

Chemical enhancement of superconductivity in LaRu_3Si_2 with mode-selective coupling between kagome phonons and flat bands

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In kagome metals, flat electronic bands induced by frustrated hopping are a platform for strong electron correlations. Here, we investigate the superconductivity in the kagome system $\text{LaRu}_3(\text{Si}_{1-x}\text{Ge}_x)_2$ by chemical pressure tuning while preserving the Ru-4d states that constitute the kagome flat bands. We observe a sizable enhancement in the density of states up to $x = 0.07$, as determined by the specific heat, with a concomitant increase in the superconducting transition temperature T_c . Ge dopants induce a uniaxial lattice expansion along the c axis. Our first-principles calculations suggest that this mitigates the detrimental effect of hybridization between kagome layers and reduces the dispersion of the Ru- $d_{x^2-y^2}$ flat band. The calculated chemical potential moves closer to the maximum in the energy-dependent density of states. Our result is consistent with a theoretical prediction of tunable flat-band superconductivity in LaRu_3Si_2 by mode-selective coupling between specific kagome phonons and the Ru- $d_{x^2-y^2}$ orbitals.

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I. INTRODUCTION

The kagome lattice is a two-dimensional network of corner-sharing triangles with distinct properties in terms of its electronic-band topology [1–3], electron-electron correlations, and phonon spectra [4]. Here, we study superconductivity in the intermetallic LaRu_3Si_2 , where the kagome lattice is formed by Ru atoms as depicted in Fig. 1(a). Considering first a single orbital model on an isolated kagome lattice in Fig. 1(b), one obtains three bands forming a flat band and a Dirac cone [Fig. 1(c)]. In particular, the dispersionless upper band originates from frustrated hopping between the three sites of the kagome lattice [5]. Kane-Mele-type spin-orbit coupling [6] further opens a gap and imparts a Chern number onto the flat band [7–9].

The single-orbital model is not sufficient to describe the topological indices and band dispersion of real-world kagome metals [10], but such materials retain key features of this simplified electronic structure if the coupling between consecutive kagome layers is weak [9,11–15]. As an example, Fig. 1(d) presents the electronic-band structure of LaRu_3Si_2 , which hosts an hourglass-shaped dispersion originating from Ru-4d orbitals along the Γ - M - K path. LaRu_3Si_2 is a rare

kagome superconductor with a flat band near the Fermi level, yet without any magnetic instability of said flat band [4,16]. In *ab initio* theory, the flat-band states couple selectively to certain acoustic kagome phonons [4], discussed further at the end of this study, and realize the highest observed transition temperature $T_c = 6.7$ K among the family of RT_3M_2 (R = rare-earth, T = transition metal, and M = main group element) [16–22] and among kagome metals as a material class [4]. At a higher temperature, other (optical) phonon modes of LaRu_3Si_2 soften and cause charge-density-wave (CDW) orders [4], possibly accompanied by breaking of time-reversal symmetry [23,24]. The phenomenology is reminiscent of the kagome superconductors AM_3Sb_5 (A = K, Rb, and Cs; M = V, Cr,...) [25,26]. In that material family, the most closely related compound is CsCr_3Sb_5 , which hosts flat bands at E_F and a charge-density wave (CDW) with the same modulation vector as LaRu_3Si_2 [27]; however, all these phenomena occur at much lower temperature in CsCr_3Sb_5 .

Real kagome metals are three-dimensional (3D), and their flat bands often exhibit strong dispersion along the k_z direction of reciprocal space [9,15,28]. This behavior is also observed in LaRu_3Si_2 along the Γ - A line in Fig. 1(d). Therefore, flat-band electrons are not fully localized in known bulk kagome metals. To achieve tailored flat bands, it has been proposed to either suppress interlayer coupling [t_{out} in Fig. 1(b)] by isolating kagome layers [29], or to introduce 3D-frustrated hopping [30]. For the latter approach, 3D flat bands have been predicted for the pyrochlore lattice [31], a 3D analog of the kagome lattice, and have recently been observed [30,32]. Despite its simplicity, the former approach has not yet been conclusively implemented to enhance electron correlation

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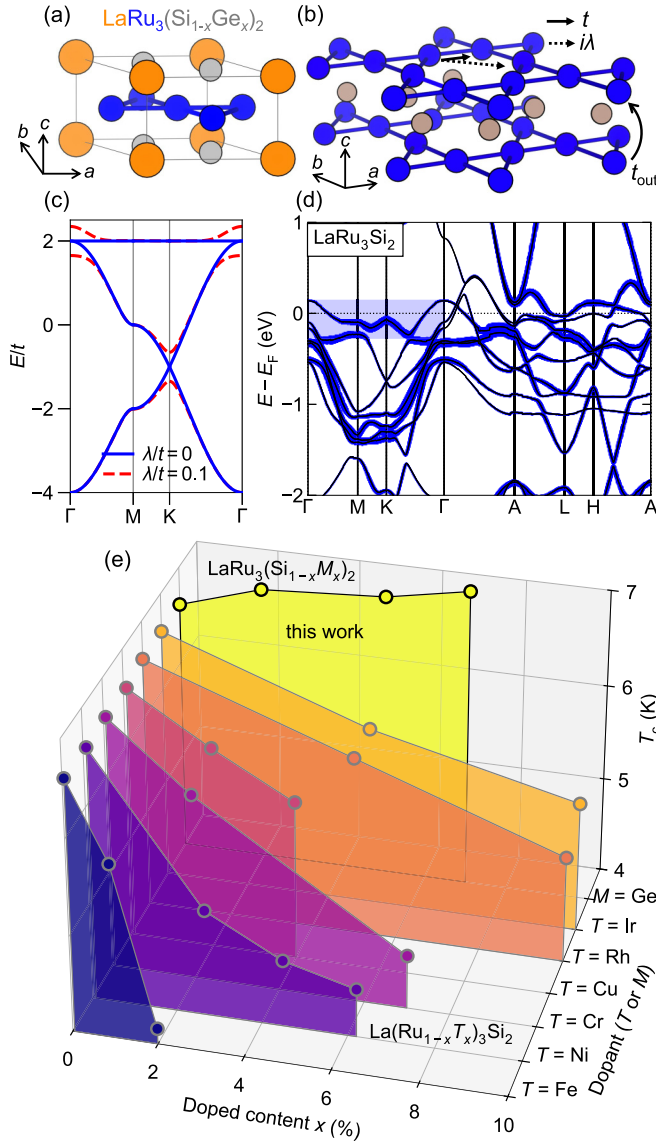


