

Supplemental Material to the article

“Electron spectrum topology and giant van Hove singularities in cubic lattices”

Formal definition of density of state reads

$$\rho(\epsilon; \tau) = \frac{1}{N} \sum_{\mathbf{k}} \delta(\epsilon - t(\mathbf{k}, \tau)), \quad (1)$$

where $t(\mathbf{k}, \tau)$ is the spectrum within tight-binding approximation. We choose the signs of transfer integrals in the spectrum as follows

$$t_{\text{sc}}(\mathbf{k}, \tau) = -2(\cos k_x + \cos k_y + \cos k_z) + 4\tau(\cos k_y \cos k_z + \cos k_z \cos k_x + \cos k_x \cos k_y),$$

$$t_{\text{bcc}}(\mathbf{k}, \tau) = -8 \cos k_x \cos k_y \cos k_z + 2\tau(\cos 2k_x + \cos 2k_y + \cos 2k_z),$$

$$t_{\text{fcc}}(\mathbf{k}, \tau) = -4(\cos k_y \cos k_z + \cos k_x \cos k_z + \cos k_x \cos k_y) + 2\tau(\cos 2k_x + \cos 2k_y + \cos 2k_z),$$

where lattice parameters are taken as unity. For the van Hove point $\bar{\mathbf{k}}$ we expand the spectrum

$$t(\mathbf{k}) = t(\bar{\mathbf{k}}) + \frac{1}{2} \sum_{ij} \frac{\partial^2 t(\bar{\mathbf{k}})}{\partial k_i \partial k_j} (k_i - \bar{k}_i)(k_j - \bar{k}_j). \quad (2)$$

Let a_i be the eigenvalues of the matrix $\partial^2 t(\bar{\mathbf{k}})/\partial k_i \partial k_j$ (inverse mass tensor). We introduce the signature as the difference between numbers of positive and negative eigenvalues of mass tensor and write it in slashes, e.g., minimum (maximum) corresponds to $/ + 3/$ ($/ - 3/$), saddle points to $/ \pm 1/$. For three-dimensional lattice in the non-degenerate case a local minimum (maximum) of the spectrum $t(\mathbf{k})$ corresponds to one-side square-root increase (decrease) of DOS as the energy ϵ deviates from ϵ_0 :

$$\rho(\epsilon) = \rho(\epsilon_0) + A\sqrt{\theta(\pm(\epsilon - \epsilon_0))|\epsilon - \epsilon_0|} + O(\epsilon - \epsilon_0) \quad (3)$$

in the vicinity of the van Hove level ϵ_0 ; a saddle-type van Hove point with the mass tensor signature $/ + 1/$ ($/ - 1/$) corresponds to one-side square-root decreasing,

$$\rho(\epsilon) = \rho(\epsilon_0) - A\sqrt{\theta(\mp(\epsilon - \epsilon_0))|\epsilon - \epsilon_0|} + O(\epsilon - \epsilon_0) \quad (4)$$

with positive constant $A = 2\pi V_{\text{BZ}} |a_1 a_2 a_3|^{-3/2}$, V_{BZ} being the Brillouin zone volume.

Figure S1 shows the spectrum for SC and BCC lattice in high-symmetry directions of the Brillouin zone for τ being in the vicinity of topological transition.

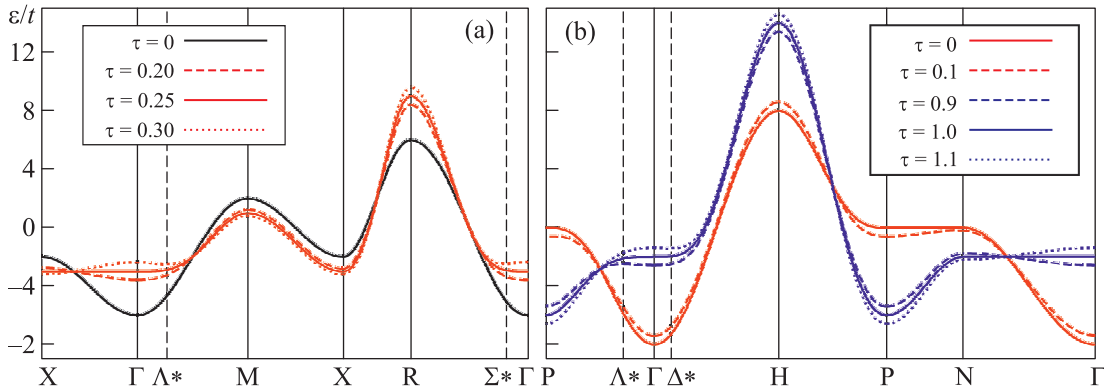


Fig. S1. Energy spectrum in high-symmetry directions of the Brillouin zone (“spaghetti”). SC (a), BCC (b) lattice, van Hove $\mathbf{k}$ points are shown

