therefore, to reveal their physical origin, one likely has to consider multi-atom cluster-mode vibrations.

Furthermore, one may expect the negative (or sign of) interatomic force constant is related to phonon topology, because it is known that two electronic FBs arising from different sign of hopping (Fig. 1(b) and 1(c)) have opposite chirality, i.e., they have opposite Chern number if SOC is added and time reversal symmetry is broken [2,5,8]. This points to an analogous correlation between the sign of force constant and phonon FB chirality. Below, we will first establish a fundamental correspondence between a collective lattice-coupling (CLC) variable of two quasi-particle quantum states in a periodic lattice with band topology via the mechanism of band inversion, and then revisit the phonon FB to explain its manifestation of a negative interatomic force constant.

We use electrons and phonons as examples, but the established correspondence principle below is generally applicable to all quasiparticles. Let us review the band topology induced by band inversion using the well-known 1D Su–Schrieffer–Heeger (SSH) model as shown in Fig. 2(a-c). Let $d_1$ ($d_2$) be the interatomic distance within (in between) unit cells, and $t_1$ ($t_2$) be the intracell (intercell) interatomic hopping as shown in Fig. 2(a). The intracell hopping $t_1$ actually defines an “on-site” level splitting within the unit cell between two electronic states of opposite parity $(|A⟩ ± |B⟩)/√2$ (odd-even). The effect of intercell hopping $t_2$ is to change the level splitting at a given momentum $k$ (i.e., band dispersion) as these two states hop in the lattice periodically from cell to cell. One notices that at the BZ boundary ($ka = ±\pi$, $a$ is lattice constant), the level splitting equals $t_1 - t_2$. Then, if $t_1 > t_2$, the order of level splitting and hence the phase of the two quantum states is unchanged as they hop over the lattice, so that the system is topological trivial (Fig. 2(b)). If $t_1 < t_2$, however, the order of level splitting will be reversed (band inversion) and the system becomes topological nontrivial (Fig. 2(c)). This observation invoked us to define a CLC of electron hopping $T_{A\rightarrow B} = t_1 + t_2 e^{-ika}$, which accounts for both interatomic hopping strength and structure factor, to capture the phase evolution of the two states $(|A⟩ ± |B⟩)/√2$ over the BZ. At the BZ boundary ($ka = ±\pi$), $T_{A\rightarrow B} = t_1 - t_2$ whose sign defines the band topology; a positive (negative) $T_{A\rightarrow B}$ corresponds to a trivial (nontrivial) band topology, as shown in Fig. 2(b) (Fig. 2(c)).

An analog of phononic SSH model can be constructed, as shown in Fig. 2(d-f). Similar to the electronic case, we define a CLC of force coefficient coupling sublattice A and B, $K^f_{A\rightarrow B} =$
\[ k_1^f + k_2^f e^{-i\kappa a}, \] which accounts for interatomic force constant and structure factor, as well as directional cosines for in-plane modes. At the BZ boundary (X point), \( K^f_{A\to B} = k_1^f - k_2^f \). Then, if \( K^f_{A\to B} > 0 \), the phonon bands are topological trivial (Fig. 2(c)); if \( K^f_{A\to B} < 0 \), they are nontrivial (Fig. 2(f)).

To better understand this, we examine the eigen modes at \( \Gamma \) and X. At \( \Gamma \) (Fig. 2(g)), the eigen modes have one acoustic branch at bottom (even parity) and another optical branch on top (odd parity). This order of modes is unchanged at X when \( K^f_{A\to B} > 0 \) (Fig. 2(h)), but reversed when \( K^f_{A\to B} < 0 \) (Fig. 2(i)). Interestingly, for \( K^f_{A\to B} < 0 \), i.e., \( k_1^f < k_2^f \), the diatomic phonon modes can be viewed shifted by half a unit cell, as shown by the dashed ovals in Fig. 2(i) shifted from Fig. 2(g), to become out of phase in the neighboring unit cells. Then the optical mode can be viewed with the two atoms in one unit cell breathing out while the two atoms in the neighboring cell breathing in (upper panel of Fig. 2(i)), as if there is no restoring force. This explains the physical underpinning of a negative CLC of force coefficient coupling the two-atom cluster modes, leading to “mode inversion” as the modes propagate over the lattice and hence a nontrivial phonon band topology. We note that while the interatomic force constant \( k_1^f \) and \( k_2^f \) are conventionally positive, the individual force coefficients \( k_2^f e^{-i\kappa a} \) (or elements of dynamic matrix) can be either positive or negative varying with momentum, because the structure factor and also direction cosines for in-plane modes change signs. However, the phonon topology corresponds to the sign of CLC of force coefficient as we define here, not the sign of individual dynamic matrix element.

