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High-temperature surface superconductivity in topological flat-band systems

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We show that the topologically protected flat band emerging on a surface of a nodal fermionic system promotes the surface superconductivity due to an infinitely large density of states associated with the flat band. The critical temperature depends linearly on the pairing interaction and can be thus considerably higher than the exponentially small bulk critical temperature. We discuss an example of surface superconductivity in multilayered graphene with rhombohedral stacking.

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Normal Fermi liquid is the generic form of a system of interacting fermions. A Fermi liquid has a finite density of states (DOS) at zero energy, which may lead to instabilities at low T with the formation of broken symmetry states with smaller DOS. However, there is a class of fermionic systems with a diverging DOS: systems with a dispersionless spectrum that has exactly zero energy (i.e., the flat band). Historically, this was first discussed in the context of Landau levels. However, flat bands may also emerge without a magnetic field; for example, in strongly interacting condensed matter systems,^{1–4} in layered systems with integer-valued pseudospin,⁵ in $2 + 1$ dimensional quantum field theory dual to a gravitational theory in the anti-de Sitter background,⁶ etc. In some cases the flat band is protected by topology in the momentum space: topologically protected zero modes emerge in cores of quantized vortices,^{7–9} on surfaces of gapless topological media such as nodal superconductors^{9–11} and multilayered graphene,^{9,12–14} as well as at the edges of graphene sheets.^{9,10}

In this Rapid Communication we consider a three-dimensional (3D) system where the topologically protected flat band with its singular DOS appears on the surface, giving rise to two-dimensional (2D) surface superconductivity. This property is generic and does not depend much on the details of the system. For illustration we use multilayered graphene with rhombohedral stacking, where a surface flat band appears in the limit of a large number of layers. We show that the superconducting critical temperature depends linearly on the pairing interaction strength and can be thus considerably higher than the usual exponentially small critical temperature in the bulk. This may open a new route to room-temperature superconductivity.⁹ Formation of surface superconductivity is already enhanced for a system having $N \geq 3$ layers where the normal-state spectrum has a power-law dispersion $\xi_p \propto |\mathbf{p}|^N$ as a function of the in-plane momentum \mathbf{p} . The DOS $\nu(\xi_p) \propto \xi_p^{(2-N)/N}$ has a singularity at zero energy which results in a drastic enhancement of the critical temperature. We also demonstrate that doping leads to a suppression of the surface critical temperature, contrary to its effect on the bulk superconductivity where the critical temperature is increased.^{15,16}

a. The model. We consider a multilayered graphene structure of N layers in the discrete representation with respect to interlayer coupling. We choose the rhombohedral

stacking configuration considered in Refs. 9,12–14 and assume for simplicity that the most important are jumps between the atoms belonging to different sublattices parametrized by a single hopping energy t . A more general form of the multilayered Hamiltonian can be found in Refs. 17 and 18. In the superconducting case the Hamiltonian has the form of a matrix in Nambu space. The Bogoliubov–de Gennes (BdG) equations are

$$\sum_{j=1}^N \begin{pmatrix} \hat{H}_{ij} - \mu_i \delta_{ij} & \Delta_i \delta_{ij} \\ \Delta_i^* \delta_{ij} & -\hat{H}_{ij} + \mu_i \delta_{ij} \end{pmatrix} \begin{pmatrix} \hat{u}_j \\ \hat{v}_j \end{pmatrix} = E \begin{pmatrix} \hat{u}_i \\ \hat{v}_i \end{pmatrix},$$

where the sum runs over the layers. The normal-state Hamiltonian is¹⁴

$$\hat{H}_{ij} = v_F (\hat{\sigma} \cdot \mathbf{p}) \delta_{i,j} - t \hat{\sigma}_+ \delta_{i,j+1} - t \hat{\sigma}_- \delta_{i,j-1}, \quad (1)$$