Table 1. Non-equivalent $\mathbf{k}$ points of van Hove singularities for SC lattice, see Fig. 1a of main text, $\tau \geq 0$. Arrow denotes a change of signature of mass tensor of van Hove $\mathbf{k}$ point as τ increases above these value $\tau_*^{\text{sc}} = 1/4$. $k_{\Sigma^*}^{\text{sc}} = \arccos[(2\tau)^{-1} - 1]$, $k_{\Lambda^*}^{\text{sc}} = \arccos[(4\tau)^{-1}]$

$\mathbf{k}$	$w^{\text{sc}} = t(\mathbf{k})$	Inverse masses	Signature
$\Gamma(0, 0, 0)$	$-6 + 12\tau$	$2(1 - 4\tau), 2(1 - 4\tau), 2(1 - 4\tau)$	$\min \xrightarrow{\tau=1/4} \max$
$R(\pi, \pi, \pi)$	$+6 + 12\tau$	$-2(1 + 4\tau), -2(1 + 4\tau), -2(1 + 4\tau)$	
$X(0, 0, \pi)$	$-2 - 4\tau$	$2, 2, 2(4\tau - 1)$	$/ + 1/ \xrightarrow{\tau=1/4} \min$
$M(0, \pi, \pi)$	$+2 - 4\tau$	$-2, -2, 2(4\tau + 1);$	$/ - 1/$
$\Sigma^*(0, k_{\Sigma^*}^{\text{sc}}, k_{\Sigma^*}^{\text{sc}})$	$-\tau^{-1} + 2 - 4\tau$	$2(4\tau - 1), 4 - \tau^{-1}, \tau^{-1} - 4$	$\tau > 1/4, / + 1/$
$\Lambda^*(k_{\Lambda^*}^{\text{sc}}, k_{\Lambda^*}^{\text{sc}}, k_{\Lambda^*}^{\text{sc}})$	$-3\tau^{-1}/4$	$\tau^{-1}((4\tau)^2 - 1), (2\tau)^{-1}(1 - (4\tau)^2), (2\tau)^{-1}(1 - (4\tau)^2)$	$\tau > 1/4, / - 1/$

Table 2. Non-equivalent $\mathbf{k}$ -points of van Hove singularities for BCC lattice, see Fig. 1b of main text, $\tau \geq 0$. The notations are the same as in the Table 1. $k_{\Lambda^*}^{\text{bcc}} = \arccos \tau$, $k_{\Delta^*}^{\text{bcc}} = \arccos \tau^{-1}$

$\mathbf{k}$	$w^{\text{bcc}} = t(\mathbf{k})$	Inverse masses	Signature
$\Gamma(0, 0, 0)$	$-8 + 6\tau$	$8(1 - \tau), 8(1 - \tau), 8(1 - \tau)$	$\min \xrightarrow{\tau=1} \max$
$H(0, 0, \pi)$	$+8 + 6\tau$	$-8(1 + \tau), -8(1 + \tau), -8(1 + \tau)$	$\max$
$P(\pi/2, \pi/2, \pi/2)$	-6τ	$8\tau, 8\tau, 8\tau$	$\min$
$N(\pi/2, \pi/2, 0)$	-2τ	$-4\tau, 4(1 + \tau), 4(-1 + \tau)$	$/ - 1/ \xrightarrow{\tau=1} / + 1/$
$\Lambda^*(k_{\Lambda^*}^{\text{bcc}}, k_{\Lambda^*}^{\text{bcc}}, k_{\Lambda^*}^{\text{bcc}})$	$2\tau(2\tau^2 - 3)$	$16\tau(1 - \tau^2), 16\tau(1 - \tau^2), -8\tau(1 - \tau^2)$	$\tau < 1, / + 1/$
$\Delta^*(0, 0, k_{\Delta^*}^{\text{bcc}})$	$2\tau - 4\tau^{-1}$	$8(\tau^{-1} - \tau), 8(\tau^{-1} - \tau), 8(\tau - \tau^{-1})$	$\tau > 1, / - 1/$