FIG. 1. Superconducting kagome metal $\text{LaRu}_3(\text{Si}_{1-x}\text{Ge}_x)_2$ (LRSG) with a flat band at the Fermi level. (a) Hexagonal structure of superconducting kagome metal LRSG. (b) The kagome motif of Ru atoms with Si and Ge between Ru layers. t and λ are the nearest-neighbor hopping and spin-orbit coupling, respectively. Uniaxial lattice expansion along the c axis suppresses out-of-plane hopping t_{out} . (c) Band dispersion of a single-orbital model on the kagome lattice, with Dirac cone and flat band (blue). The introduction of spin-orbit coupling opens a gap between the Dirac cone and the flat band (red). (d) Band structure of LaRu_3Si_2 . Blue shading highlights a flat band in the k_x - k_y plane. Thick blue color: density of states for the $\text{Ru-}4d_{x^2-y^2}$ orbital. (e) Superconducting transition temperature T_c for alloyed LaRu_3Si_2 . This work demonstrates enhancement of T_c by chemical pressure tuning, in contrast to previous attempts at band-filling tuning. $T_c(x)$ is shifted so that $T_c(0)$ in each report becomes 6.6 K.

phenomena and superconductivity, possibly driven by specific phonon modes, on the kagome lattice.

Here, we engineer the electronic structure of LaRu_3Si_2 by substituting Si with the larger volume element Ge. We observe a uniaxial lattice expansion along the c axis and a marked

increase of the superconducting critical temperature T_c . An enhancement of the total density of states (DOS) with Ge doping underpins the observed evolution of T_c , as confirmed by specific heat measurements. Our electronic-structure calculations reproduce these behaviors; they suggest the bandwidth of the flat band decreases due to suppression of interlayer hopping t_{out} by the anisotropic lattice expansion. The calculations also suggest an effective hole doping through chemical pressure, moving the flat band closer to the Fermi level. The increase in T_c is thus broadly consistent with the scenario of mode-selective coupling to kagome phonons in LaRu_3Si_2 [4]. As summarized in Fig. 1(e), our results are in stark contrast to previous attempts to tune superconductivity in LaRu_3Si_2 by chemical substitution at the Ru site, which generally results in a sharp decrease of T_c [33–35].

II. METHODS

Crystals are obtained by the arc-melting technique; see Appendixes A and B. In Fig. 2(a), the crystal structure of LaRu_3Si_2 is confirmed by powder x-ray diffraction (XRD). The absence of the LaRu_2Si_2 phase is confirmed. Figures 2(c) and 2(d) show the hexagonal lattice constants of $\text{LaRu}_3(\text{Si}_{1-x}\text{Ge}_x)_2$ (LRSG) extracted from XRD and their evolution with x based on LeBail analysis in the $P6/mmm$ structure. This neglects the minor effects of the reduction in symmetry into an orthorhombic structure and charge order in this family of compounds [23]. We find a robust value of a and a linear expansion of the out-of-plane lattice constant c , which in combination give a linear volume expansion in Fig. 2(e). The latter is consistent with Vegard’s law, and in good agreement with the trend derived from structure-relaxation calculations of LaRu_3Si_2 and LaRu_3Ge_2 .

III. RESULTS

Magnetization and specific heat measurements are performed in a commercial cryostat (see Appendixes D and E). To confirm the bulk superconducting state in LRSG, we show the magnetic susceptibility χ in Fig. 3(a). Above the transition temperature T_c , χ is small and positive, consistent with the weak paramagnetic Pauli susceptibility of LaRu_3Si_2 [36]. Strong diamagnetism accompanying the superconducting transition appears as a sharp drop in χ around 6 ~ 7 K.

To precisely determine T_c , we measure the specific heat $C(T)$ in zero field and at 5 T, which is high enough to entirely suppress the superconductivity [Fig. 3(b)]. In the former traces, a sharp kink appears at T_c , the second-order transition into the superconducting state. We model the normal-state contribution C_N by electronic and phonon terms, viz., $C_N(T) = \gamma T + \beta T^3 + \eta T^5$ [lines in Fig. 3(b)]. The higher-order phonon contribution ηT^5 is necessary to describe the data [37]. After subtraction of $C_N(T)$, we fit the superconducting specific heat $C(T) - C_N(T)$ to the prediction of Bardeen-Cooper-Schrieffer (BCS) theory by equal-area construction in Fig. 3(c) [38], confirming an enhancement in T_c with x in Fig. 3(d), reaching up to 7.1 K for $x = 0.07$.

In Fig. 3(e), a positive slope of $\gamma(x)$ is reported. Error analysis and the evolution of β , from which we calculate Θ_D , are discussed in Appendix E; see also Fig. 4(f). Given the formula

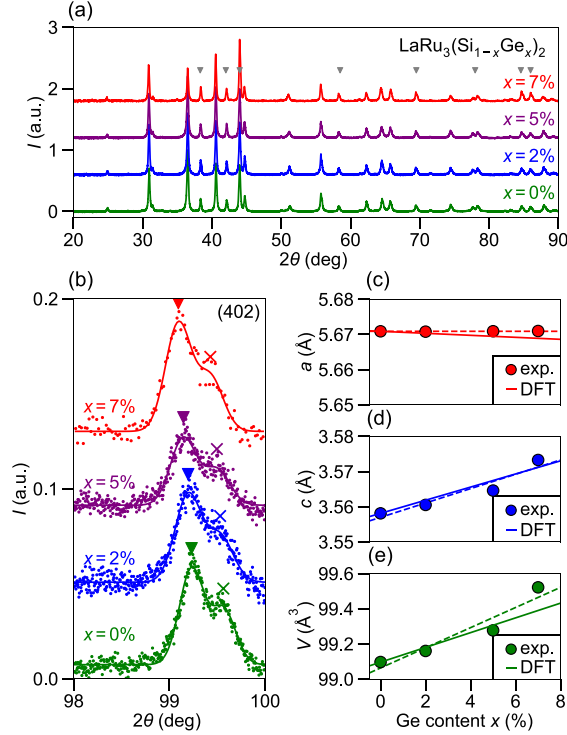


FIG. 2. Structural evolution of $\text{LaRu}_3(\text{Si}_{1-x}\text{Ge}_x)_2$ (LRSg). (a) Powder x-ray diffraction (XRD) pattern for four compositions of LRSg with normalized intensity. Impurity lines from excess Ru metal are indicated by grey triangles. (b) Systematic shift of the (402) reflection as a function of x , measured using $\text{Cu-K}\alpha_1$ (triangle) and $\text{Cu-K}\alpha_2$ (cross) x-rays. The lines indicate a double-Gaussian fit to the data. Offsets are applied to each compound for clarity in panels (a),(b). (c)–(e) Evolution of lattice constants a , c , and unit cell volume V for LRSg from LeBail analysis of the powder XRD (filled circle) and density-functional theory (DFT) calculations (solid line) in the approximate hexagonal structure. Dotted lines correspond to linear fits to the data. Solid lines are derived from structure optimization by DFT calculations for LaRu_3Si_2 and LaRu_3Ge_2 . A constant offset is applied to the DFT data to align with the experimental values at $x = 0$.