The above correspondence between the CLC variable of two quantum states and topology is general and equally applicable to 2D lattices. For example, consider the graphene lattice (see detailed discussion in Section II in SM [6]), there are two \( \pi \) and \( \pi^* \) electronic states per unit cell resulting from linear combination of \( p_z \)-orbitals on A and B sublattices \((|p_{z,A}\rangle \pm |p_{z,B}\rangle)/\sqrt{2}\), whose CLC of electron hopping is calculated as \( T_{A\to B} = t_1 + t_2 (e^{-i\kappa a_1} + e^{-i\kappa a_2}) \), where the first \( (t_1) \) term is the intracell and the second \( (t_2) \) term is the intercell NN hopping, respectively, and \( a_1 \) \( (a_2) \) are lattice vectors. Note that \( T_{A\to B} \) can be viewed as the CLC between sublattice A and B for a bipartite lattice like graphene. By C\( _3 \) rotation symmetry \( (t_1 = t_2) \), one can see that \( T_{A\to B} = 0 \) at the corners of BZ (K and K' points). Thus, \( T_{A\to B} = 0 \) corresponds to a Dirac semimetal state protected by symmetry. Following the original work by Kane and Mele [9], if one breaks inversion symmetry by adding an on-site energy difference between A and B
sublattice, the system opens a trivial gap becoming a normal insulator, which can be reinterpreted now as it effectively increases $t_1$ making $T_{A\rightarrow B}$ positive at $(K, K')$. On the other hand, if one adds SOC, it effectively adds a phase to the $t_2$ term making $T_{A\rightarrow B}$ negative at $(K, K')$, so that the system opens a nontrivial gap becoming a topological insulator.

For electrons, the CLC-topology correspondence established above applies also to cases of single atom per unit cell, because atomic valence orbitals have different $(s, p, d \ldots)$ parities and interatomic electron hopping can be positive or negative. One can reformulate the band inversion model of $(s, p_x, p_y)$ bands in a rectangle [10], triangle [11] and square lattice (see detailed discussion in Section III in SM [6]) by defining a CLC of electron hopping $T_{s\rightarrow p}$ between the $s$- and $p$-orbitals in presence of the $p$-orbital-originated SOC. For phonons, however, the correspondence principle applies only to multi-atom per unit cell, because single atomic vibrations have only $p$-symmetry and interatomic force constant is always positive so that the CLC can be defined. This means phonons are always topological trivial in all materials with single atom per unit cell.

Now we come back to analyze phonon FB in terms of both the CLC of force coefficient and interatomic force constant. As established above, a topological phonon Dirac state corresponds to a zero CLC at the Dirac $k$-points. It represents a local phase cancellation of Bloch wavefunction to form a Berry flux center at the Dirac $k$-points. Strikingly, a topological phonon FB corresponds to a zero CLC (i.e. phase cancellation of Bloch wavefunction) at all the $k$-points in the BZ. This can be inferred from the FB real-space wave function, the so-called compact localized state, as shown in Fig. 3(a), calculated from Fig. 1(e). It has six nodal points at the vertices of a hexagon with red and blue circles denoting the positive (up) and negative (down) displacement along z-axis, respectively. Thus, the FB-phonon mode is completely localized in real space, as reflected by cancellation of pair-wise restoring forces acting outside the hexagon (red and blue dashed arrows in Fig. 3(a)). This signifies a destructive quantum interference of phonon wavefunctions, in analogy to compact localized state of electronic FB [12,13]. The FB has a singular band touching point at $\Gamma$ (Fig. 1(e)) which is a Berry flux center in analogy to Dirac point [12-14].