Consider exact expressions for the density of states in the SC and BCC lattice within the tight-binding approximation (see main text). The DOS can be presented as a sum of three contributions

$$\rho(\epsilon; \tau) = \mathcal{R}_\psi(\epsilon, \tau) + \mathcal{R}_{\varphi'}(\epsilon, \tau) + \mathcal{R}_\varphi(\epsilon, \tau). \quad (5)$$

For SC lattice, depending on τ value the contributions $\mathcal{R}_i^{\text{sc}}$ read (arguments are omitted for brevity)

1. $\tau \leq 1/4$. $\mathcal{R}_\psi^{\text{sc}} = \mathcal{R}_{\varphi'}^{\text{sc}} = 0$

$$\mathcal{R}_\varphi^{\text{sc}} = \begin{cases} \Phi_{\text{sc}}(x_{\psi 1}^{\text{sc}}, +1), & w_{\Gamma}^{\text{sc}} < \epsilon < w_X^{\text{sc}}(\tau) \\ \Phi_{\text{sc}}(-1, +1), & w_X^{\text{sc}}(\tau) < \epsilon < w_M^{\text{sc}}(\tau) \\ \Phi_{\text{sc}}(-1, x_{\psi 2}^{\text{sc}}), & w_M^{\text{sc}}(\tau) < \epsilon < w_R^{\text{sc}}. \end{cases} \quad (6)$$

2. $1/4 < \tau \leq 1/2$.

$$\mathcal{R}_\psi^{\text{sc}} = \begin{cases} 2\Psi_{\text{sc}}(x_{\varphi}^{\text{sc}}, +1), & w_X^{\text{sc}} < \epsilon < w_{\Sigma^*}^{\text{sc}} \\ 2\Psi_{\text{sc}}(x_{\zeta-}^{\text{sc}}, x_{\zeta+}^{\text{sc}}), & w_{\Sigma^*}^{\text{sc}} < \epsilon < w_{\Lambda^*}^{\text{sc}}, \end{cases} \quad (7)$$

$$\mathcal{R}_{\varphi'}^{\text{sc}} = \begin{cases} 2[\Phi_{\text{sc}}(x_{\psi 1}^{\text{sc}}, x_{\zeta-}^{\text{sc}}) + \Phi_{\text{sc}}(x_{\zeta+}^{\text{sc}}, +1)], & w_{\Sigma^*}^{\text{sc}} < \epsilon < w_{\Lambda^*}^{\text{sc}} \\ 2\Phi_{\text{sc}}(x_{\psi 1}^{\text{sc}}, +1), & w_{\Lambda^*}^{\text{sc}} < \epsilon < w_{\Gamma}^{\text{sc}}, \end{cases} \quad (8)$$

$$\mathcal{R}_\varphi^{\text{sc}} = \begin{cases} \Phi_{\text{sc}}(-1, x_{\psi 1}^{\text{sc}}), & w_X^{\text{sc}} < \epsilon < w_{\Gamma}^{\text{sc}} \\ \Phi_{\text{sc}}(-1, +1), & w_{\Gamma}^{\text{sc}} < \epsilon < w_M^{\text{sc}} \\ \Phi_{\text{sc}}(-1, x_{\psi 2}^{\text{sc}}), & w_M^{\text{sc}} < \epsilon < w_R^{\text{sc}}. \end{cases} \quad (9)$$

Table 3. Non-equivalent $\mathbf{k}$ points of van Hove singularities for FCC lattice, see Fig. 2a of main text. The notations are the same as in the Table 1. $k_{\Sigma^*}^{\text{fcc}} = \arccos(2\tau - 1)^{-1}$, $k_{\Delta^*}^{\text{fcc}} = \arccos \tau^{-1}$. $a_{\Delta^* 1}^{\text{fcc}} = 4(\tau^{-1} - 1)(1 + 2\tau)$, $a_{\Delta^* 2}^{\text{fcc}} = 8\tau^{-1}(\tau^2 - 1)$, $a_{\Sigma^* 1}^{\text{fcc}} = 8(\tau - 1)(1 + 2\tau)/(1 - 2\tau)$, $a_{\Sigma^* 2}^{\text{fcc}} = 16\tau(\tau - 1)(1 + 2\tau)(1 - 2\tau)^{-2}$, $a_{\Sigma^* 3}^{\text{fcc}} = 16\tau(\tau - 1)(2\tau - 1)^{-1}$