$\gamma = \pi^2 k_B^2 N(E_F)/3$ with $N(E_F)$ being the density of states at the Fermi energy E_F , the enhancement of γ corresponds to an increase of $N(E_F)$ [Fig. 3(e)]. The trend is reproduced by our density-functional theory (DFT) calculations, where $N(E_F)$ increases from 2.9 /eV/u.c./spin to 3.3 /eV/u.c./spin when going from LaRu_3Si_2 to LaRu_3Ge_2 , c.f. Fig. 3(f). Electronic structure calculations at an intermediate x value are discussed in Appendix C.

IV. DISCUSSION

We now take a closer look at the electronic bands to understand the behavior of $N(E_F, x)$. The projected band structures for LaRu_3Ge_2 and LaRu_3Si_2 are shown in Figs. 4(a) and 4(b). Focusing on the Γ -A line, which is parallel to the k_z axis, we find that substitution of Si with Ge decreases the bandwidth of the flat band at E_F ; the uniaxial lattice expansion along the c axis by Ge doping suppresses interlayer coupling between kagome layers.

In the partial density of states (PDOS) of LaRu_3Ge_2 , Figs. 4(c) and 4(d), the contribution of $4d_{z^2}$ grows weaker while the PDOS peak of $4d_{x^2-y^2}$ sharpens, corresponding to a narrowing of the flat band through chemical pressure tuning. Moreover, the calculations indicate a slight shift of the PDOS peak towards E_F . From the viewpoint of superconductivity, Ge doping has the favorable effect of reducing the bandwidth, but it also helps to drive E_F into the fractionally filled flat band. Note that recent theory work predicts an enhancement of T_c by hole doping LaRu_3Si_2 [4].

To discuss these results, we consider the McMillan formalism for BCS,

$$T_c = \frac{\langle \omega \rangle}{1.20} \exp \left(\frac{-1.04(1 + \lambda)}{\lambda - \mu^*(1 + 0.62\lambda)} \right), \quad (1)$$

where $\langle \omega \rangle$ is a characteristic phonon frequency after weighting by the electron-phonon interaction and μ^* is the Coulomb pseudopotential [39]. The electron-phonon coupling constant λ can be expressed as

$$\lambda = 2 \frac{N(E_F)}{N} \frac{\hbar \langle g^2 \rangle}{\hbar^2 \langle \omega^2 \rangle}, \quad (2)$$

where N and $\langle g^2 \rangle$ represent the number of sites and the weighted phonon linewidth [39]. For LaRu_3Si_2 we expect $\lambda < 1$ based on (i) recent *ab initio* modeling, which predicts $\lambda \approx 0.8$, and (ii) $\Delta C/(\gamma T_c)$ in Fig. 4(h), which is characteristic of moderate coupling strength.

According to recent theory, $d_{x^2-y^2}$ flat bands have a mode-selective electron-phonon coupling to the B_{3u} kagome phonon [4]. This low-energy mode corresponds to a planar oscillation into and out of the large hexagonal plaquette in the kagome lattice, illustrated in Fig. 4(e). In the scenario of Deng *et al.* [4], the widely used [40]

$$\langle \omega \rangle \approx 0.828 \Theta_D \quad (3)$$

cannot be valid for $\text{LaRu}_3(\text{Si}_{1-x}\text{Ge}_x)_2$: the Debye temperature is an average over the phonon spectrum $F(\omega)$ that is not weighted by the electron-phonon coupling $\alpha^2(\omega)$, unlike $\langle \omega \rangle = \int d\omega \alpha^2(\omega) F(\omega) / [\int d\omega \alpha^2(\omega) F(\omega) / \omega]$ [39–41]. For the sake of argument, we apply Eq. (3) to LaRu_3Si_2 with $N(E_F)$ from γ and show $N\hbar\langle \omega^2 \rangle / \langle g^2 \rangle$ from Eq. (2) in Fig. 4(g). While the measured Θ_D softens with x , the latter quantity grows in equal measure. This lack of agreement between Figs. 4(f) and 4(g) confirms that the *mode-independent* approximation for $\alpha^2(\omega)$, Eq. (3), is not suitable in LaRu_3Si_2 . However, BCS theory and Eq. (1) remain valid for this kagome metal, even with mode-selective electron-phonon coupling. In our scenario, despite the change in Θ_D , $N(E_F)$ and the reported flattening of the $4d_{x^2-y^2}$ band, not changes in the phonon spectrum, predominantly drive a Ge-induced enhancement of superconductivity; see Appendix E for further discussion.

V. CONCLUSION

In summary, we control superconductivity in LaRu_3Si_2 by chemical pressure and use specific heat measurements—which are not accessible for recent studies of enhanced superconductivity in LaRu_3Si_2 under high external pressure [42,43]—to track the electronic density of states and Debye