On the other hand, the property of CLC for a FB that vanishes at all momenta is independent of the sign of interatomic force constant ($k_f$). However, a topological phonon FB will only manifest a positive $k_f$ in a Kagome lattice with one atom per lattice site (Fig. 1(d)).
Therefore, one must consider multi-atom phonon modes in a Kagome lattice, i.e., multi atoms per Kagome lattice site, to derive a FB of a negative $k_f$. For example, we have found that out-of-plane vibrational modes of di-atomic and tri-atomic Kagome lattices can have FBs manifesting a negative effective interatomic (i.e., inter-Kagome-lattice-site) force constant (see Fig. S3 and Section IV in SM [6]). Here, we focus on explaining the surprising results of Kagome-BN in Fig. 1(h) by considering the in-plane vibration modes from a four-atom cluster on each Kagome lattice site (Fig. 1(g)). As shown in Fig. 3(b), there are three different springs: N-N bond ($k_{11}$), B-N bond ($k_{12}$) and B-B bond ($k_{22}$), and two atoms of different mass: B (11 amu) and N (14 amu). From the calculated phonon spectra which contains 24 bands (see Fig. S6 in SM [6]), one can indeed find two isolated sets of Kagome bands in the frequency range of ~25-50 THz, as shown in Fig. 3(d), which agree nicely with the density-functional-theory (DFT) results featured with two FBs manifesting a negative interatomic force constant. It is worth noting that the model calculations are done by setting $k_{11} = 8000$ N/m, $k_{12} = 5600$ N/m, $k_{22} = 2500$ N/m, which are perfectly consistent with the order of DFT bond lengths (N-N bond: 1.02 Å, B-N bond: 1.36 Å, B-B bond: 1.70 Å) or strength.

We next show that the established CLC-topology correspondence can be generalized to high-order topological insulators (HOTI). We use 2D Kekulé lattice[15] as an example which is known to host HOTI corner states[16,17]. Kekulé lattice can be considered as deformed from hexagonal lattice as shown in Fig. 4(a), with the intracell and intercell hopping $t_1$ and $t_2$, respectively. Topological corner states will emerge in a finite sample when $t_2 > t_1$ as shown in Fig. 4(b). As an alternative understanding of 2D HOTI, namely a 1D first-order TI, one can consider a 1D sublattice of the 2D lattice, by cutting a ribbon along certain directions. Then, to apply the newly established correspondence principle, one can define a 1D CLC of electron hopping for the two states near Fermi level, which turns out to be $T_a = 2(t_1 - t_2)$ at $\Gamma$ for the armchair ribbon as shown in Fig. 4(c) (see details in Section IV in SM [6]). Consequently, similar to 1D SSH model, if $T_a < 0$, the 1D armchair ribbon is topological nontrivial, characterized with one pair of in-gap topological “corner” states (Fig. 4(d)) to appear at the two ends of a finite ribbon with broken stronger $t_2$ bonds (Fig. 4(c)). In contrast, a zigzag ribbon cut from the Kekulé lattice is metallic and topological trivial as shown in Fig. S5(g) (See SM [6]). This analysis explains straightforwardly why the topological corner states exist on all the six corners of a hexagonal sample (Fig. 4(b)), but only on
two corners of a rhombus sample, because they appear only at two ends along the nontrivial armchair direction but not the trivial zigzag direction (see Fig. S5(h) in SM [6]).