$\mathbf{k}$	$w^{\text{fcc}} = t(\mathbf{k})$	Inverse masses	Signature
$\Gamma(0, 0, 0)$	$-12 + 6\tau$	$8(1 - \tau), 8(1 - \tau), 8(1 - \tau)$	$\min \xrightarrow{\tau=1} \max$
$X(0, 0, \pi)$	$+4 + 6\tau$	$-8\tau, -8\tau, -8(1 + \tau)$	$\min \xrightarrow{\tau=-1} / + 1/ \xrightarrow{\tau=0} \max$
$W(0, \pi/2, \pi)$	$+4 + 2\tau$	$-4(1 + 2\tau), 8\tau, 8\tau$	$/ + 1/ \xrightarrow{\tau=-1/2} \max \xrightarrow{\tau=0} / - 1/$
$L(\pi/2, \pi/2, \pi/2)$	-6τ	$4(1 + 2\tau), 4(1 + 2\tau), 8(\tau - 1)$	$\max \xrightarrow{\tau=-1/2} / + 1/ \xrightarrow{\tau=-1} \min$
$\Delta^*(0, 0, k_{\Delta^*}^{\text{fcc}})$	$-2\tau^{-1}(2 + 2\tau - \tau^2)$	$a_{\Delta^* 1}^{\text{fcc}}, a_{\Delta^* 1}^{\text{fcc}}, a_{\Delta^* 2}^{\text{fcc}}$	$/ - 1/, \tau > +1; / + 1/, \tau < -1$
$\Sigma^*(0, k_{\Sigma^*}^{\text{fcc}}, k_{\Sigma^*}^{\text{fcc}})$	$4(1 - 2\tau)^{-1} - 2\tau$	$a_{\Sigma^* 1}^{\text{fcc}}, a_{\Sigma^* 2}^{\text{fcc}}, a_{\Sigma^* 3}^{\text{fcc}}$	$/ + 1/, \tau > +1; / - 1/, \tau < 0$

3. $\tau > 1/2$. The kinks of the functions $\mathcal{R}_\varphi^{\text{sc}}$ and $\mathcal{R}_{\varphi'}^{\text{sc}}$ at $\epsilon = w_0^{\text{sc}}(\tau) = 4\tau - \tau^{-1}$ cancel each other.

$$\mathcal{R}_\psi^{\text{sc}} = \begin{cases} 2\Psi_{\text{sc}}(x_\varphi^{\text{sc}}, +1), & w_X^{\text{sc}} < \epsilon < w_{\Sigma^*}^{\text{sc}} \\ 2\Psi_{\text{sc}}(x_{\zeta^-}^{\text{sc}}, x_{\zeta^+}^{\text{sc}}), & w_{\Sigma^*}^{\text{sc}} < \epsilon < w_{\Lambda^*}^{\text{sc}}, \end{cases} \quad (10)$$

$$\mathcal{R}_{\varphi'}^{\text{sc}} = \begin{cases} 2\Phi_{\text{sc}}(x_{\zeta^+}^{\text{sc}}, \min[x_{\psi_2}^{\text{sc}}, +1]) + 2\Phi_{\text{sc}}(x_{\psi_1}^{\text{sc}}, x_{\zeta^-}^{\text{sc}}), & w_{\Sigma^*}^{\text{sc}} < \epsilon < w_{\Lambda^*}^{\text{sc}} \\ 2\Phi_{\text{sc}}(x_{\psi_1}^{\text{sc}}, \min[x_{\psi_2}^{\text{sc}}, +1]), & w_{\Lambda^*}^{\text{sc}} < \epsilon < w_0^{\text{sc}}, \end{cases} \quad (11)$$

