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Theory of Superconductivity in LaRu_3Si_2 and Predictions of New Kagome Flat Band Superconductors

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Abstract

Kagome flat bands can enhance superconductivity, but the same flat-band density of states also amplifies repulsive interactions, so partially filled flat bands often favor magnetic or other competing instabilities. The conditions under which flat bands can promote superconductivity in real materials therefore remain unclear. Here, we present a combined *ab initio*, analytical, and high-throughput study of 1:3:2 kagome compounds, using LaRu_3Si_2 as a representative case. This family realizes a distinct filling regime in which a kagome-derived quasi-flat band, predominantly of local $d_{x^2-y^2}$ character, lies near the Fermi level but remains nearly filled, allowing superconductivity to persist. This contrasts with the van Hove physics often associated with 1:3:5 compounds and the magnetism that partial flat-band filling can favor in the 1:6:6 family. The electron-phonon coupling is strongly mode-selective, dominated by the coupling between kagome B_{3u} phonons, corresponding to local x -direction displacements toward kagome hexagon centers, and kagome flat-band electrons. We derive an analytical expression for this coupling and show that the mode selectivity originates from kagome geometry and persists in 1:3:2 compounds with similar low-energy electronic and phononic structures. Light hole doping toward the flat band, of order one hole per unit cell, enhances the electron-phonon coupling and raises T_c by over 50%, whereas heavier hole doping induces ferromagnetism and structural instability. Extending beyond LaRu_3Si_2 , high-throughput screening of 3063 stable 1:3:2 kagome compounds identifies 385 candidates with predicted $T_c \geq 1 \text{ K}$, reaching a maximum of 15 K. These results establish the 1:3:2 family as a rare materials class for flat-band-assisted superconductivity mediated by mode-selective electron-phonon coupling, and clarify the intrinsic limits of flat-band-driven superconductivity in real materials. Possible measurements of the electronic structure and lattice dynamics are proposed to assess the role of the flat band and its coupling to phonons.

1 Introduction

Kagome materials, with their characteristic lattice geometry and distinctive electronic structure, provide a fertile ground for realizing emergent quantum phenomena. The kagome lattice naturally hosts flat bands (FBs), Dirac cones, and van Hove singularities at specific electron fillings [1–3], enabling a rich interplay between band topology and electronic interactions. These features have led to the discovery of non-trivial topological states [4–6], charge density waves (CDWs) [7–10], superconductivity (SC) [11–13], and quantum spin-liquid phases [14–17]. A central question is whether the large density of states (DOS) and nontrivial quantum geometry associated with kagome FBs can enhance SC in real materials [18–21]. The difficulty is that the same FB DOS also amplifies repulsive interactions, so that when the FB is partially filled, magnetic or other competing instabilities are often favored over SC. Thus, for real materials, the central issue is not simply whether a kagome compound hosts an FB, but whether the FB can lie close to the Fermi level while remaining sufficiently filled or empty to avoid competing instabilities. A further question is whether materials with such an FB condition can have the interactions needed for SC, for example, sufficient coupling of the FB electrons to phonons.

Among recently discovered kagome materials, the 1:3:5, 1:1, and 1:6:6 families have attracted significant interest. The vanadium-based kagome metal AV_3Sb_5 ($A = K, Rb, Cs$), a representative of the 1:3:5 family, is one of the most extensively studied examples [6, 11, 22–28]. It hosts a $\mathbb{Z}_2$ -nontrivial band topology [6, 11], a CDW transition at $T_{CDW} \sim 80\text{--}104\text{ K}$ [7–10, 29], and SC with $T_c \sim 0.9\text{--}2.5\text{ K}$ [12, 13, 30, 31]. Elemental substitution in this family has yielded titanium-based $CsTi_3Bi_5$ [32–36] and chromium-based $CsCr_3Sb_5$ [37–40]. However, although both AV_3Sb_5 and $CsTi_3Bi_5$ are superconducting, their Fermi levels (E_F) lie near van Hove singularities rather than FBs [10, 32, 33]. Meanwhile, $CsCr_3Sb_5$ hosts FBs near E_F [38, 39], but its SC with $T_c^{\max} \sim 6.4\text{ K}$ emerges only under applied pressures of 3.65–8.0 GPa [37].

Unlike the 1:3:5 family, which includes superconducting members, the 1:1 and 1:6:6 kagome families primarily exhibit CDW and magnetic transitions [41–45]. Representative examples include ScV_6Sn_6 and $FeGe$, both exhibiting CDW behavior, with $FeGe$ also showing pressure-sensitive ordering [44, 46–49]. Their electronic structures can be understood through a LEGO-like framework, where kagome d orbitals decouple into hybridized subsets [50]. These materials accommodate broad chemical substitutions [51], with E_F often near van Hove singularities or FBs. However, when FBs approach E_F , magnetism typically emerges, polarizing and shifting the bands away from E_F , thereby suppressing SC [42, 45, 51]. These examples illustrate the practical challenge of FB SC: the FB must lie close enough to E_F to strengthen pairing, yet remain sufficiently filled or empty to avoid magnetic instabilities.

The 1:3:2 kagome compounds occupy a distinctive filling regime: a kagome-derived FB can lie near E_F while remaining nearly filled. This differentiates them from 1:3:5 kagome superconductors, whose low-energy physics is often associated with van Hove singularities, and from 1:6:6-type FB systems, in which partial FB filling tends to favor magnetic order. Several 1:3:2 compounds are superconducting, including $CeRu_3Si_2$ with $T_c \sim 1\text{ K}$ [52–54], YRu_3Si_2 with $T_c \sim 3\text{ K}$ [55, 56], $ThRu_3Si_2$ with $T_c \sim 3.8\text{ K}$ [57], and $LaIr_3Ga_2$ with $T_c \sim 5.2\text{ K}$ [58]. This makes the 1:3:2 family a well-defined

materials platform for testing whether a kagome FB can strengthen superconducting pairing without inducing magnetic order. Within this family, LaRu_3Si_2 is the most extensively studied superconducting example. It exhibits ambient-pressure SC with $T_c \sim 7.8$ K, among the highest reported values for kagome superconductors, and hosts high-temperature CDW transitions at ~ 400 K with wave vector $(1/4, 0, 1/2)$ and at 80-170 K with wave vector $(1/6, 0, 1/2)$ [59–66]. First-principles calculations indicate a quasi-FB near E_F [67], while experiments report a nodeless s -wave superconducting gap [68] and possible two-gap behavior [69]. Together with the absence of reported magnetic order, these features make LaRu_3Si_2 an experimentally grounded test case for FB-assisted SC. However, the microscopic origin of its SC and the role of the structural distortion remain unresolved.