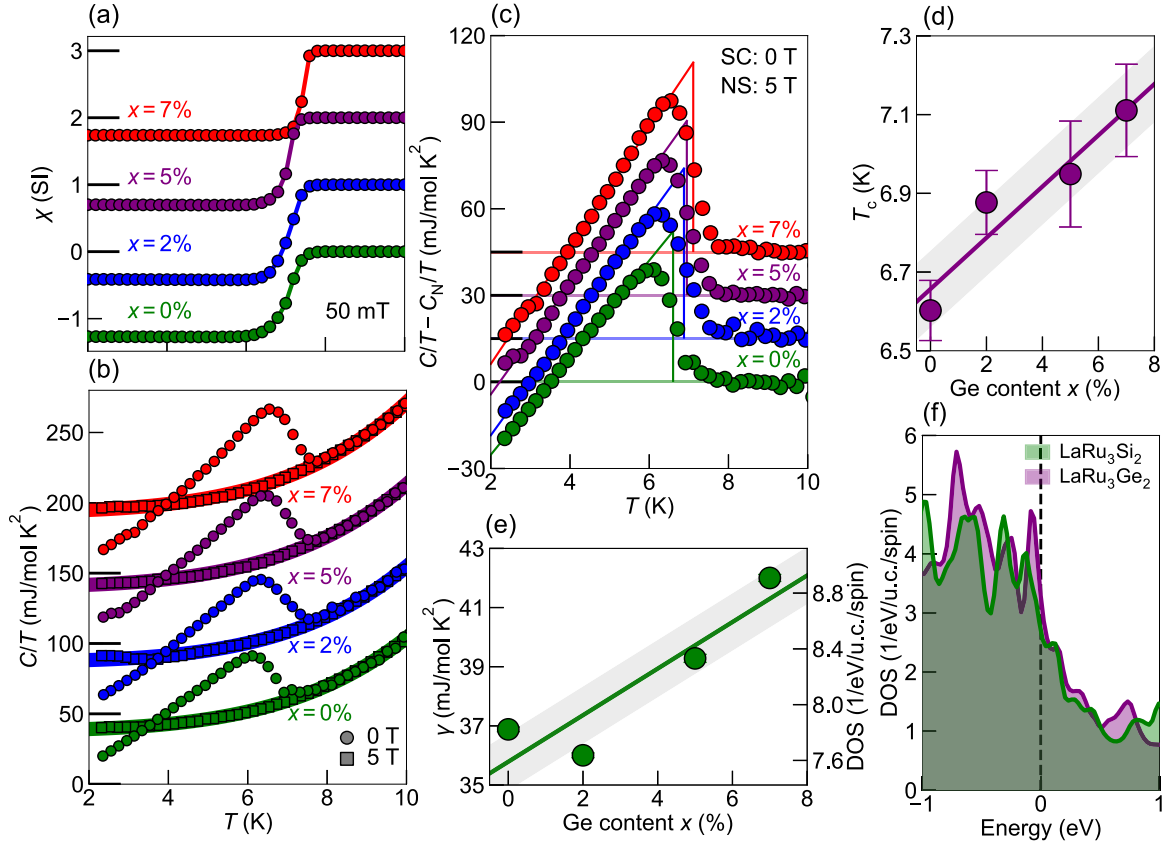


FIG. 3. Enhancement of superconductivity by chemical pressure tuning in $\text{LaRu}_3(\text{Si}_{1-x}\text{Ge}_x)_2$ (LRSG). (a) Magnetic susceptibility $\chi = M/H$ in SI units. The onset of a rapid drop indicates the Meissner effect of a bulk superconducting state; demagnetization correction is applied. (b) Specific heat $C(T)$ in zero magnetic field (round symbols) and in a field large enough to suppress the superconducting state (square symbols). Lines are a fit to the normal-state specific heat $C_N(T)$ using $C_N(T) = \gamma T + \beta T^3 + \eta T^5$. (c) After subtraction of $C_N(T)$, we perform a linear fit for $C(T) - C_N(T)$ by equal-area construction (solid lines). Offsets are applied to each dataset for clarity, with the zero values marked by bold ticks in panels (a)–(c). (d) Evolution of electronic specific heat coefficient γ extracted from $C_N(T)$ as a function of Ge content x . (e) Superconducting transition temperature T_c . The error bars are estimated by the bootstrap method, as explained in Appendix E. (f) Density of states (DOS) from density-functional theory for LaRu_3Si_2 and (hypothetical) LaRu_3Ge_2 . The DOS at the Fermi level E_F is 2.9 /eV/u.c./spin and 3.3 /eV/u.c./spin for LaRu_3Si_2 and LaRu_3Ge_2 , respectively.

temperature. Although chemical pressure tuning has been implemented in a number of superconductors, as summarized in Appendix F, simultaneous reports of T_c and γ are less common, and none such has targeted kagome metals. Tuning the flat band by uniaxial strain, using large single crystals, remains a challenge for future research.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX A: CRYSTAL GROWTH

Crystals of $\text{LaRu}_3(\text{Si}_{1-x}\text{Ge}_x)_2$ (LRSG) are prepared by arc melting in an argon atmosphere after careful evacuation to 10^{-3} Pa. The ingot is turned and remelted at least three times, and weight loss is typically around 0.5%. To stabilize the LaRu_3Si_2 structure over the competing phase LaRu_2Si_2 , excess Ru metal is added to the starting compo-