Finally, we comment on some general implications of the newly established CLC-topology correspondence, which provides a new and unified view of three common classes of topological materials: topological semimetal, insulator and FB materials. First, a topological semimetal corresponds to a zero CLC at special $k$-points. This can be generally achieved for both fermions and bosons by symmetry operations in a crystal. Most topological phonons found in real materials belong to this category, such as phononic Dirac/Weyl point [18-22] and nodal-line states [23-28]. Secondly, a TI state corresponds to a negative CLC at the special $k$-points. It requires the coupling strength to increase with the increasing interatomic distance without SOC, for example, $t_2 > t_1$ or $k_2^2 > k_1^2$ for $d_2 > d_1$ in the SSH model. This is rather counterintuitive, but achievable for both electrons and phonons through alternation of single and double bonds between the same atoms, such as Graphdiyne for realizing the Kekulé model [16]. Also, starting from a topological semimetal or a narrow-gap semiconductor with $s$- and $p$-state band edges, most TIs are achieved by adding SOC to turn the CLC negative. In this sense, all electronic materials could be topological with SOC, provided it has the right lattice constant and position of Fermi level [29]. However, it is much harder for phonon modes lacking SOC to attain a negative CLC, because for the same atoms the longer the bonds, the softer the bonds. Another fundamental difference is that the electronic bands of single atom per unit cell can be topological because a CLC, such as between atomic $s$- and $p$-valence, can be defined; while the phonon bands of single atom per unit cell are always trivial because a CLC cannot be defined. For these reasons, so far phonon TIs have been studied by models implicitly assuming a negative CLC of force coefficient [30-33], but rarely in real materials. On the other hand, the correspondence principle we established for phonons can be readily applied to designing bosonic TIs in artificial, such as photonic, acoustic and mechanical-wave systems, where CLC can be manipulated by design [33-37]. Finally, FB corresponds to a zero CLC at all $k$-points in the whole BZ. Intriguingly, a phonon FB can manifest a negative interatomic force constant. So more generally, bosonic FBs of opposite chirality can be manufactured in artificial systems by designing a positive or negative “interatomic” coupling.
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Fig. 1 [Full Column] **Illustration of electron (phonon) FB with positive interatomic hopping (force constant) vs. negative interatomic hopping (force constant).** (a) The electronic Kagome lattice with hopping $t$. (c) The electron band structure for $t > 0$. (e) The electron band structure for $t < 0$. (d) Spring-mass model for Kagome lattice with out-of-plane z-mode force constant $k_f$. (e) The phonon spectra for $k_f > 0$. (f) The phonon spectra for $k_f < 0$. (g) The structure of 2D Kagome-BN, B and N atoms are denoted by green and grey sphere, respectively. (h) The DFT calculated phonon spectra for Kagome-BN. (i) Two sets of Kagome bands between 25-50THz, the DFT and spring-mass model results are shown in red solid and blue dashed lines, respectively.
Fig. 2 [Full Column] **Illustration of electron (phonon) band topology in association with positive vs. negative CLC in SSH model.** (a) Electronic SSH model. The red dashed lines mark the unit cell. (b) Band structure for $T > 0$ ($t_1 > t_2$). The even (odd) parity of the band is marked by red and blue color, respectively. (c) Band structure for $T < 0$ ($t_1 < t_2$). (d) Phononic SSH model. (e) The phonon spectra for $K_f > 0$ ($k_1^f > k_2^f$). (f) The phonon spectra for $K_f < 0$ ($k_1^f < k_2^f$). (g) The eigenmodes at $\Gamma$ point. (h) The eigenmodes at X point for $K_f > 0$. (i) The eigenmodes at X point for $K_f < 0$.

Fig. 3 [Half Column] **Illustration of FB manifesting positive (negative) “interatomic” force constant.** (a) The compact localized state of Kagome FB. (b) Lattice model of Kagome-BN. (c) The comparison between model and DFT results. The model phonon bands and DFT phonon bands are plotted by blue dashed and red lines, respectively.
Fig. 4 [Half Column] **Demonstration of the CLC-topology correspondence for 2D HOTI.** (a) The structure of Kekulé lattice, intra- and inter-cell hopping are denoted as $t_1$ and $t_2$, respectively. Red box marks the unit cell. (b) The corner states of a hexagonal sample. Six corner states can be seen as three sets of boundary states of 1D TI as marked by three colored bands. (c) The boundary states of a 1D armchair nanoribbon. Red dashed lines mark the unit cell. (d) The energy spectrum of the armchair nanoribbon in (c). Red dashed box marks the in-gap boundary states, as shown by red dots in (c).
I. Methods

I. a Spring-mass model

Within the harmonic-oscillator approximation (spring-mass model), the eigen equation of phonon dynamical matrix \( \mathbf{D} \) is written as:

\[
(\omega^2 - \mathbf{D})\mathbf{u} = 0,
\]