In this work, we use LaRu_3Si_2 as a representative member of the 1:3:2 kagome family to determine how a nearly filled kagome FB near E_F contributes to SC in real materials. Combining first-principles calculations with analytical modeling, we show that SC in LaRu_3Si_2 is dominated by strongly mode-selective electron-phonon coupling (EPC) between Ru B_{3u} phonons, corresponding to local- x displacements toward kagome hexagon centers, and Ru A_g FB states derived mainly from local $d_{x^2-y^2}$ orbitals. Doping calculations further reveal the potential and limitations of FB-driven SC: light hole doping toward the FB (~ 1 hole per unit cell) enhances EPC and raises T_c by over 50%, whereas heavier doping destabilizes the structure and induces magnetism. Extending the analysis to the broader 1:3:2 family, high-throughput screening identifies 3063 candidate materials, including 385 predicted superconductors, with the highest T_c reaching 15 K. Taken together, these results identify 1:3:2 kagome compounds as a rare realization of FB-assisted SC in real materials, where FB states contribute directly to pairing through mode-selective EPC. They also show that this mechanism is limited by competing magnetic and structural instabilities that emerge as the FB approaches partial filling.

2 Structural stability and lattice dynamics

The structural transitions of LaRu_3Si_2 make the choice of reference phase important for the EPC analysis. X-ray diffraction (XRD) reveals several temperature-dependent phases [65, 66]. Above 620 K, it adopts the high-symmetry space group (SG) $P6/mmm$ (No. 191), featuring a Ru kagome lattice at $z = c/2$, a Si honeycomb lattice, and a La triangular lattice at $z = 0$, occupying Wyckoff positions $3g$, $2c$, and $1a$, respectively [Fig. 1a]. However, the harmonic phonon spectrum [Fig. 1b] shows dynamic instability at low temperatures, with imaginary modes on the $q_z = \pi/c$ plane, an instability that persists even at elevated temperatures (see Supplementary Section S2.3.1).

We analyze the irreducible representations (irreps) of the imaginary phonon modes at the high-symmetry point $A = (0, 0, \pi/c)$ in $P6/mmm$ and their associated distortion patterns [Table 1]. The one-dimensional (1D) irrep A_4^+ , corresponding to a Ru B_{3u} mode involving local x -displacements toward the kagome hexagon center (1a site), drives in-plane torsional distortions [inset, Fig. 1b]. Its maximal subgroup is $P6_3/mcm$ [70, 71], while powder XRD reports a lower-symmetry $P6_3/m$ (No. 176) phase [72], which breaks the nonsymmorphic in-plane symmetry $\tilde{C}_{2x} = \{C_{2x}|0, 0, 1/2\}$

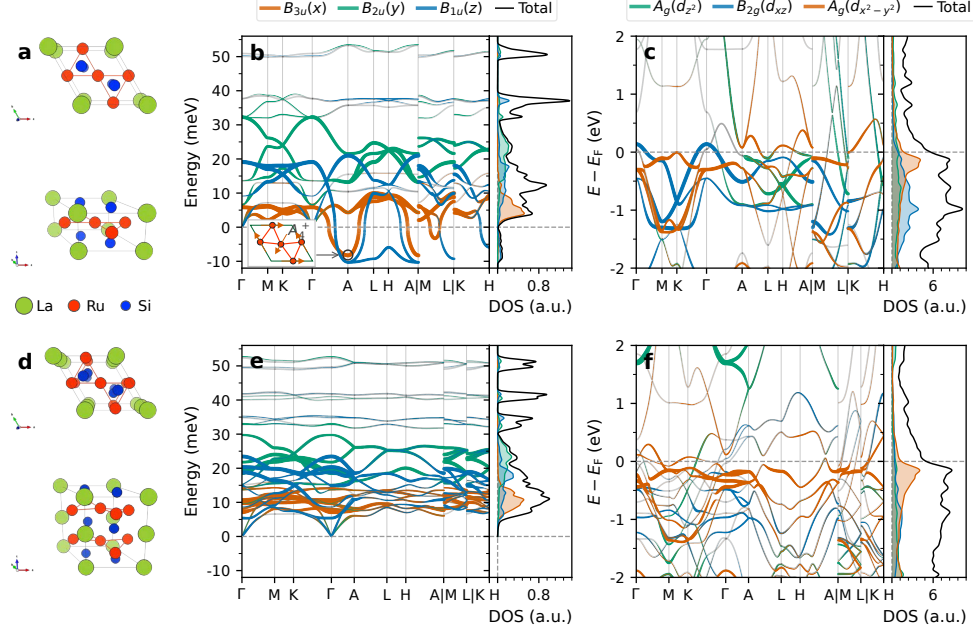


Fig. 1 Structural, phonon, and electronic properties of LaRu_3Si_2 in the $P6/mmm$ and $Cccm$ phases. **a–c** Crystal structure in primitive cell, phonon dispersion, and band structure of the $P6/mmm$ phase. **d–f** Corresponding results for the $Cccm$ phase. Phonon bands are coloured according to the Ru displacement weight in the local axis and electronic bands according to the Ru local d -orbital weight. The side panels give the corresponding projected DOS using the same colour scheme. The inset in **b** shows the eigenvector of the unstable A_4^+ mode circled at A . The $1 \times 1 \times 2$ reconstruction in the $Cccm$ phase folds the bands from the $k_z = 0$ and $k_z = \pi/c$ planes of the $P6/mmm$ Brillouin zone onto the $k_z = 0$ plane of the $Cccm$ Brillouin zone (see Supplementary Section S2.4).

present in $P6_3/mcm$ (No. 193). First-principles relaxations starting from $P6_3/m$ converge to $P6_3/mcm$, which is also energy favored [Table 2]. However, phonon spectra reveal that both are dynamically unstable (see Supplementary Section S2.3.2) and, thus, are not considered further.