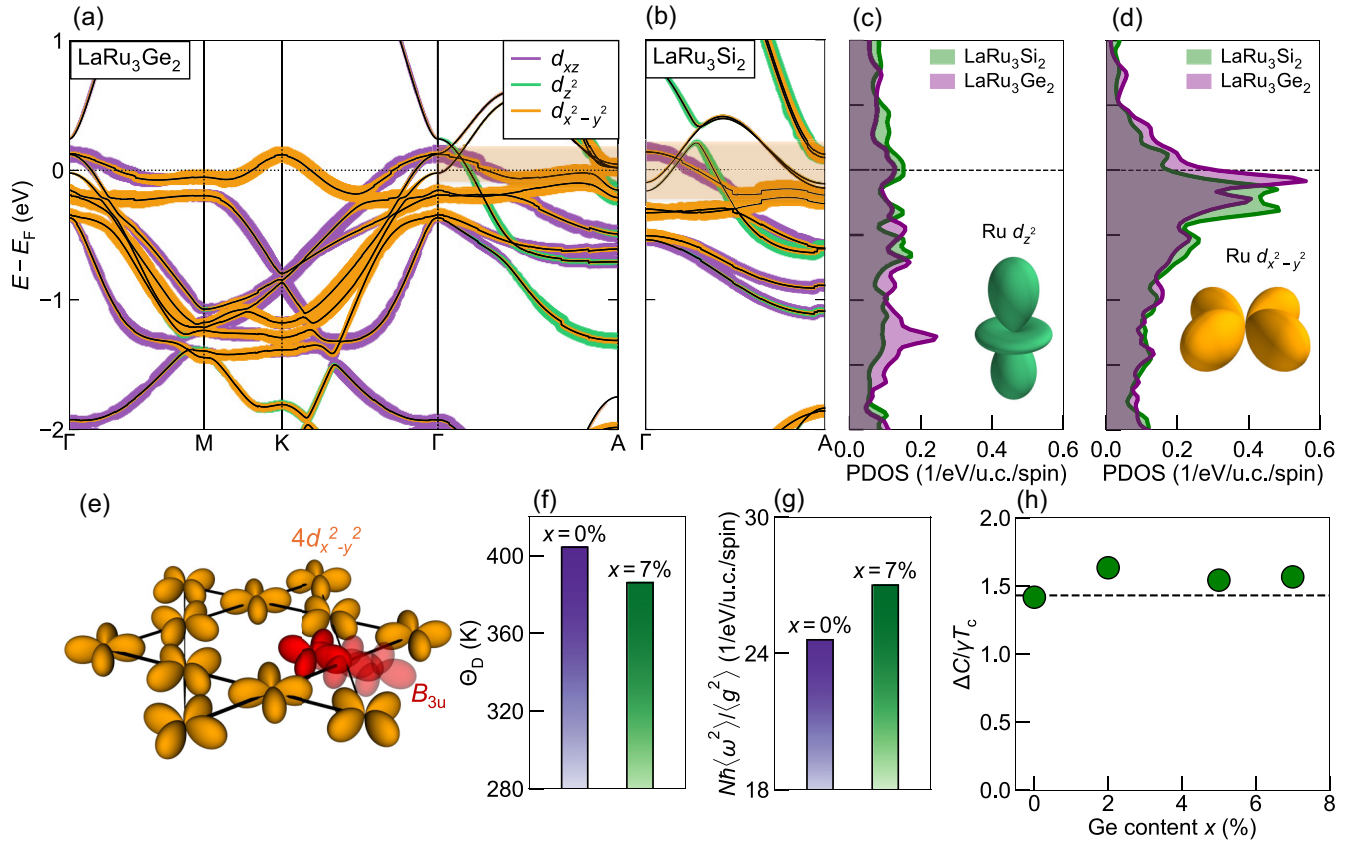


FIG. 4. Electronic structure of LaRu₃Ge₂ in comparison with LaRu₃Si₂ and mode-selective electron-phonon coupling in LaRu₃(Si_{1-x}Ge_x)₂. (a) Projected band structure of LaRu₃Ge₂ in the k_x - k_y plane and along the Γ -A line. Bands that are flat in the k_x - k_y plane are highlighted in orange along the path parallel to the k_z axis. (b) Projected band structure of LaRu₃Si₂ along the Γ -A line. The bandwidth of the flat band along this path is wider for LaRu₃Si₂. (c),(d) Partial density of states (PDOS) for Ru- d_{z^2} and Ru- $d_{x^2-y^2}$ states of LaRu₃Si₂ and LaRu₃Ge₂. The contributions of d_{z^2} and $d_{x^2-y^2}$ at E_F are suppressed and enhanced by replacing Si with Ge, respectively. (e) Illustration of $d_{x^2-y^2}$ orbitals on the lattice and kagome phonon mode B_{3u} , discussed by Deng *et al.* [4]. B_{3u} corresponds to vibration into and out of the central hexagon of the kagome pattern (red highlight, with shading indicating time dependence). (f),(g) Evolution of Θ_D extracted from the specific heat measurement and $2N(E_F)/\lambda$ from Eq. (2). (h) Specific heat jump ΔC at T_c , normalized by electronic specific heat just above the transition temperature. Dashed line: weak coupling BCS value.

sition [16,17,36,37,44]. The solution limit of Ge is found to be $x = 0.07$, and the required amount of Ru increases when approaching this value: We use a melt of starting composition LaRu_{4.5}(Si_{1-x}Ge_x)₂ for $x = 0, 0.02, 0.05$, and LaRu₅(Si_{1-x}Ge_x)₂ for $x = 0.07$.

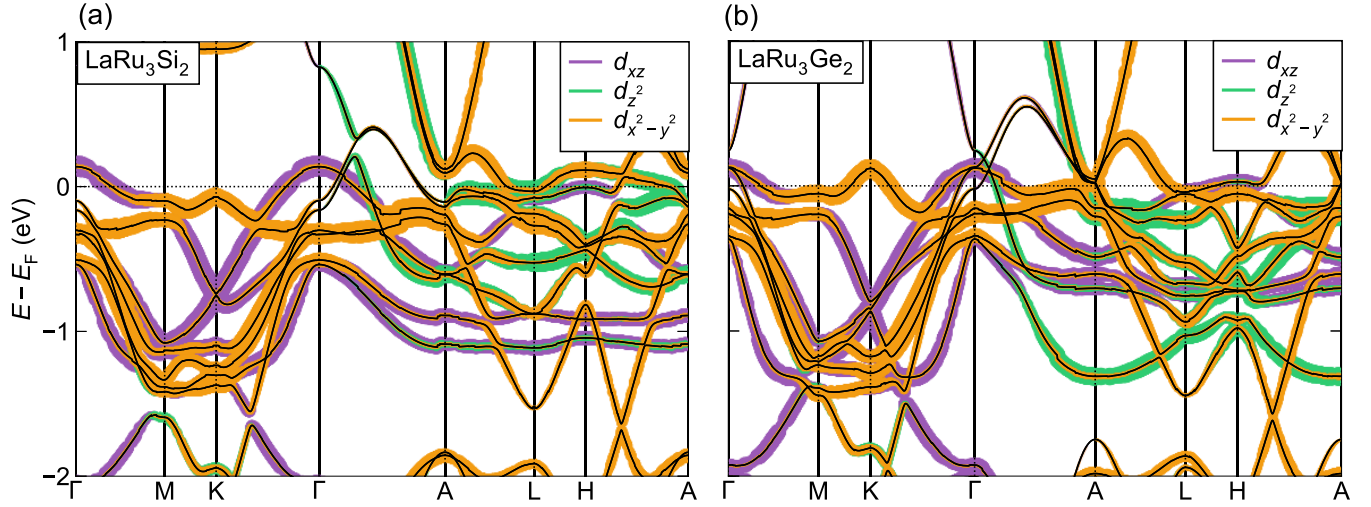
APPENDIX B: POWDER X-RAY DIFFRACTION

We perform powder x-ray diffraction (XRD) to confirm the formation of LRSG as well as the absence of the competing LaRu₂Si₂. The data include reflections from nonmagnetic, elemental Ru, because Ru is added to the melt to destabilize the chemically stable LaRu₂Si₂ phase.

APPENDIX C: DENSITY-FUNCTIONAL CALCULATION

First-principles calculations are carried out using the WIEN2k software package, which employs the full-potential linearized augmented plane-wave (FP-LAPW) method with local orbitals [45]. The exchange-correlation energy is treated

within the generalized gradient approximation (GGA) using the functional formulated by Perdew, Burke, and Ernzerhof (PBE) [46] in the $P6/mmm$ structure. We employ a uniform grid of 4096 k points to ensure accurate sampling of the Brillouin zone and relax the lattice constants a and c . This yields $a = 5.8260$ Å, $c = 3.5666$ Å for LaRu₃Si₂ and $a = 5.7967$ Å, $c = 3.7538$ Å for hypothetical LaRu₃Ge₂. We calculate the band structures and the density of states in the presence of spin-orbit coupling (SOC). For the density of states (DOS) and partial density of states (PDOS), we divide the calculated values by 2 to express them in units of eV⁻¹ per unit cell (u.c.) per spin. A previous report on the band structure of LaRu₃Si₂ assumes the $P6_3/m$ structure with two times larger unit cell [16]. However, a recent study shows that the proper structure is orthorhombic [23]. Due to the different structure and band folding in the $P6_3/m$ space group, slight differences can be seen in our calculation results compared to the previous study. On the other hand, our calculations are largely consistent with the most recent theoretical work on LaRu₃Si₂ [4]. For our calculations, we ignore the structural transition from $P6/mmm$ to $Cccm$ and subsequent CDW


 FIG. 5. Projected band structure of LaRu_3Si_2 (a) and LaRu_3Ge_2 (b) in the full Brillouin zone.

transitions [23]. Theory shows that the flat band persists in the orthorhombic $Cccm$ phase [4].