$$\mathcal{R}_\varphi^{\text{sc}} = \begin{cases} \Phi_{\text{sc}}(-1, x_{\psi_1}^{\text{sc}}), & w_X^{\text{sc}} < \epsilon < w_M^{\text{sc}} \\ \Phi_{\text{sc}}(-1, x_{\psi_1}^{\text{sc}}) + \Phi_{\text{sc}}(x_{\psi_2}^{\text{sc}}, +1), & w_M^{\text{sc}} < \epsilon < w_0^{\text{sc}} \\ \Phi_{\text{sc}}(-1, x_{\psi_2}^{\text{sc}}) + \Phi_{\text{sc}}(x_{\psi_1}^{\text{sc}}, +1), & w_0^{\text{sc}} < \epsilon < w_\Gamma^{\text{sc}} \\ \Phi_{\text{sc}}(-1, x_{\psi_2}^{\text{sc}}), & w_\Gamma^{\text{sc}} < \epsilon < w_R^{\text{sc}}. \end{cases} \quad (12)$$

In these equations $F(x, y) = K(1 - y/x)/\sqrt{x}$ is symmetric function, which is infinite when x or y tends to zero,

$$K(m) = \int_0^{\pi/2} \frac{d\phi}{\sqrt{1 - m \sin^2 \phi}}$$

being full elliptic integral of the first kind

$$\Psi_{\text{sc}}(x_1, x_2; \epsilon, \tau) = \frac{2}{\pi^3} \int_{x_1}^{x_2} \frac{dx F(-\zeta_{\text{sc}}(x; \epsilon, \tau), \psi_{\text{sc}}(x; \epsilon, \tau))}{\sqrt{1 - x^2}}, \quad (13)$$

$$\Phi_{\text{sc}}(x_1, x_2; \epsilon, \tau) = \frac{2}{\pi^3} \int_{x_1}^{x_2} \frac{dx F(\zeta_{\text{sc}}(x; \epsilon, \tau), \varphi_{\text{sc}}(x; \epsilon, \tau))}{\sqrt{1 - x^2}}, \quad (14)$$

where

$$\zeta_{\text{sc}}(x; \epsilon, \tau) = 16(\tau(\epsilon + 2x) + (1 - 2\tau x)^2), \quad (15)$$

$$\varphi_{\text{sc}}(x; \epsilon, \tau) = (\epsilon + 2x + 4\tau)^2, \quad (16)$$

$$\psi_{\text{sc}}(x; \epsilon, \tau) = (\epsilon + 2x - 4\tau)^2 - 16(1 - 2\tau x)^2, \quad (17)$$

the x integration bounds are $x_{\psi_s}^{\text{sc}}(\epsilon, \tau) = (1/2)(4((-1)^s + \tau) - \epsilon)/(1 + 4(-1)^s \tau)$, $s = 1, 2$; $x_\varphi^{\text{sc}}(\epsilon, \tau) = -2\tau - \epsilon/2$, $x_{\zeta^\pm}^{\text{sc}}(\epsilon, \tau) = (\frac{1}{2} \pm \sqrt{-\frac{3}{4} - \tau\epsilon})/2\tau$, at $\epsilon < w_{\Lambda^*}^{\text{sc}}(\tau)$. Plots of DOS for different values of τ for SC lattice are presented in Fig. S2a.

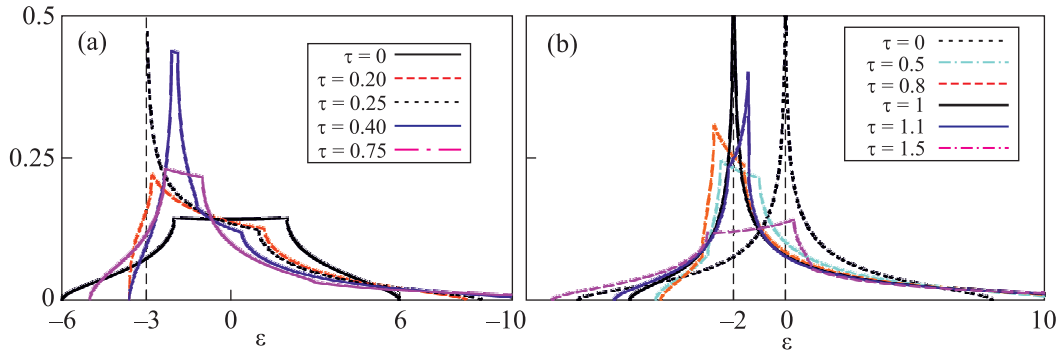


Fig. S2. DOS $t\rho(\epsilon)$ for SC (a) and BCC (b) lattices at different τ . Vertical dashed lines show the position of giant van Hove singularities