In addition to the A_4^+ mode, a 2D soft mode with irrep A_5^+ breaks C_{3z} symmetry and can lower the structure to subgroups $Cccm$ (No. 66), $Cmmm$ (No. 65), or $P2_1/m$ (No. 10). First-principles relaxations suggest that the $Cccm$ phase is energetically favored (Table 2) and dynamically stable [Fig. 1e], consistent with recent experimental refinements in LaRu_3Si_2 for $400 \text{ K} < T < 620 \text{ K}$ [65, 66] and in YRu_3Si_2 for $T > 800 \text{ K}$ [56]. In this $Cccm$ phase, the original A_4^+ mode becomes hardened, while upon further cooling, a 1D mode at Γ with irrep Γ_3^+ softens, though it remains positive. This mode involves the same atomic displacements as A_4^+ in the $P6/mmm$ phase (see Supplementary Section S2.3.3). Importantly, the A_4^+ mode in the $P6/mmm$ phase, and the corresponding Γ_3^+ mode in the lower-symmetry $Cccm$ phase, harden with increasing electronic temperature (see Supplementary Section S2.3), in close analogy to the soft-mode behavior reported in 1T transition-metal dichalcogenides [73, 74],

MgB₂ [75, 76], and KV₃Sb₅ [77]. This points to an EPC-driven origin of the instability. Its softening on cooling should therefore be accompanied by phonon self-energy effects, such as anomalous temperature dependence and possible linewidth broadening, providing direct experimental signatures in Raman spectroscopy and inelastic X-ray or neutron scattering. In addition, pressure-dependent phonon calculations indicate that the same Γ_3^+ mode in the *Cccm* phase becomes unstable near 13 GPa (see Supplementary Section S2.3.6), consistent with recent experiments that report anomalous behavior of T_c in the same pressure range [63, 64].

Below 400 K, LaRu₃Si₂ exhibits two CDW phases: a $4 \times 4 \times 2$ phase near 400 K and a $6 \times 6 \times 2$ phase at 80 K (170 K in Fe-doped samples) [65, 66]. The $4 \times 4 \times 2$ phase has *Pmma* (No. 51) symmetry, whereas the $6 \times 6 \times 2$ phase has *Pbam* (No. 55) symmetry [65, 66]. Such CDW superstructures appear to be a common motif in the 1:3:2 family and have been reported not only in LaRu₃Si₂ [65, 66] but also in YRu₃Si₂ [56] and NdRu₃Si₂ [78]. Structural refinements indicate that the distortions from the high-temperature *Cccm* phase to the low-temperature *Pmma* and *Pbam* phases are dominated by Si displacements. Consistently, orbital-resolved unfolded band structures show that the Ru-local $d_{x^2-y^2}$ quasi-FB and its associated DOS peak persist in both low-temperature CDW phases, and the phonon spectra remain qualitatively similar (see Supplementary Section S2.3.5).

Because the key electronic and phononic ingredients are largely preserved across these low-temperature CDW transitions, we focus our EPC and SC analysis on the $1 \times 1 \times 2$ *Cccm* phase, which is sufficient to isolate the leading electronic and phononic ingredients of the proposed mechanism. A detailed first-principles treatment of EPC and SC in the *Pmma* and *Pbam* supercells is left for future work because of the substantially increased computational cost.

Table 1 Possible subgroups of SG *P6/mmm* (No. 191) driven by imaginary phonon modes at high symmetry point *A* in LaRu₃Si₂.

$\omega(\text{meV})$	Irrep (ρ)	Subgroup
-8.384	A_4^+ (1D)	SG <i>P6₃/mcm</i> (No. 193)
-10.342	A_5^+ (2D)	SG <i>Cccm</i> (No. 66)

Table 2 Total energy of LaRu₃Si₂ in different structures, with $\Delta E = E_{\text{SG}} - E_{P6/mmm}(\text{meV/atom})$.

SG	<i>P6/mmm</i>	<i>P6₃/m</i>	<i>P6₃/mcm</i>	<i>Cccm</i>
$\Delta E(\text{meV/atom})$	0	+13.690	-2.539	-13.738

3 Kagome-derived quasi-flat band near the Fermi level

To identify the orbital character of the low-energy states in the $Cccm$ phase, we first analyze the electronic structure of the higher-symmetry $P6/mmm$ phase and then track the evolution of these states under the structural distortion. The triangular, honeycomb, and kagome sublattices occupy Wyckoff positions $1a$, $2c$, and $3g$, with site-symmetry groups D_{6h} , D_{3h} , and D_{2h} , respectively. The bands near E_F arise primarily from Ru $4d$ and Si $3p$ orbitals. At the $3g$ site, the Ru $4d$ orbitals transform according to four distinct irreps of D_{2h} , distinguished by their eigenvalues under the three twofold rotations (see Supplementary Section S2.4). The orbital-resolved band structure [Fig. 1c] reveals a quasi-FB with predominantly Ru A_g (local $d_{x^2-y^2}$) character, which produces a peak in the total DOS 150 meV below E_F (see Supplementary Section S2.4). The same orbital also gives rise to a large Fermi surface (FS) that, as shown below, plays a key role in SC.

To evaluate the role of electron correlations, we performed embedded dynamical mean-field theory (eDMFT) calculations using WIEN2k and the Rutgers eDMFT code [79–83], with interaction parameters $U = 6$ eV and $J_H = 0.9$ eV. The spectral function obtained at $T = 100$ K closely reproduces the *ab initio* band structure, as does the FS (see Supplementary Section S2.4). The largest mass renormalization factor is $Z \simeq 0.66$, indicating relatively weak correlations. These results establish that LaRu_3Si_2 is a weakly correlated, itinerant metal in which SC is primarily driven by EPC rather than strong electronic correlations. Correlation effects are therefore neglected in the following analysis.

Upon cooling, LaRu_3Si_2 undergoes a structural transition driven by condensation of the 2D soft phonon mode A_g^+ , which doubles the unit cell along z and lowers the symmetry from $P6/mmm$ to $Cccm$ [Fig. 1d]. In this $Cccm$ phase, the kagome lattice becomes distorted along z , breaking the C_{3z} rotational symmetry. Although the symmetry breaking induces hybridization between the original D_{2h} irreps, the essential electronic features remain intact. In particular, the quasi-FB originated from Ru A_g orbitals, together with the associated DOS peak, persists in the $Cccm$ phase [Fig. 1f] (see Supplementary Section S2.4).