We provide projected band structures in the full Brillouin zone for LaRu_3Si_2 and LaRu_3Ge_2 in Fig. 5.

To check the impact of spin-orbit coupling (SOC), we compare band structure and DOS with and without SOC in Fig. 6. For both cases, the flat band is present at the Fermi energy, and LaRu_3Ge_2 has a larger DOS than LaRu_3Si_2 .

In addition to LaRu_3Si_2 and LaRu_3Ge_2 , we illustrate in Fig. 7 the calculations performed for LRSg with $x = 8\%$ by the virtual-crystal approximation (VCA) [47]. The DOS systematically increases around the Fermi level upon doping Ge [Fig. 7(a)]. These calculations are done with VASP 6 [48–50], using the PBE functional [46]. The pseudopotentials used in

the calculations are La, Ru_{pv} , Si, and Ge [51,52]. We use a gamma-centered $15 \times 15 \times 19$ grid for sampling reciprocal space. Spin-orbit coupling as implemented in VASP is added to the calculations [53]. Geometries are optimized using the residual-minimization method, direct inversion in the iterative subspace (RMM-DIIS) algorithm, with a step size of 0.25 [54].

APPENDIX D: MAGNETIC SUSCEPTIBILITY MEASUREMENT

We perform magnetization measurements to detect the superconducting Meissner effect in a low magnetic field of $\mu_0 H = 0.05$ T. Samples of mass ~ 100 mg are mounted in

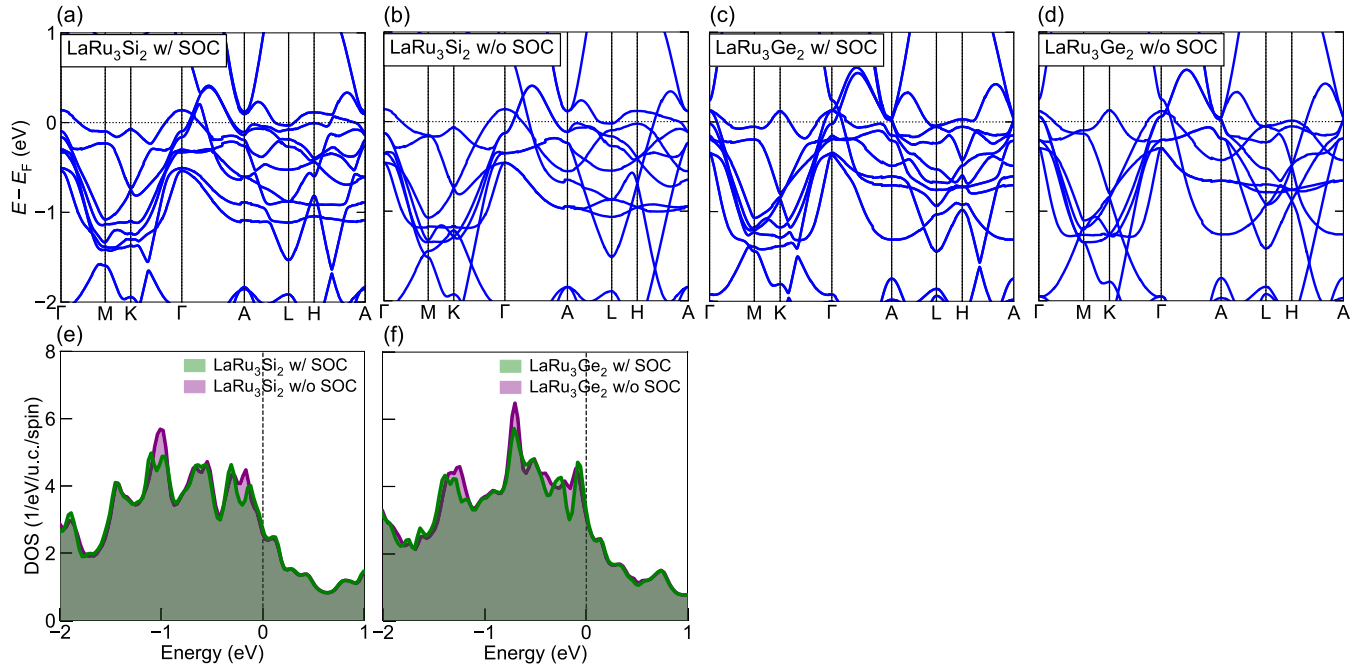


FIG. 6. Comparison of *ab initio* calculations with and without SOC. (a),(b) Band structure for LaRu_3Si_2 with and without spin-orbit coupling (SOC). (c),(d) Band structure for LaRu_3Ge_2 with and without SOC. (e) Density of states (DOS) for LaRu_3Si_2 with and without SOC. (f) DOS for LaRu_3Ge_2 with and without SOC.