where $\hat{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y)$, $\hat{\sigma}_\pm = (\hat{\sigma}_x \pm i \hat{\sigma}_y)/2$, and \hat{u}_i, \hat{v}_i are matrices and spinors in the pseudospin space associated with two sublattices. This Hamiltonian acts on the envelope function of the in-plane momentum \mathbf{p} taken near one of the Dirac points; that is, for $|\mathbf{p}| \ll \hbar/a$ where a is the interatomic distance within a layer; $v_F = 3t_0 a / (2\hbar)$ where t_0 is the hopping energy between nearest-neighbor atoms belonging to different sublattices on a layer. The particle-like, \hat{u}_i , and hole-like, \hat{v}_i , wave functions near the Dirac point are coupled via the superconducting order parameter Δ_i that can appear in the presence of a pairing interaction. Here we do not specify the nature of pairing which can be either due to the electron-phonon interaction or due to other interactions that have been suggested as a source for intrinsic superconductivity in graphene, see Ref. 19. As a reasonable starting point we assume s -wave symmetry for the order parameter and neglect fluctuations for simplicity, although they could, in principle, be relevant for 2D superconductivity. The excitation energy for particles and holes is measured upward or downward, respectively, from the Fermi level, which can be shifted with respect to the Dirac point. We assume that the shifts at the outermost layers may be different from the bulk chemical potential due to the presence of a surface charge (i.e., $\mu_i = \mu$ for $i \neq 0, N$ while $\mu_{1,N} = \mu + \delta\mu_{1,N}$). The order parameter and the Fermi-level shifts μ_i are scalars in the pseudospin space. We assume that Δ_i and μ_i are much smaller than the interlayer coupling energy $t > 0$, which in turn is $t \ll t_0$. Usually, $t \sim 0.1 t_0$ where $t_0 \sim 3 \text{ eV}$.¹⁸

b. Spectrum. We decompose the wave function

$$\begin{pmatrix} \hat{u}_n \\ \hat{v}_n \end{pmatrix} = \left[\begin{pmatrix} \alpha_n^+ \\ \beta_n^+ \end{pmatrix} \otimes \hat{\Psi}^+ + \begin{pmatrix} \alpha_n^- \\ \beta_n^- \end{pmatrix} \otimes \hat{\Psi}^- \right] \quad (2)$$

into the spinor functions localized at each sublattice:

$$\hat{\Psi}^+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \hat{\Psi}^- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The BdG equations take the form

$$\check{\tau}_3[v_F(p_x - ip_y)\check{\alpha}_n^- - t\check{\alpha}_{n-1}^- - \mu\check{\alpha}_n^+] = E\check{\alpha}_n^+, \quad n \neq 1, \quad (3)$$

$$\check{\tau}_3[v_F(p_x + ip_y)\check{\alpha}_n^+ - t\check{\alpha}_{n+1}^+ - \mu\check{\alpha}_n^-] = E\check{\alpha}_n^-, \quad n \neq N. \quad (4)$$

We introduce matrices and vectors in the Nambu space:

$$\check{\tau}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \check{\Delta}_n = \begin{pmatrix} 0 & \Delta_n \\ \Delta_n^* & 0 \end{pmatrix}, \quad \check{\alpha}_n^\pm = \begin{pmatrix} \alpha_n^\pm \\ \beta_n^\pm \end{pmatrix}.$$

In Eqs. (3) and (4) we assume that $\Delta_n \neq 0$ only at the outermost layers, while $\Delta_n = 0$ for $n \neq 1, N$. The arguments supporting this model are given below. We also neglect Δ_n as compared to t in Eqs. (3) and (4) for $n = N$ and $n = 1$, respectively, as they lead to higher-order corrections in Δ/t . The particle and hole channels are thus decoupled if $n \neq 1, N$, which determines the coefficients $\check{\alpha}_n^\pm = \check{A}^\pm e^{ip_z d n}$ and the energy in terms of the transverse momentum p_z (d is the interlayer distance):¹⁴

$$E^2 = v_F^2 p^2 - 2tv_F p \cos(p_z d - \phi) + t^2, \quad (5)$$

where $p = \sqrt{p_x^2 + p_y^2}$ and $e^{i\phi} = (p_x + ip_y)/p$.