4 Mode-selective electron-phonon coupling

An exact FB arising from lattice geometry [84] is known to exhibit superfluid weight proportional to its quantum geometry under attractive interactions [18]. In dispersive bands, the quantum geometry of the FS can also contribute to EPC [85], thereby influencing SC. However, in 3D systems, partially filled FBs are often susceptible to magnetism due to Coulomb repulsion [20, 21], which can suppress SC. LaRu_3Si_2 , with the highest known $T_c \sim 7.8$ K among kagome superconductors [55, 57–60, 68], features a quasi-FB 150 meV below E_F . To assess its role in driving SC, we examined EPC via *ab initio* calculations using the EPW code [86–89] for both the high-symmetry $P6/mmm$ and the distorted $Cccm$ phases.

Although the $P6/mmm$ phase is dynamically unstable, it provides insight into the underlying EPC physics, as the symmetry-breaking distortion in the $Cccm$ phase introduces only perturbative changes to the electronic structure. Fig. 2a,b show the phonon linewidth $\Pi''_{\mathbf{q},\nu}$, Eliashberg function $\alpha^2 F(\omega)$, and cumulative EPC strength $\lambda(\omega)$ of the $Cccm$ phase, which are qualitatively similar to those of the $P6/mmm$ phase (see Supplementary Section S2.5). Phonons with energies below 15 meV dominate the EPC in both phases, accounting for 95.9% and 76.4% of the total EPC strength in the $P6/mmm$ and $Cccm$ phases, respectively. Mode-resolved analysis identifies the kagome-lattice B_{3u} (local x) phonon as the dominant EPC channel in this energy range, although the B_{3u} and B_{2u} (local y) modes have comparable linewidths. Decomposing $\alpha^2 F(\omega)$ of the $Cccm$ phase into contributions from displacements along the local axes at each site, we find that phonons below 15 meV account for 99% of $\lambda_{\text{Ru},x}$, compared with 25-31% of $\lambda_{\text{Ru},y}$. In the undoped cell, $\lambda_{\text{Ru},x}/\lambda_{\text{Ru},y} = 3.2$ (see Supplementary Section S2.5). The EPC between Ru A_g electrons and the B_{3u}/B_{2u} phonon modes in the kagome lattice was further examined by projecting the *ab initio* EPC tensor from EPW [86–89] onto the local Wannier basis, yielding the real-space EPC tensor. The results show that the coupling strengths of Ru A_g electrons to the B_{3u} and B_{2u} phonons are nearly identical, with values of 0.0201 Ry/Bohr and 0.0204 Ry/Bohr, respectively (see Supplementary Section S2.5).

To better understand this behavior, we parameterize the hopping terms using Slater-Koster integrals [90] within the Gaussian approximation [85] (see Supplementary Section S3.1). Specifically, the hopping between A_g ($d_{x^2-y^2}$) orbitals on sublattices m and n is given by $t_{mn}(\mathbf{r}) = f_{mn}(\mathbf{r})V^d(\mathbf{r}) - V_\pi(\mathbf{r})/2$, where $\mathbf{r}$ is the hopping vector, and $f_{mn}(\mathbf{r})$ is a geometric factor depending on the direction cosines of $\mathbf{r}$ (i.e., $r_\mu/|\mathbf{r}|$, $\mu \in \{x, y, z\}$) (see Supplementary Section S3.1). The terms $V_\pi(\mathbf{r})$ and $V^d(\mathbf{r}) = [V_\delta(\mathbf{r}) - 4V_\pi(\mathbf{r}) + 3V_\sigma(\mathbf{r})]/8$ represent Slater-Koster integrals for d orbitals [90] (see Supplementary Section S3.1). In the framework of the Gaussian approximation, all hopping integrals follow a Gaussian decay: $V_i(\mathbf{r}) = V_{i,0} \exp(-\gamma_i |\mathbf{r}|^2/2)$, with $i \in \sigma, \pi, \delta$, where $V_{i,0}$ sets the strength and γ_i controls the decay rate.

Using this framework, we analyze the EPC. Due to mirror symmetry $\mathcal{M}_z$, out-of-plane atomic motions do not couple to electrons in the ideal kagome layer of the $P6/mmm$ phase. Therefore, EPC $g_{mn,\nu}(\mathbf{k}, \mathbf{q})$ is nonzero only for in-plane atomic displacements, i.e., $\nu = x, y$. In the $Cccm$ phase, as well as in the lower-temperature phases, the symmetry-lowering distortion acts only as a weak perturbation to the kagome-derived low-energy states and does not qualitatively alter the dominant in-plane EPC channel (see Supplementary Section S2.5). For nearest-neighbor hopping between A_g ($d_{x^2-y^2}$) orbitals, the EPC can be decomposed into radial and angular components (see Supplementary Section S3.1). The total coupling amplitude is given by:

$$g_{mn;\nu}(\mathbf{r}) = \frac{\partial t_{mn}(\mathbf{r})}{\partial r_\nu} = \frac{\partial f_{mn}(\mathbf{r})}{\partial r_\nu} V^d(\mathbf{r}) + f_{mn}(\mathbf{r}) \frac{\partial V^d(\mathbf{r})}{\partial r_\nu} - \frac{1}{2} \frac{\partial V_\pi(\mathbf{r})}{\partial r_\nu}, \quad (1)$$

where the radial terms (second and third) scale with the projection of $\mathbf{r}$ onto direction ν , while the angular term (first) depends on the directional derivative of the geometric