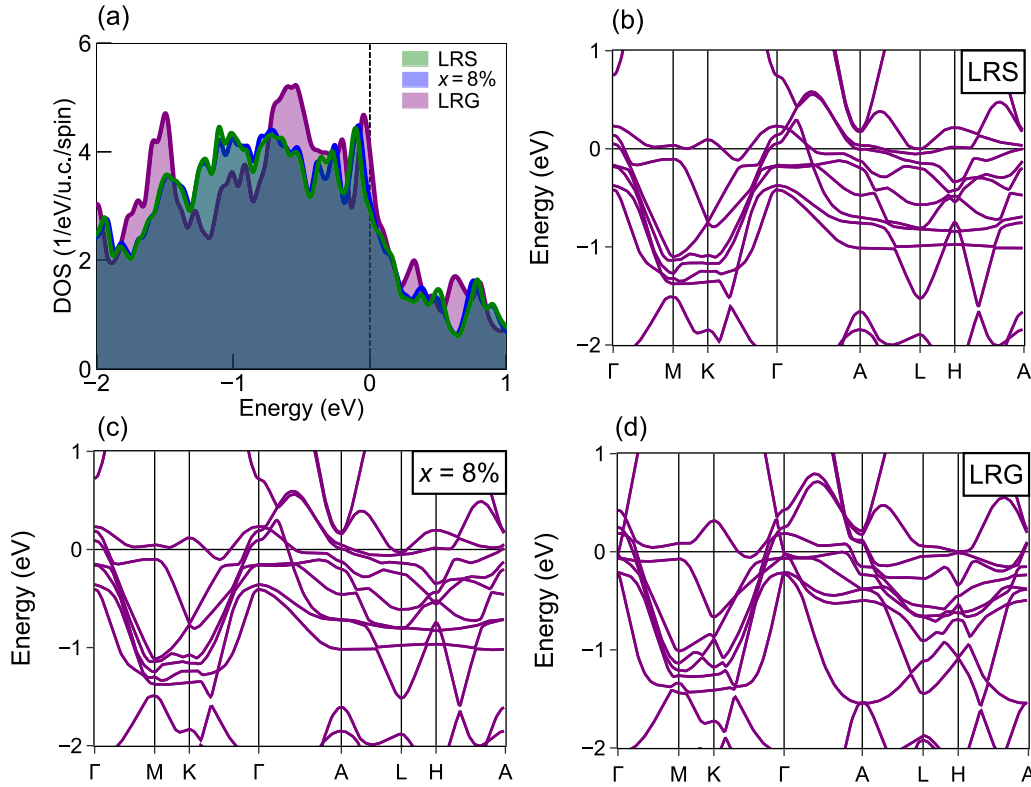


FIG. 7. First-principle calculations for $\text{LaRu}_3(\text{Si}_{1-x}\text{Ge}_x)_2$ (LRS) with $x = 0, 0.08, 1$ performed in VASP. For $x = 0.08$, the virtual-crystal approximation is employed. (a) Comparison of the DOS. (b)–(d) Band structure for LaRu_3Si_2 (LRS), LRS ($x = 0.08$), and LaRu_3Ge_2 (LRG).

a Quantum Design Magnetic Properties Measurement System (MPMS). We correct for the demagnetization effect in χ by approximating our roughly shaped crystals as a sphere, which has a demagnetization factor $N = 1/3$. The intrinsic susceptibility is then obtained using the relation $\chi = \chi_{\text{exp}}/(1 - N\chi_{\text{exp}})$. Slightly smaller values than the ideal $\chi = -1$ (perfect Meissner shielding) may arise due to deviations from the spherical approximation.

APPENDIX E: SPECIFIC HEAT MEASUREMENT

1. Measurement details

We measure specific heat by the relaxation technique in a Quantum Design Physical Properties Measurement System (PPMS). For each measurement, the addenda (with Apiezon N grease mounted on the stage) are measured before setting the sample for the main measurement. To eliminate contributions from nonmagnetic impurity Ru metal, we subtract $\gamma_{\text{Ru}} = 2.8 \text{ mJ/molK}^2$ and $\beta_{\text{Ru}} = 0.068 \text{ mJ/molK}^4$ from the total γ and β values [37,55]. These values are scaled by the impurity fraction, given by $y/3$, where y denotes the amount of excess Ru. Specifically, $y = 1.5$ for $x = 0, 0.02$, and 0.05 , and $y = 2$ for $x = 0.07$. We summarize γ and β values before and after the subtraction of the Ru contribution in Table I.

2. Evaluation of errors

Errors for the fitting parameters β and γ are estimated by the bootstrap method. This allows us to evaluate errors or the stability of fitting while incorporating systematic mea-

surement errors. The procedure is as follows: We first fit the data and calculate residuals. We then compute the total measurement error for each data point by performing the relaxation-method measurement 3 times at each temperature and then calculating the mean and standard deviation $\sigma(T)$. Next, we randomly sample values from zero to $\sigma(T)$, add them to the experimental data, and obtain fit parameters for this perturbed data. This is repeated 100 times. We take an average of these trials as a central value for β and γ ; we also use its standard deviation as a fit error for these parameters. Other errors, such as sample mass and batch dependence, are ignored as we precisely measured the mass and uniformly melted all samples.

3. Electronic and phononic specific heat

We estimate the density of states (DOS) at the Fermi energy $N(E_F)$ using the relation

$$N(E_F) = \frac{3\gamma}{\pi^2 k_B^2}, \quad (\text{E1})$$

which has units of J^{-1} . We convert this to eV^{-1} per unit cell (u.c.). Furthermore, since γ is calculated assuming a spinless electronic structure, we divide by 2 to obtain $N(E_F)$ in units of eV^{-1} per unit cell per spin [38,56]. The errors of $N(E_F)$ in Fig. 3(e) are estimated by the error propagation of γ . In Table I, we also present the Debye temperature Θ_D calculated

TABLE I. Properties of $\text{LaRu}_3(\text{Si}_{1-x}\text{Ge}_x)_2$ probed by specific heat measurements. For the electron and phonon contributions γ and β , we give values before and after subtracting a subtle contribution from Ru impurity in $\text{LaRu}_3(\text{Si}_{1-x}\text{Ge}_x)_2 + y\text{Ru}$. $\Delta C(T_c)$ denotes the specific heat jump at T_c , and $\Delta C(T_c)/\gamma T_c = 1.43$ holds for weakly coupled superconductors. $N(E_F)$ and λ denote the DOS and the electron-phonon coupling constant, respectively.

Ge content x	0	0.02	0.05	0.07
γ (mJ/molK ²)	38.3	37.4	40.7	43.8
$\gamma' = \gamma - y/3 \cdot \gamma_{\text{Ru}}$ (mJ/molK ²)	36.9	36.0	39.3	42.0
β (mJ/molK ⁴)	0.21	0.19	0.25	0.25
$\beta' = \beta - y/3 \cdot \beta_{\text{Ru}}$ (mJ/molK ⁴)	0.18	0.15	0.21	0.20
Θ_D (K)	405	423	379	384
$\Delta C(T_c)/\gamma' T_c$	1.42	1.64	1.54	1.57
$N(E_F)$ (1/eV/u.c./spin)	7.82	7.64	8.33	8.90
λ	0.635	0.635	0.659	0.659
$N(E_F)/(1 + \lambda)$ (1/eV/u.c./spin)	4.78	4.68	5.03	5.36

from β as

$$\Theta_D = \left(\frac{12\pi^4 N k_B}{5\beta} \right). \quad (\text{E2})$$

In the main text, we discuss the observed reduction of Θ_D which is summarized in Table I. Assuming Eq. (3) of the Main Text, this may be understood to imply a softening of $\langle \omega \rangle$ with x for the phonon modes relevant to the superconducting T_c . However, softening appears unreasonable considering the dominant role of the B_{3u} phonon in DFT [4], its nature as a vibration in the hexagonal ab plane, and the lack of a lattice expansion along a in Fig. 2(c). The observed softening of Θ_D with x should then be attributed to the elastic coupling between kagome layers, which is irrelevant to the superconductivity [4].