A finite order parameter Δ couples the particle and hole channels at the outermost layers, $i = 1$ and $i = N$,

$$\check{\tau}_3 v_F(p_x - ip_y)\check{\alpha}_1^- - \check{\tau}_3 \mu_1 \check{\alpha}_1^+ = E\check{\alpha}_1^+ - \check{\Delta}_1 \check{\alpha}_1^+, \quad (6)$$

$$\check{\tau}_3 v_F(p_x + ip_y)\check{\alpha}_N^+ - \check{\tau}_3 \mu_N \check{\alpha}_N^- = E\check{\alpha}_N^- - \check{\Delta}_N \check{\alpha}_N^-. \quad (7)$$

Boundary conditions (6) and (7) select p_z and determine 2N particle and hole branches of the energy spectrum. Looking for the branches that belong to the surface states with energies of the order of Δ and μ , we solve these equations for $E \ll t$. Since Eqs. (3) and (4) do not contain Δ , one can use the coefficients as obtained in Ref. 14:

$$\begin{aligned} \check{\alpha}_n^+ &= \frac{C}{\sqrt{2}} \left[\left(\frac{v_F p}{t} \right)^{n-1} \check{A}^+ \right. \\ &\quad \left. + \left(\frac{v_F p}{t} \right)^{N-n} \frac{v_F p (\check{\tau}_3 E + \mu)}{v_F^2 p^2 - t^2} \check{A}^- \right] e^{i(n-1-\frac{N}{2})\phi}, \\ \check{\alpha}_n^- &= \frac{C}{\sqrt{2}} \left[\left(\frac{v_F p}{t} \right)^{N-n} \check{A}^- \right. \\ &\quad \left. + \left(\frac{v_F p}{t} \right)^{n-1} \frac{v_F p (\check{\tau}_3 E + \mu)}{v_F^2 p^2 - t^2} \check{A}^+ \right] e^{i(n-\frac{N}{2})\phi}. \end{aligned}$$

Here C is a normalization constant. We include the first-order corrections in energy. Having an imaginary momentum p_z for $v_F p < t$, these solutions decay away from the surfaces and thus describe the surface states. The vectors $\check{A}^\pm = (A^\pm, B^\pm)^T$ do not depend on n . Equations (6) and (7) yield

$$\check{\tau}_3 \xi_p \check{A}^- = (\check{E} + \check{\tau}_3 \check{\mu}_1) \check{A}^+ - \check{\Delta}_1 \check{A}^+, \quad (8)$$

$$\check{\tau}_3 \xi_p \check{A}^+ = (\check{E} + \check{\tau}_3 \check{\mu}_N) \check{A}^- - \check{\Delta}_N \check{A}^-, \quad (9)$$

where $\xi_p = t(v_F p/t)^N$, $\check{\mu}_{1,N} = \check{\mu} + \delta\mu_{1,N}$, and

$$E = \check{E}(1 - v_F^2 p^2/t^2), \quad \mu = \check{\mu}(1 - v_F^2 p^2/t^2). \quad (10)$$

Equations (8) and (9) provide the surface-state spectrum

$$\begin{aligned} &[\check{E}^2 - \check{\mu}_N^2 - |\Delta_N|^2][\check{E}^2 - \check{\mu}_1^2 - |\Delta_1|^2] + \xi_p^4 \\ &- \xi_p^2 [2\check{E}^2 + 2\check{\mu}_1 \check{\mu}_N - \Delta_1^* \Delta_N - \Delta_1 \Delta_N^*] = 0. \quad (11) \end{aligned}$$

If $\Delta_1 = \Delta_N$ we have from Eq. (11)

$$\check{E}_\pm^2 = [\check{\mu}_0 \mp \sqrt{\xi_p^2 + (\delta\mu)^2}]^2 + |\Delta|^2, \quad (12)$$

where $\delta\mu = (\mu_1 - \mu_N)/2$ and $\check{\mu}_0 = (\check{\mu}_1 + \check{\mu}_N)/2$. Equations (8) and (9) determine four independent states. If $\mu = \delta\mu = 0$ they are (i) $\check{E}_1 = \check{E}$ and $A_1^\pm = u$, $B_1^\pm = v$, (ii) $\check{E}_2 = -\check{E}$ and $A_2^\pm = v$, $B_2^\pm = -u$, (iii) $\check{E}_3 = \check{E}$ and $A_3^\pm = \pm v$, $B_3^\pm = \pm u$, and (iv) $\check{E}_4 = -\check{E}$ and $A_4^\pm = \pm u$, $B_4^\pm = \mp v$. Here, $\check{E} = \sqrt{\xi_p^2 + \Delta^2}$ and

$$u = \frac{1}{\sqrt{2}}[1 + \xi_p/\check{E}]^{\frac{1}{2}}, \quad v = \frac{1}{\sqrt{2}}[1 - \xi_p/\check{E}]^{\frac{1}{2}}. \quad (13)$$