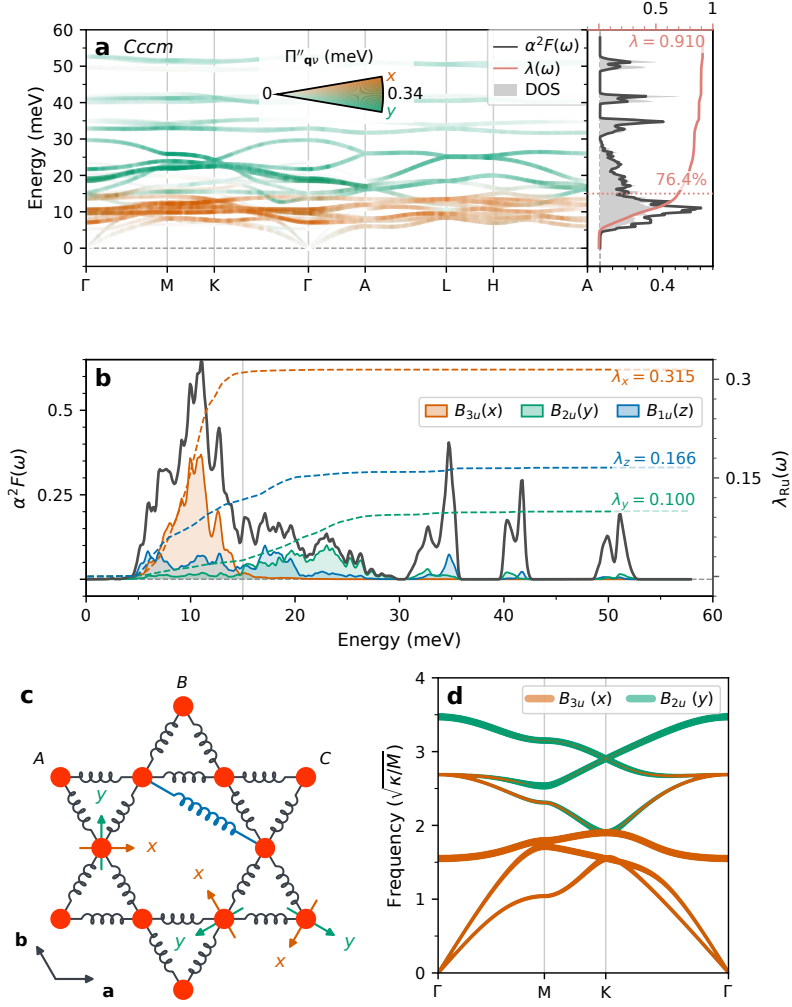


Fig. 2 EPC in the $Cccm$ phase of LaRu_3Si_2 . **a** Phonon dispersion, with modes coloured according to their Ru displacement character: B_{3u} (local x , orange) or B_{2u} (local y , green). The colour intensity indicates the linewidth $\Pi''_{\mathbf{q}\nu}$, as shown in the inset wedge-shaped legend. The side panel shows the Eliashberg spectral function $\alpha^2F(\omega)$ (black), the cumulative EPC strength $\lambda(\omega)$, and the phonon DOS (grey shading). The dotted line marks 15 meV. Phonons below this energy contribute 76.4% of the total $\lambda = 0.91$. **b** The same $\alpha^2F(\omega)$, with the kagome Ru contribution resolved along the three local axes of the $3g$ site: $B_{3u}(x)$, $B_{2u}(y)$, and $B_{1u}(z)$. The cumulative EPC strength of each channel is plotted against the right axis. The shaded areas show only the Ru contributions, which account for 64% of the total λ . **c** Schematic of the kagome spring-ball model, with the local coordinate frame (x, y) shown at one site of each sublattice. **d** Mode-resolved phonon spectrum of the spring-ball model, with ribbon widths and colours indicating the mode weights along the local x (B_{3u}) and y (B_{2u}) axes at each site. The $P6/mmm$ counterpart of panel **a** is shown in Supplementary Section S2.5.

factor f_{mn} . For the ideal nearest-neighbor kagome lattice, f_{mn} is stationary along the bond direction, so the angular term vanishes at the equilibrium bond and only the radial terms survive. Symmetry then fixes the radial coupling to the B_{2u} mode at $\sqrt{3}$ times that to the B_{3u} mode, where $\sqrt{3} = \tan(\pi/3)$ is set by the geometry of the kagome lattice. Using Slater-Koster parameters extracted from first-principles calculations (see Supplementary Section S3.1), we obtain coupling strengths of 0.0192 and 0.0334 Ry/Bohr between A_g electronic states and the B_{3u} and B_{2u} phonons, respectively. These values are of the same order as the corresponding full *ab initio* values of 0.0201 and 0.0204 Ry/Bohr (see Supplementary Section S2.5). The single-orbital model thus captures the overall coupling scale, while the near-equality of the two coupling strengths can be recovered by including an interorbital A_g - B_{1g} coupling channel (see Supplementary Section S3.1).

The bulk EPC constant is given by $\lambda = 2 \int d\omega \alpha^2 F(\omega)/\omega$, where $\alpha^2 F(\omega)$ is the Eliashberg function [91, 92]. Alternatively, it can be expressed as $\lambda = 2 \frac{D(\mu)}{N} \frac{\hbar \langle g^2 \rangle}{\hbar^2 \langle \omega^2 \rangle}$, where $D(\mu)$ is the electronic DOS at the chemical potential μ , N the number of lattice sites, and $\langle \omega^2 \rangle$ the McMillan average phonon frequency. The comparable *ab initio* real-space couplings do not by themselves explain the larger local- x contribution to λ .

We therefore examine the phonon-frequency hierarchy using a nearest-neighbor kagome spring-ball model [Fig. 2c]. The mode-resolved spectrum in Fig. 2d reveals that the B_{3u} phonon (orange) consistently has lower frequency than the B_{2u} phonon (green) across the Brillouin zone. An accidental degeneracy at the K point is lifted by including next-nearest-neighbor springs (blue curve in Fig. 2c, see Supplementary Section S3.2). The frequency difference originates from the distinct restoring forces: vertical displacements (associated with B_{2u}) experience stronger potential gradients than horizontal ones (B_{3u}), leading to higher phonon energies. This trend, derived analytically from our spring-ball model, is consistent with the high-throughput calculations (see Supplementary Section S5), in which low-frequency phonons likewise dominate the EPC of the transition-metal kagome compounds. Our model thus provides a simple yet quantitative framework for understanding the kagome phonon spectrum.

5 Superconductivity and competing instabilities

We next analyze SC mediated by EPC in LaRu₃Si₂. As shown in Fig. 3a, the superconducting gap function $\Delta_{\mathbf{k}n}$ is strongly anisotropic, running from 0.86 to 2.01 meV at $T = 2.5$ K with an area-weighted mean of 1.37 meV, and is largest on the FS dominated by Ru A_g ($d_{x^2-y^2}$) orbitals (see Supplementary Section S2.5). Averaged over each FS the gap spans 1.13 to 1.53 meV, a spread that a single isotropic gap cannot describe and that is consistent with recent observations of a two-gap $s + s$ structure in LaRu₃Si₂ [69]. This anisotropy is likely due to the high DOS and the large FS from the quasi-FB formed by the Ru A_g ($d_{x^2-y^2}$) orbitals. Additionally, since the superconducting gap is smaller than the bandwidth of the nearly FB, the conventional contribution to the superfluid weight dominates over the quantum geometric component (see Supplementary Section S4).