For BCC lattice we present the following form for the contributions $\mathcal{R}_i^{\text{bcc}}$

1. $\tau \leq 1$.

$$\mathcal{R}_\psi^{\text{bcc}} = \begin{cases} 2\Psi_{\text{bcc}}(0, x_\varphi^{\text{bcc}}), & w_P^{\text{bcc}} < \epsilon < w_{\Lambda^*}^{\text{bcc}} \\ 2\Psi_{\text{bcc}}(0, x_\zeta^{\text{bcc}}), & w_{\Lambda^*}^{\text{bcc}} < \epsilon < w_N^{\text{bcc}}, \end{cases} \quad (18)$$

$$\mathcal{R}_{\varphi'}^{\text{bcc}} = \begin{cases} 2\Phi_{\text{bcc}}(x_{\zeta}^{\text{bcc}}, x_{\psi_1}^{\text{bcc}}), & w_{\Lambda^*}^{\text{bcc}} < \epsilon < w_{\text{N}}^{\text{bcc}} \\ 2\Phi_{\text{bcc}}(0, x_{\psi_1}^{\text{bcc}}), & w_{\text{N}}^{\text{bcc}} < \epsilon < w_0^{\text{bcc}}, \end{cases} \quad (19)$$

$$\mathcal{R}_{\varphi}^{\text{bcc}} = \Phi_{\text{bcc}}(x_{\psi_1}^{\text{bcc}}, +1). \quad (20)$$

2. $\tau > 1$.

$$\mathcal{R}_{\psi}^{\text{bcc}} = \begin{cases} 2\Psi_{\text{bcc}}(0, x_{\varphi}^{\text{bcc}}), & w_{\text{P}}^{\text{bcc}} < \epsilon < w_{\text{N}}^{\text{bcc}} \\ 2\Psi_{\text{bcc}}(x_{\zeta}^{\text{bcc}}, +1), & w_{\text{N}}^{\text{bcc}} < \epsilon < w_{\Delta^*}^{\text{bcc}}, \end{cases} \quad (21)$$

$$\mathcal{R}_{\varphi'}^{\text{bcc}} = \begin{cases} 2\Phi_{\text{bcc}}(0, x_{\zeta}^{\text{bcc}}), & w_{\text{N}}^{\text{bcc}} < \epsilon < w_{\Delta^*}^{\text{bcc}} \\ 2\Phi_{\text{bcc}}(0, x_{\psi_1}^{\text{bcc}}) \\ + 2\Phi_{\text{bcc}}(x_{\psi_2}^{\text{bcc}}, +1), & w_{\Delta^*}^{\text{bcc}} < \epsilon < w_{\Gamma}^{\text{bcc}}. \end{cases} \quad (22)$$

$$\mathcal{R}_{\varphi}^{\text{bcc}} = \begin{cases} \Phi_{\text{bcc}}(x_{\psi_1}^{\text{bcc}}, x_{\psi_2}^{\text{bcc}}), & w_{\Delta^*}^{\text{bcc}} < \epsilon < w_{\Gamma}^{\text{bcc}} \\ \Phi_{\text{bcc}}(x_{\psi_1}^{\text{bcc}}, +1), & w_{\Gamma}^{\text{bcc}} < \epsilon < w_{\text{H}}^{\text{bcc}}, \end{cases} \quad (23)$$

The kinks of the functions $\mathcal{R}_{\varphi}^{\text{bcc}}, \mathcal{R}_{\varphi'}^{\text{bcc}}$ at $\epsilon = w_0^{\text{bcc}} = 2\tau$ cancel each other.