(S1)

where \( \omega \) is the phonon frequency, \( \mathbf{u} = (u_{1x}, u_{1y}, u_{1z}, u_{2x}, u_{n,\alpha})^\dagger \) is the atomic displacement. \( D_{\alpha\beta}^{mn} = \sum_{m,n} \frac{1}{\sqrt{M_m M_n}} (C_{\alpha\beta}^{mn}(R)) e^{ik(r_m - r_n + R)} \), where \( R, M \) are the lattice vector and mass; \( m, n \) are the atom indices; \( \alpha, \beta \) denote the directions of vibrations. \( C_{\alpha\beta}^{mn} = k_{f\alpha\beta}^{mn} S_{\alpha\beta}^{mn} \) is the force coefficient, \( k_{f\alpha\beta}^{mn} \) is the interatomic force constant which can only take positive values, while \( S_{\alpha\beta}^{mn} \) and \( D_{\alpha\beta}^{mn} \), containing the structure factor and direction cosines, can be either positive or negative. Each atom in a lattice has three phonon modes, corresponding to vibrations in the \( x, y, \) and \( z \) directions. In a planar 2D lattice, out-of-plane mode (\( z \)-mode) is decoupled from the in-plane \( x \)- and \( y \)-modes; \( C_{\alpha\beta}^{mn} = k_{fz}^{mn} \) for the \( z \)-mode, and \( C_{\alpha\beta}^{mn} = k_{f\alpha\beta}^{mn} \cos(\theta_\alpha) \cos(\theta_\beta) \)
for the in-plane modes, where $\theta_i$ is angle between the bond direction and $i$-axis.

I. b Density-functional theory (DFT) calculation

The phonon calculations for Kagome-BN were performed using Vienna ab initio simulation package (VASP) [1] within the framework of DFT. The Perdew-Burke-Ernzerhof functional within the generalized gradient approximation was adopted [2-4]. The cutoff energy is set to 400 eV and a 3*3*1 Monkhorst-Pack k-points grid is used to sample the Brillion zone [5]. The structure was fully relaxed until the forces on each atom are smaller than 0.001 eV/Å. And a 15 Å thick vacuum layer was used to ensure the decoupling between neighboring slabs. The phonon spectra are calculated using PHONOPY package [6] based on the finite displacement method using a 3*3*1 supercell.

I. c Tight-binding (TB) calculation

TB models are constructed using Slater-Koster parameters [7] to explore the correspondence between topology and collective lattice coupling (CLC) of electron hopping in the $s, p_z$-Kagome lattice, 1D $s, p_z$-SSH model, $s, p_z$-hexagonal lattice, $sp^2$-square lattice, $s, p_z$-Kekulé lattice.

II. Correspondence between the collective lattice-coupling variable of two quantum states and their topology in graphene lattice

As shown in Fig. S1(a), in graphene lattice, each sublattice A site can hop to three nearest
neighbor B sites, including one intracell \( (t_1) \) and two intercell \( (t_2) \) hoppings. Thus, the collective lattice coupling (CLC) of electron hopping can be calculated as \( T_{A \rightarrow B} = t_1 + t_2 (e^{-i k a_1} + e^{-i k a_2}) \), which is effectively the coupling of two sub lattices A and B of a bipartite lattice. By \( C_3 \) rotation symmetry \( (t_1 = t_2) \), one finds that \( T_{A \rightarrow B} = t_1 (1 + e^{-i k a_1} + e^{-i k a_2}) = 0 \) at corners of Brillouin zone (BZ) \( (K \text{ and } K') \) points) which corresponds to a topological semimetal state protected by symmetry as shown in Fig. S1(b) (Dirac cone at K point). The \( T_{A \rightarrow B} = 0 \) at the Dirac points represents a condition for local phase cancellation of Bloch wavefunction, leading to formation of Berry flux center at \( K \) and \( K' \). If one breaks inversion symmetry of the system by adding an on-site energy difference between A and B sublattice, for example adding 0.5 eV on-site energy to A sublattice as shown in Fig. S1(c, d), the system opens a trivial gap, becoming a normal insulator, which can be reinterpreted now as it effectively increases \( t_1 \) making \( T_{A \rightarrow B} \) positive at \( (K, K') \). On the other hand, if one adds spin-orbital coupling (SOC, \( \lambda = 0.5 \) eV) as shown in Fig. S1(e, f), it effectively adds a phase to the \( t_2 \) term making \( T_{A \rightarrow B} \) negative at \( (K, K') \), so that the system opens a nontrivial gap becoming a topological insulator.