4. Specific heat jump at T_c

For the superconducting state, the specific heat can be fitted by an analytical expression within the framework of the BCS theory. Here, we approximate the temperature dependence to be linear below T_c , which is valid for our temperature range (>2 K) [20]. This method allows us to precisely determine T_c by the equal-area construction, which is crucial for tracking the evolution of T_c in our crystals: We first numerically calculate the area under the curve of $\Delta C/T = C/T - C_N/T$ below 8 K, denoted as S [Fig. 8(a)]. We then fit $\Delta C/T$ below 6 K by a linear function $\Delta C/T = aT + b$. Imposing entropy conservation, the area under the curve is thus given by

$$S = \frac{1}{2}(T_c - T_0)(aT_c + b) - \frac{1}{2}(T_0 - T_{\min})|aT_{\min} + b|, \quad (\text{E3})$$

where $T_0 = -b/a$ is the intercept of the linear fit, and $T_{\min}$ is the lowest temperature at which data are taken. The first term corresponds to the area for $T_0 \leq T \leq T_c$ and the second to that for $T_{\min} \leq T \leq T_c$, as illustrated in Fig. 8(b). Solving this equation, we analytically determine the transition temperature as

$$T_c = \frac{-b + \sqrt{b^2 + 2aS + a^2T_{\min}^2 + 2abT_{\min}}}{a}. \quad (\text{E4})$$

Furthermore, we obtain the specific heat jump at T_c as

$$\Delta C(T_c)/T_c = aT_c + b. \quad (\text{E5})$$

The errors of a and b are evaluated by the same method as for β , γ , and T_c described above and shown in Fig. 3. Error propagation is carefully considered.

We provide the calculated ratio $\Delta C(T_c)/\gamma T_c$ in Table I. A slight deviation from the BCS value of 1.43 may suggest a moderate superconducting coupling strength. This behavior is consistent with a previous report [35]. Given that the Sommerfeld coefficient of pure Ru is small ($\gamma_{\text{Ru}} = 2.8$ mJ/mol K²), the residual specific-heat contribution from the Ru impurity is expected to be negligible.

5. Electron-phonon coupling strength and bare density of states

Using Eqs. (1) and (3) of the main text, we estimate the electron-phonon coupling constant λ . Setting $\mu^* = 0.13$, we estimate λ to be $0.63 \sim 0.66$, as summarized in Table I. The enhanced electron-phonon coupling constant $\lambda > 0.5$ suggests a moderately coupled superconductor. This is consistent with $\Delta C(T_c)/\gamma T_c > 1.43$ in Fig. 4(h).

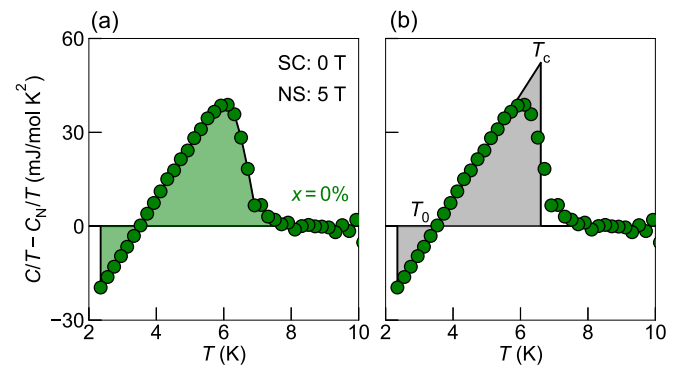


FIG. 8. Fitting of superconducting specific heat $\Delta C = C - C_N$ and equal-area construction. As a representative example, we show the procedure for LaRu_3Si_2 . (a) The area under the curve (green) is calculated numerically. (b) $\Delta C/T$ is fitted by a linear approximation of the BCS expression. T_c is identified such that the gray areas equal the green area in panel (a). T_0 denotes the intercept of the fit.

TABLE II. Superconducting transition temperatures T_c for a pure and maximally doped sample ($x = x_0$) for each material system listed. ΔT_c denotes a change of ΔT_c compared to the pure sample. The columns of $N(E_F)_{\text{exp}}$ and $N(E_F)_{\text{DFT}}$ represent whether the DOS at the Fermi level is determined by experiments or DFT calculations, respectively. Note that $4H_b\text{-Ta}(\text{S}_{1-x}\text{Se}_x)_2$ exhibits a decrease of T_c above $x_0 = 30\%$.

Material	$T_c(0)$ (K)	x_0 (%)	$T_c(x_0)$ (K)	ΔT_c (%)	$\Delta T_c/x_0$	$N(E_F)_{\text{exp}}$	$N(E_F)_{\text{DFT}}$	Reference
$\text{InTe}_{1-x}\text{Se}_x$	2.6	30	5.0	92	3	×	×	[58]
$1\text{T-Pd}(\text{Te}_{1-x}\text{Se}_x)$	1.64	50	2.7	67	1	○	×	[61]
$\text{Sn}_{1-x}\text{Ge}_x\text{Te}$	2.1	1.2	1.3	-38	-32	×	×	[60]
$\text{Sn}_{1-x}\text{Pb}_x\text{Te}$	2.1	12	1.9	-10	-0.8	×	×	[60]
$\text{K}_{0.8}\text{Fe}_2(\text{Se}_{1-x}\text{Te}_x)_2$	31	25	14.9	-52	-2	×	×	[59]
$4H_b\text{-Ta}(\text{S}_{1-x}\text{Se}_x)_2$	2.8	30	4.0	43	1	×	×	[57]
$\text{Cs}(\text{V}_{1-x}\text{Nb}_x)_3\text{Sb}_5$	2.9	7	4.5	55	8	×	×	[62]
$\text{Cs}(\text{V}_{1-x}\text{Ta}_x)_3\text{Sb}_5$	3.1	16	5.3	71	4	×	×	[63]
$\text{LaRu}_3(\text{Si}_{1-x}\text{Ge}_x)_2$	6.6	7	7.1	7	1	○	○	this work

With λ determined, we compute the bare density of states $N_{\text{bare}}(E_F)$ using

$$N_{\text{bare}}(E_F) = \frac{N(E_F)}{1 + \lambda}, \quad (\text{E6})$$

which allows for comparison to band-structure calculations. Here, $N_{\text{bare}}(E_F)$ has the same unit as $N(E_F)$ because λ is dimensionless. This yields approximately $N_{\text{bare}}(E_F) = 5 \text{ eV/u.c./spin}$ and reasonably corresponds to the calculated DOS at $E = -0.1 \text{ eV}$ in Fig. 3(f).

APPENDIX F: STRENGTH OF DOPING EFFECT ON T_c

Table II shows examples of superconductors with isovalent doping [57–63]. Since the solution limit x_0 —the maximum doping value studied—is different for various systems, we compare the enhancement of T_c , ΔT_c , divided by x_0 . Crucially, our study systematically traces the evolution of $N(E_F)$ and compares the results to first-principle calculations, revealing the origin of the enhanced T_c . We note that $4H_b\text{-Ta}(\text{S}_{1-x}\text{Se}_x)_2$ shows a decreasing T_c above $x_0 = 30\%$ and CsV_3Sb_5 is doped at the transition-metal site (V), in contrast to other systems.

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