$$\Psi_{\text{bcc}}(x_1, x_2; \epsilon, \tau) = \frac{2}{\pi^3} \int_{x_1}^{x_2} \frac{dx F(-\zeta_{\text{bcc}}(x; \epsilon, \tau), \psi_{\text{bcc}}(x; \epsilon, \tau))}{\sqrt{x(1-x)}}, \quad (24)$$

$$\Phi_{\text{bcc}}(x_1, x_2; \epsilon, \tau) = \frac{2}{\pi^3} \int_{x_1}^{x_2} \frac{dx F(\zeta_{\text{bcc}}(x; \epsilon, \tau), \varphi_{\text{bcc}}(x; \epsilon, \tau))}{\sqrt{x(1-x)}}, \quad (25)$$

where

$$\zeta_{\text{bcc}}(x; \epsilon, \tau) = 16(\tau(\epsilon + 2\tau) + 4(1 - \tau^2)x), \quad (26)$$

$$\varphi_{\text{bcc}}(x; \epsilon, \tau) = (6\tau + \epsilon - 4\tau x)^2, \quad (27)$$

$$\psi_{\text{bcc}}(x; \epsilon, \tau) = (\epsilon - 2\tau - 4\tau x)^2 - 64x, \quad (28)$$

and the x integration boundaries read $x_{\varphi}^{\text{bcc}}(\epsilon, \tau) = (\epsilon + 6\tau)/4\tau$, at $w_{\text{P}}^{\text{bcc}} < \epsilon$, $x_{\zeta}^{\text{bcc}}(\epsilon, \tau) = \tau(\epsilon + 2\tau)/4(\tau^2 - 1)$, at $(\epsilon - w_{\zeta}^{\text{bcc}})(\tau - 1) > 0$, $x_{\psi_1, 2}^{\text{bcc}}(\epsilon, \tau) = \left(\mp 2 + \sqrt{\tau(\epsilon - 2\tau) + 4}\right)^2 / (4\tau^2)$, at $\epsilon > w_{\Delta^*}^{\text{bcc}}$. DOS plots for different values of τ for BCC lattice are shown in Fig. S2b.

Full understanding for the dependence of DOS on τ can be obtained using the τ dependence of $\rho(w_i^{\text{vHS}}(\tau), \tau)$ at the levels of van Hove points $\epsilon = w_i^{\text{vHS}}(\tau)$. These plots are shown in Fig. S3. For SC lattice, the maximal value of DOS at $\tau > 1/4$ is achieved at the levels $\epsilon = w_{\Sigma^*}^{\text{sc}}$ and $w_{\Lambda^*}^{\text{sc}}$. These values slowly decrease as τ is shifted from $1/4$ ($\rho_{\text{sc}}(w_{\Sigma^*}^{\text{sc}}(\tau), \tau) \approx \rho_{\text{sc}}(w_{\Lambda^*}^{\text{sc}}(\tau), \tau) \sim (\tau - 1/4)^{-1/2}$). For BCC lattice, the maximal value of DOS is always achieved at the energy level corresponding to inner points of the Brillouin zone: $\epsilon = w_{\Lambda^*}^{\text{bcc}}$ at $\tau < 1$, $\epsilon = w_{\Delta^*}^{\text{bcc}}$ at $\tau > 1$.

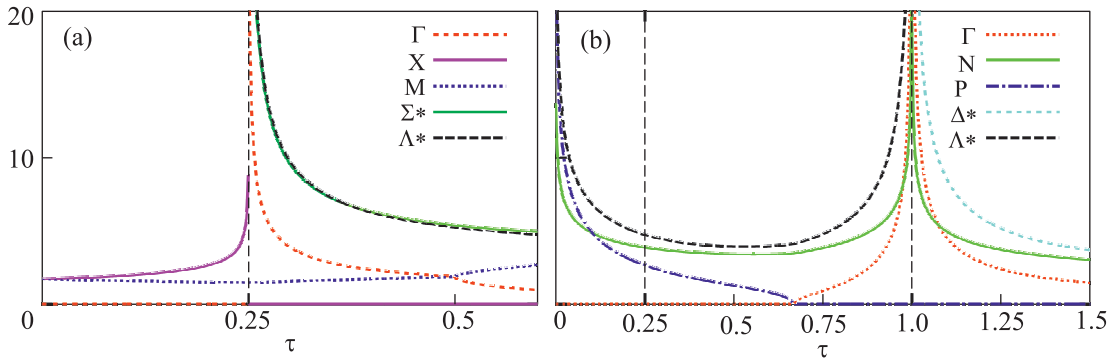


Fig. S3. τ dependence of DOS $W\rho(\epsilon; \tau)$ at each van Hove singularity level for SC (a) and BCC (b) lattices (W is the bandwidth). In the case (a), DOS values at $w_{\Lambda^*}^{\text{sc}}$ and $w_{\Sigma^*}^{\text{sc}}$ are almost equal, see main text