Fig S1 Illustration of the CLC-topology correspondence in graphene lattice. (a) Graphene lattice. Intra- and inter-cell hopping is marked as \( t_1 \) and \( t_2 \), respectively. Sublattice A(B) is denoted by red (blue) circles. (b) The band structure for \( t_1 = t_2 \). (c-d) The band structure and edge states for \( t_1 = t_2 \) and \( \epsilon_A = 0.5 \) eV, \( \epsilon_B = 0 \) eV. (e-f) The band structure and edge states for \( t_1 = t_2 \), \( \epsilon_A = \epsilon_B = 0 \) and \( \lambda = 0.5 \) eV.
III. Electronic \( sp^2 \) model in a square lattice

In this section, we will demonstrate that our established CLC-topology correspondence can be applied to cases of single atom per unit cell for electronic states. Here, we take a \( sp^2 \) square lattice as an example, as shown in Fig. S2(a). The Hamiltonian for the system can be written as Eq. S2 using \( (s, px + ipy, px - ipy) \) basis:

\[
H = \begin{pmatrix}
\epsilon_s + 2t_{ss\sigma}(\cos(k_x) + \cos(k_y)) & \sqrt{2}t_{sp\sigma}(i \sin(k_x) - \sin(k_y)) & \sqrt{2}t_{sp\sigma}(i \sin(k_x) + \sin(k_y)) \\
\sqrt{2}t_{sp\sigma}(-i \sin(k_x) - \sin(k_y)) & \epsilon_p + \lambda + (t_{pp\sigma} + t_{pp\pi})(\cos(k_x) + \cos(k_y)) & -(t_{pp\sigma} - t_{pp\pi})(\cos(k_x) - \cos(k_y)) \\
\sqrt{2}t_{sp\sigma}(-i \sin(k_x) + \sin(k_y)) & -(t_{pp\sigma} - t_{pp\pi})(\cos(k_x) - \cos(k_y)) & \epsilon_p - \lambda + (t_{pp\sigma} + t_{pp\pi})(\cos(k_x) + \cos(k_y))
\end{pmatrix}
\]  

(S2)

Without SOC \( (\lambda = 0) \), two \( p \)-bands are degenerate at \( \Gamma \) point as shown in Fig. S2(b) \( t_{ss\sigma} = t_{sp\sigma} = 1, \ t_{pp\sigma} = -1, \ t_{pp\pi} = -0.1, \ \epsilon_s = -4.5 \) and \( \epsilon_p = 2 \). If one gradually increases SOC strength \( \lambda \), two \( p \)-bands will be separated. And if the SOC is strong enough, one of the \( p \)-band will further be inverted with \( s \)-band at \( \Gamma \) and a topological gap opens as shown in Fig. S2(c-d) with \( s-p \) band inversion.

To show that our newly established correspondence principle can be applied to explain the topological phase transition in this system, we first expand Eq. S2 to the 1\textsuperscript{st} order around \( \Gamma \) as shown in Eq. S2:

\[
H(\Gamma) = \begin{pmatrix}
\epsilon_s + 4t_{ss\sigma} & -\sqrt{2}t_{sp\sigma} k_y + i\sqrt{2} t_{sp\pi} k_x & \sqrt{2}t_{sp\sigma} k_y + i\sqrt{2} t_{sp\pi} k_x \\
-\sqrt{2}t_{sp\sigma} k_y - i\sqrt{2} t_{sp\pi} k_x & \epsilon_p + \lambda + 2(t_{pp\sigma} + t_{pp\pi}) & 0 \\
\sqrt{2}t_{sp\sigma} k_y - i\sqrt{2} t_{sp\pi} k_x & 0 & \epsilon_p - \lambda + 2(t_{pp\sigma} + t_{pp\pi})
\end{pmatrix}
\]  

(2)