The orbital dependence of the gap motivates testing the role of the quasi-FB by varying the band filling. We therefore study doping in $Cccm$, tracking changes in EPC together with structural and magnetic stability. As shown in Fig. 3b, the structure remains dynamically stable under weak hole doping ($N_{\text{hole}} < 2$ per unit cell), although phonon softening indicates proximity to an instability. As E_F approaches the FB, the nonmagnetic state becomes unstable toward ferromagnetism. At three holes per unit cell, a spin-polarized solution is obtained with a small magnetic moment of $0.27 \mu_B$ on each kagome Ru atom ($0.13 \mu_B$ per atom averaged over the unit cell) and a total energy 1.4 meV/atom lower than that of the nonmagnetic state [Fig. 3c] [20, 21]. The doping dependence of T_c , calculated within the rigid-band approximation and shown in Fig. 3d, further supports this picture: light hole doping ($N_{\text{hole}} < 1$ per unit cell) enhances T_c by over 50% through an increased DOS associated with the Ru A_g FB and stronger EPC, whereas electron doping suppresses SC [93–95]. This enhancement is mode-selective rather than uniform. At $E_F - \mu = +150$ meV, the local x (B_{3u}) coupling on Ru is enhanced by a factor of 2.3 relative to its undoped value, compared with a factor of 1.6 for the local y channel. Consequently, the ratio $\lambda_{\text{Ru},x}/\lambda_{\text{Ru},y}$ increases from 3.2 to 4.6 (see Supplementary Section S2.5). Shifting E_F toward the quasi-FB thus strengthens the B_{3u} channel that already dominates the EPC in the undoped system, with the strongest mode selectivity occurring at the filling where both λ and T_c reach their maxima.

These results demonstrate that the FB in LaRu_3Si_2 is essential: it enhances SC under moderate hole doping but drives magnetism and structural instability as its DOS peak approaches E_F . This prediction can be examined experimentally—via angle-resolved photoemission spectroscopy (ARPES) to determine the FB position relative to E_F , and through controlled substitution or gating to probe the non-monotonic doping dependence of T_c . Notably, chemical-pressure tuning achieved by substituting Si with Ge in LaRu_3Si_2 has already shifted the Ru- A_g FB toward E_F and enhanced T_c by $\sim 7\%$ [96], consistent with our theory. Such measurements offer a valuable opportunity to evaluate our predictions and clarify the central role of the FB in the SC of 1:3:2 kagome compounds.

6 Superconducting candidates in the 1:3:2 family

Chemical substitution is the most practical route to doping in real materials. We therefore performed a high-throughput structural search for 1:3:2 compounds sharing the same $P6/mmm$ structure and stoichiometry as LaRu_3Si_2 . Within an energy range up to 100 meV/atom above the convex hull, 3063 such compounds were identified. Of these, 385 are predicted to exhibit SC with $T_c \geq 1$ K, including 58 with $T_c \geq 5$ K. Full lists of thermodynamically ($E_{\text{hull}} < 100$ meV/atom) and dynamically stable superconductors are provided in Supplementary Section S5, along with detailed information on the electronic structures, phonon dispersions, and Eliashberg functions for those with $T_c \geq 1$ K and $E_{\text{hull}} < 30$ meV/atom.

These predicted kagome superconductors fall into two broad classes. The first resembles LaRu_3Si_2 , with kagome bands derived from transition metal d orbitals

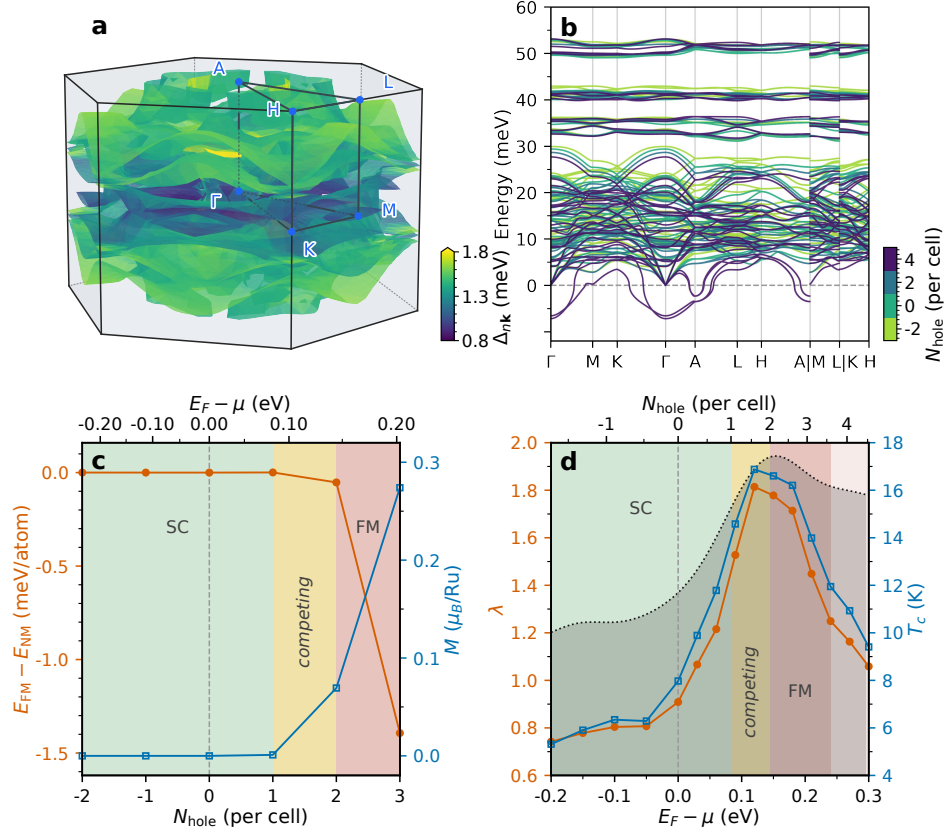


Fig. 3 Superconducting properties of LaRu_3Si_2 under doping. **a** Superconducting gap function $\Delta_{\mathbf{k}n}$ on the FS of LaRu_3Si_2 in the $Cccm$ phase, from the anisotropic Migdal-Eliashberg solution at $T = 2.5$ K. **b** Phonon spectra of LaRu_3Si_2 in the stable $Cccm$ phase as a function of hole doping. **c** Total-energy difference (meV/atom) between calculations initialized in nonmagnetic (NM) and ferromagnetic (FM) states, together with the magnetic moment of the kagome Ru atoms (μ_B/Ru) as a function of hole-doping level N_{hole} (per unit cell) in the $Cccm$ phase. The magnetization resides almost entirely on the kagome Ru sites. Lattice instabilities appear for $N_{\text{hole}}/\text{unit cell} > 2$. Here NM and FM refer to the *initial* magnetic configurations used in the self-consistent calculations. A zero energy difference indicates that the FM-initialized calculation relaxes to the NM state. **d** EPC constant λ and estimated superconducting T_c as a function of chemical potential shift $E_F - \mu$ (eV) within the rigid-band approximation. The gray background shows the total DOS of LaRu_3Si_2 .