Then, the CLC of electron hopping between \( s \) and \( (px - ipy) \) around \( \Gamma \) can be obtained by the on-site energy difference (can be viewed as intracell hopping) between two states plus the lattice hopping (can be viewed as intercell hopping), \( T_{s\to px-ipy}(\Gamma) = \epsilon_p - \lambda + 2(t_{pp\sigma} + t_{pp\pi}) - \epsilon_s - 4t_{ss\sigma} + \sqrt{2}t_{sp\sigma} k_y + i\sqrt{2} t_{sp\pi} k_x \), which reduces to \( 0.3 - \lambda \) for \( t_{ss\sigma} = t_{sp\sigma} = 1, \ t_{pp\sigma} = -1, \)
\[ t_{ppn} = -0.1, \ \varepsilon_s = -4.5, \ \varepsilon_p = 2 \ \text{and} \ k_x = k_y = 0. \] Thus, if \( \lambda < 0.3 \), \( T_{s\rightarrow p_x-\ell_y} > 0 \), the system is trivial as shown in Fig. S2(b); if \( \lambda = 0.3 \), \( T_{s\rightarrow p_x-\ell_y} = 0 \), the system is a topological semimetal as shown in Fig. S2(c); if \( \lambda > 0.3 \), \( T_{s\rightarrow p_x-\ell_y} < 0 \), the system opens a topological gap at \( \Gamma \) point as shown in Fig. S2(d).

**Fig. S2.** Illustration of CLC-topology correspondence in single atom per unit cell for \( sp^2 \) states in a square lattice. (a) Electronic \( sp^2 \) square lattice. \( s, p_x, p_y \) orbitals are colored in black, red and blue, respectively. (b) The band structure for \( \lambda = 0 \). The s-orbital contribution and p-orbitals contribution are denoted by red and blue color. (c) The band structure for \( \lambda = 0.3 \). (d) The band structure for \( \lambda = 0.5 \).

**IV. Out-of-plane phonon bands of di- and tri-atomic Kagome lattices**

In order to derive a FB manifesting a negative interatomic force constant, here we use di- and tri-atomic Kagome lattice as examples to demonstrate the condition for a positive versus
negative interatomic force constant that couples the FB-modes of opposite chirality. Let’s assume
the two (three) atoms on each lattice site are coupled with a force constant \( k_1^f \) and they are
coupled with each other on different lattice sites with \( k_2^f \), as shown in Fig. S3(a, d).
Interestingly, one can define an effective “interatomic” (i.e., inter-Kagome-lattice-site) force
constant, \( k_e^f = 2k_1^f - 3k_2^f \), which couples the FB-modes of a superatom (i.e. a cluster contains
two or three atoms). When \( k_e^f > 0 \), there are two (three sets) of Kagome bands, all having the
FB above the Dirac bands, as shown in Fig. S3(b, e). If \( k_e^f < 0 \), the FB in the lower set of
Kagome bands will move up to the upper set sitting below the Dirac bands. Consequently, the FB
will now manifest a negative interatomic force constant, as shown by the red FB in Fig. S3(c, f).

Fig S3  Di- and tri-atomic Kagome lattice model. (a) Di-atomic Kagome lattice. The black dashed ovals mark the
Kagome-lattice-site. (b) The phonon spectrum for \( k_e^f > 0 \). The red line marks the FB manifesting positive interatomic
force constant between superatoms on each Kagome-lattice-site. (c) The phonon spectrum for \( k_e^f < 0 \). The red line
marks the FB manifesting negative interatomic force constant between superatoms on each Kagome-lattice-site. (d)
Tri-atomic Kagome lattice. The black dashed ovals mark the Kagome-lattice-site. (e) The phonon spectrum for \( k_e^f > 0 \).
The red lines mark the set of Kagome bands manifesting positive interatomic force constant between superatoms
on each Kagome-lattice-site. (f) The phonon spectrum for \( k_e^f < 0 \). The red lines mark the set of Kagome bands
manifesting negative interatomic force constant between superatoms on each Kagome-lattice-site.
V. High-order topological states in Kekulé lattice

In this section, we will elaborate on an alternative understanding of 2D high-order topological states based on our newly established CLC-topology correspondence, using the well-known Kekulé lattice as shown in Fig. S4(a). One can cut a 1D armchair ribbon along lattice vector $\vec{a}$ direction as shown in Fig. S4(b). By tuning the intracell and intercell hopping $t_1$ and $t_2$, there will be a gap closing and reopening process near Fermi level as shown in Fig. S4(c-e).

To show the band inversion (topology) of the gap, we plot the $\Gamma$-point wavefunction of the two bands near Fermi level as shown by the inset of Fig. S4(c, e). One can easily see that when $t_2 > t_1$, the wavefunction of two bands is inverted, indicating a topological nontrivial gap, similar with 1D SSH model. We numerically calculated the relationship between the gap at $\Gamma$ and $(t_1 - t_2)$ as shown in Fig. S4(f), one can see that the gap is linear to the absolute value of $(t_1 - t_2)$.

Thus, the CLC of electron hopping (gap) between the two states at $\Gamma$ around Fermi level can be expressed as $T = 2(t_1 - t_2)$.

Fig. S4. Illustration of high-order topological states in Kekulé lattice. (a) Kekulé Lattice. (b) 1D armchair nanoribbon of Kekulé lattice. (c) The band structure for nanoribbon when $t_2 < t_1$, the insets show the $\Gamma$ point
wavefunction. (d) The band structure for nanoribbon when $t_2 = t_1$. (e) The band structure for nanoribbon when $t_2 > t_1$, the insets show the $\Gamma$ point wavefunction. (f) The plot of gap as a function of $(t_1 - t_2)$.

Next, to show the correspondence between CLC of hopping and topology, one can make a finite-length armchair ribbon with strong bond ($t_2$) broken as shown in Fig. S5(a). For $T > 0$ ($t_2 < t_1$), the energy spectrum is shown in Fig. S5(b) which shows a trivial gap without corner states in the gap. For $T < 0$ ($t_2 > t_1$), there are two topological in-gap states as shown in the red dashed box in Fig. S5(c), which are similar to 1D SSH model with strong bond ($t_2$) broken in Fig. 2(c). We plot these two states in real-space which are localized at two ends of the ribbon as shown by red dots in Fig. S5(a). Thus, the six corner states of a hexagon flake of Kekulé lattice (see Fig. 4) can be understood as three pairs of in-gap “end” states of 1D armchair ribbon. Also similar with 1D SSH model (Fig. 2(b)), assuming $t_2 > t_1$, if one makes a finite-length ribbon with weak bond ($t_1$) broken as shown in Fig. S5(e), there will be no topological in-gap states as shown in Fig. S5(d).

On the other hand, for 1D zigzag ribbon as shown in Fig. S5(f), it is a metallic ribbon with many trivial dangling-bond edge states around the zero energy (Fermi level) as shown in Fig. S5(g), similar to zigzag graphene ribbon[8-10]. Consequently, the 1D zigzag ribbon is trivial without in-gap topological states. To further confirm this, one can plot the states near the Fermi level (marked by dashed red box) in real-space as shown Fig. S5(g) which are indeed localized at zigzag edge rather than at two corners. In this way, two corners of a rhombus sample having corner states can be understood as topological “end” states of one topological nontrivial armchair chain, while the other two corners without corner states are ends of one topological trivial zigzag chain, as shown in Fig. S5(h).
Fig. S5. Illustration of topological “end” state in Finite-size Kekulé ribbon. (a) The upper figure shows the way to cut an armchair ribbon with strong bond ($t_2$) broken. The lower figure shows the finite-size armchair ribbon the in-gap topological states. (b) The energy spectrum for $T > 0$ ($t_2 < t_1$). (c) The energy spectrum for $T < 0$ ($t_2 > t_1$). The red dashed box marks the in-gap topological “end” states. (d) The upper figure shows the way to cut an armchair ribbon with weak bond ($t_1$) broken. The lower figure shows the finite-size armchair ribbon. (e) The energy spectrum of finite size ribbon in Fig. S5(d) when $t_2 > t_1$. (f) The way of cutting a 1D zigzag ribbon with strong bond ($t_2$) broken. (g) The energy spectrum of the zigzag chain in Fig. S5(f). The red box marks the dangling-bond states on zigzag edge. The lower figure shows the real-space distribution of the dangling-bond states. (h) The corner states of a rhombus sample. The grey and pink band mark the zigzag and armchair ribbon, respectively.
Fig S6 The in-plane phonon bands of the four-atomic Kagome lattice model. There is a nonuple-degenerate flat band at zero frequency, because we only consider the stretching restoring force for springs in our in-plane model which can generate collective modes with no restoring forces (floppy mode)[11,12]. Such floppy modes can be stabilized by considering a weak bending restoring force.
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