and EPC dominated by low-frequency phonons. Most of these materials are effectively electron-doped analogs of LaRu_3Si_2 and therefore have lower T_c . Among the 65 promising compounds in this class with $E_{\text{hull}} < 30$ meV/atom (see Supplementary Section S5.1), notable candidates include SrIr_3Ni_2 ($T_c \sim 7$ K) and CaRh_3Ga_2 ($T_c \sim 6$ K). By contrast, hole-doped variants such as RRu_3B_2 ($R = \text{Tm, Er, Dy}$) tend to magnetize and are structurally unstable in the paramagnetic phase [60], in line with the FB-instability trend identified above. The recent synthesis of YRu_3B_2 , together with the related isostructural compound LuRu_3B_2 , already provides a proof of principle for

this screening strategy [97–99], offering encouraging evidence that machine-learning-aided materials screening can successfully identify new superconductors within this structural family.

The second class comprises compounds whose kagome nets are formed by main-group elements, mainly Be and Al, and whose relevant bands derive from p electrons. Among the 20 compounds in this class with $E_{\text{hull}} < 30$ meV/atom, notable examples include $X\text{Be}_3\text{Ni}_2$ ($X = \text{Zr}, \text{Sc}$), with estimated $T_c \sim 2$ K.

It should be emphasized that the EPC mechanism identified above for LaRu_3Si_2 is not intended to represent a universal mechanism for all candidate compounds, but rather applies to those that retain a kagome-derived quasi-FB near E_F and a comparable hierarchy of phonon frequencies. Given the broad chemical diversity of these ternary compounds, both the electronic structures and the microscopic pairing mechanisms can vary substantially from material to material.

7 Discussion

In summary, we have systematically investigated LaRu_3Si_2 as a representative 1:3:2 kagome superconductor with a kagome-derived FB near E_F and ambient-pressure SC with the highest reported $T_c \sim 7.8$ K among kagome compounds. Our study focuses on its structural stability, EPC, and superconducting properties, and uses this compound to identify a broader mechanism in the 1:3:2 kagome family. Contrary to earlier reports suggesting a structure in SG $P6_3/m$ (No. 176) [72], our *ab initio* calculations and analysis demonstrate that the stable structure of LaRu_3Si_2 above the CDW transition temperature is stabilized by condensation of the 2D A_5^+ soft phonon mode, consistent with recent XRD refinements in both LaRu_3Si_2 [65, 66] and YRu_3Si_2 [56]. The EPC in LaRu_3Si_2 is strongly mode-selective, dominated by coupling between kagome B_{3u} phonons (local x direction) and Ru A_g (local $d_{x^2-y^2}$) electrons. This behavior arises from a universal feature of kagome systems: the B_{3u} phonon consistently exhibits a significantly lower frequency than the B_{2u} (local y direction) phonon. A spring-ball model and high-throughput screening suggest that this mode-selective EPC can persist in a large subset of related 1:3:2 kagome materials with similar low-energy electronic and phononic structures. Doping calculations further reveal both the potential and the limitations of FB-driven SC: light hole doping toward the FB, of order one hole per unit cell, enhances EPC and raises T_c by over 50%, whereas heavier hole doping destabilizes the structure and induces magnetism. Extending beyond LaRu_3Si_2 , high-throughput screening of the 1:3:2 family identifies 3063 stable kagome compounds with the same structural motif, among which 385 are predicted to be superconducting with $T_c \geq 1$ K. Notably, we also identify candidate kagome superconductors whose FBs are primarily derived from p electrons.

Placed in a broader context, these findings clarify a central issue in FB physics. In most systems, the large DOS of FBs favors magnetism, which competes directly with SC. This behavior is consistent with numerous experimental observations in kagome and related materials [39, 40, 42, 45]. The 1:3:2 family represents a rare exception: here, the FB is nearly filled, magnetization is inefficient, and mode-selective EPC dominates the pairing mechanism. This duality clarifies the central question of FB

SC—FBs can enhance T_c , but only within a narrow regime where magnetic instabilities are avoided. These results identify 1:3:2 kagome compounds as a rare realization of FB-assisted SC in real materials, while also clarifying the intrinsic filling limit of this mechanism. Experimental probes such as ARPES and inelastic X-ray or neutron scattering can test these predictions by resolving the FB character of the A_g states and probing the associated kagome phonons, providing a direct route to assess the proposed mode-selective EPC mechanism.

Methods

Ab initio calculations

First-principles calculations were performed based on density functional theory (DFT), using the projector augmented wave method [100, 101], as implemented in the Vienna *ab initio* Simulation Package (VASP) [102, 103] and the QUANTUM ESPRESSO package [104, 105]. The generalized gradient approximation was used, incorporating the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional [106]. The internal atomic positions within the structures were relaxed until the forces on each atom were reduced to less than 0.1 meV/Å. A kinetic energy cutoff of 500 eV or 100 Ry was set for the plane-wave basis set. The Brillouin zone was sampled using the Monkhorst-Pack method [107] with a Γ -centered $\mathbf{k}$ -point grid of $9 \times 9 \times 12$ and $9 \times 9 \times 6$ for LaRu₃Si₂ in the SG 191 and SG 66 ($1 \times 1 \times 2$) phase respectively.

Phonon spectra were calculated via VASP using the frozen phonon method in conjunction with the PHONOPY package [108, 109] and via the QUANTUM ESPRESSO package in the framework of density functional perturbation theory (DFPT). Irreps were determined using IRVSP [110, 111]. Wannier-based calculations were done with WANNIERTOOLS [112]. The band representation analysis was conducted on the website BRdecomp. Furthermore, a Wannier-based tight-binding Hamiltonian was constructed using WANNIER90 [113, 114], with La- d , Ru- s , d and Si- p orbitals.

EPC properties were computed using the EPW package [86–89], included within QUANTUM ESPRESSO [104, 105]. Electron-phonon matrix elements were first computed on coarse $\mathbf{k}$ -point and $\mathbf{q}$ -point meshes, $9 \times 9 \times 12$ and $3 \times 3 \times 4$ for the SG 191 phase and $9 \times 9 \times 6$ and $3 \times 3 \times 2$ for the SG 66 phase, and then interpolated onto finer grids using maximally localized Wannier functions. The fine meshes for the SG 66 phase were $24 \times 24 \times 16$ for $\mathbf{k}$ and $12 \times 12 \times 8$ for $\mathbf{q}$, with a 1 eV Fermi window and a 0.20 meV phonon smearing. Phonon dispersions and linewidths $\Pi''_{\mathbf{q}\nu}$ were evaluated along the high-symmetry path, whereas $\alpha^2F(\omega)$, the cumulative $\lambda(\omega)$ and the phonon DOS were obtained as Brillouin-zone averages on those meshes.

Superconducting properties

The isotropic Eliashberg spectral function $\alpha^2F(\omega)$ and the EPC constant $\lambda = 2 \int d\omega \alpha^2F(\omega)/\omega$ were evaluated from the interpolated electron-phonon matrix elements on those same meshes. Superconducting transition temperatures were then estimated from the Allen-Dynes-modified McMillan equation [92, 115, 116] with a

Coulomb pseudopotential $\mu^* = 0.10$ and the logarithmic average phonon frequency $\omega_{\log}$ obtained from $\alpha^2 F(\omega)$.

The momentum-resolved gap function $\Delta_{\mathbf{k}n}$ of Fig. 3a was obtained by solving the anisotropic Migdal-Eliashberg equations on the imaginary axis [91, 117], as implemented in EPW [88, 89], followed by Padé continuation to the real axis. The values reported are those at $T = 2.5$ K, the lowest temperature solved. States within 1.0 eV of E_F were retained, with a Fermi-surface broadening of 20 meV and a Matsubara frequency cutoff of 0.1 eV, and the electron-phonon matrix elements were interpolated onto fine $24 \times 24 \times 16$ $\mathbf{k}$ - and $24 \times 24 \times 16$ $\mathbf{q}$ -meshes, the two taken equal so that the fine $\mathbf{k}$ - and $\mathbf{q}$ -grids are the same set of points. The Coulomb pseudopotential was $\mu^* = 0.10$, the same value used for the Allen-Dynes estimates.

DMFT calculations

First-principles calculations combining DFT and eDMFT were performed using WIEN2k and the Rutgers eDMFT code [79, 80]. The local-density approximation [118] was employed, as it provides optimal results for lattice properties when combined with eDMFT [81, 82]. Coulomb repulsion and Hund’s coupling parameters were set to $U = 6.0$ eV and $J_H = 0.9$ eV, respectively. The auxiliary impurity problem in eDMFT was solved using a continuous-time quantum Monte Carlo impurity solver [83].

High-throughput *ab initio* calculations

High-throughput *ab initio* calculations were performed to study the kagome family RT_3X_2 , crystallizing in SG 191 ($P6/mmm$). The chemical space was explored by systematically substituting elements up to Bi in all possible combinations within the prototype structure. From the resulting compounds, we selected those with distances to the convex hull below 100 meV/atom (calculated within the PBE approximation [106] against the ALEXANDRIA database [119, 120]), metallic, and nonmagnetic. For the resulting 3063 candidate materials, we performed DFPT calculations to obtain the EPC constants. All calculations were performed using QUANTUM ESPRESSO (version 7.1) [104, 105] with the Perdew-Burke-Ernzerhof generalized gradient approximation for solids (PBEsol) [121], and we chose the PBEsol pseudopotentials from the PSEUDODOJO project [122], specifically the stringent, scalar-relativistic norm-conserving set. Geometry optimizations were performed using uniform Γ -centered $\mathbf{k}$ -point grids with a density of 1500 $\mathbf{k}$ -points per reciprocal atom. Convergence thresholds for energies, forces, and stresses were set to 1×10^{-8} a.u., 1×10^{-6} a.u., and 5×10^{-2} kBar, respectively. For electron-phonon calculations, we used the double-grid technique, using the previous $\mathbf{k}$ -grid as the coarse grid and a quadrupled $\mathbf{k}$ -grid for the fine sampling. Phonon $\mathbf{q}$ -points were sampled at half the initial $\mathbf{k}$ -point grid. The Eliashberg function was obtained through double delta integration using Methfessel-Paxton smearing [123] of 0.03 Ry. Materials exhibiting imaginary frequencies at explicitly calculated $\mathbf{q}$ -points were excluded from further analysis, while those developing instabilities during Fourier interpolation were retained but flagged as potentially unstable. In both cases, the materials might stabilize in a lower symmetry ground state, as is characteristic of LaRu_3Si_2 and other kagome phases [51]. We

leave a more detailed study on the CDW phases and SC properties of these materials for future work. Superconducting transition temperatures were estimated using the McMillan formula [92, 115], with $\mu^* = 0.10$.

Data availability

All data generated in this study are included in the main text and the Supplementary Information. Further data are available from the authors on reasonable request.

Code availability

All calculations in this work used publicly available packages, cited in Methods: QUANTUM ESPRESSO, WANNIER90, EPW, WANNIERTOOLS, VASP, PHONOPY, IRVSP, and WIEN2k with Rutgers eDMFT. The custom scripts used to post-process their output and to generate the figures are available from the corresponding authors on reasonable request.

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Author contributions

J.D., Y.J., H.H., D.C., and H.P. contributed to the first-principles calculations, theoretical model development, and analysis under the supervision of P.T. and B.A.B. T.F.T.C. and M.A.L.M. performed the high-throughput calculations and materials screening. K.H. performed the dynamical mean-field theory calculations. E.O.L. performed the superfluid-weight analysis. E.M., T.N., S.B.-C., C.F., Z.W., and M.G.V. contributed theoretical and experimental insights and participated in interpreting the results. J.D., Y.J., and B.A.B. prepared the original draft. J.D., Y.J., T.F.T.C., M.A.L.M., and E.O.L. collaboratively wrote the Methods and Supplementary Information. All authors reviewed and contributed to editing the final manuscript.

Competing interests

The authors declare no competing interests.

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