The overall normalization requires $d \sum_{n=1}^N [|\alpha_n^+|^2 + |\beta_n^+|^2 + |\alpha_n^-|^2 + |\beta_n^-|^2] = 1$. For $\xi_p \ll t$ this gives

$$|C|^2 = d^{-1} t [1 - (v_F p/t)^2]. \quad (14)$$

Note that Eqs. (11)–(14) hold for $\xi_p \ll t$. The spectrum is plotted in Fig. 1.

If $N \rightarrow \infty$ and $\xi_p \rightarrow 0$ for any $v_F p/t < 1$, the surface-state part localized at $n = N$ (with the coefficients \check{A}^-) decouples from that (with \check{A}^+) which is localized at $n = 1$. For a ‘‘flat band’’ $\xi_p \rightarrow 0$, Eq. (11) yields

$$\check{E}_+^2 = \check{\mu}_N^2 + |\Delta_N|^2 \quad \text{or} \quad \check{E}_-^2 = \check{\mu}_1^2 + |\Delta_1|^2. \quad (15)$$

This shows that the different signs in Eq. (12) belong to the surface states localized at the corresponding layers.

c. Flat band, zero doping. The gap at layer N is

$$\begin{aligned} \Delta_N &= \int \frac{d^2 p}{(2\pi\hbar)^2} \sum_{k=1}^N V_{\mathbf{p}, p_z(k)} \text{Tr}[\hat{u}_N(\mathbf{p}, k) \hat{v}_N^*(\mathbf{p}, k)] \\ &\quad \times [1 - 2f(E_{\mathbf{p}, k})], \end{aligned}$$

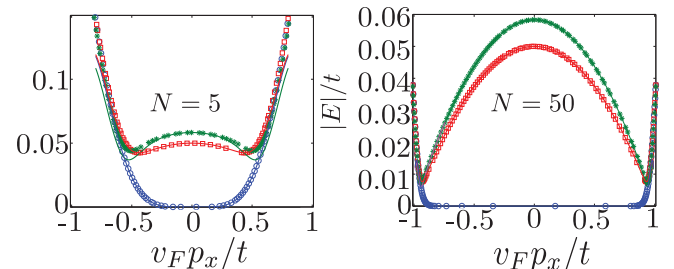


FIG. 1. (Color online) Spectrum of surface states for different numbers of layers. $N = 5$ (left) and $N = 50$ (right). The symbols have been calculated by exact diagonalization and the solid lines are computed from Eq. (12) up to the point where the approximation in it is valid. The three cases are: normal case with $\mu_n \equiv 0$ (blue circles), $\Delta = 0.05t, \mu_n \equiv 0$ (red squares), and $\Delta = 0.05t, \mu_1 = \mu_N = 0.03t$ (green crosses).

where $f(E)$ is the Fermi distribution function. We assume that the cutoff momentum p_c of the pairing potential V is larger than $p_{\text{FB}} = t/v_F$. The sum includes one $n = N$ surface state which we label by $k = 0$ and the bulk states specified by the transverse momenta $p_z(k)$, where $k = 1, 2, \dots, N-1$ with the spectrum of Eq. (5). Therefore, $\Delta_N = \Delta_S + \Delta_B$ where the surface contribution comes from the flat band area $p < p_{\text{FB}}$,

$$\Delta_S = V \int_{p < p_{\text{FB}}} \frac{d^2 p}{(2\pi\hbar)^2} \text{Tr}[\hat{u}_N(\mathbf{p}, 0) \hat{v}_N^*(\mathbf{p}, 0)] [1 - 2f(E_{\mathbf{p}, 0})]. \quad (16)$$

The bulk contribution comes from the momenta $p > p_{\text{FB}}$. For such momenta, the surface state $k = 0$ will also extend to the bulk, giving rise to (for $T = 0$)

$$\Delta_B = V \int_{p_{\text{FB}} < p < p_c} \frac{d^2 p}{(2\pi\hbar)^2} \left\{ \text{Tr}[\hat{u}_N(\mathbf{p}, 0) \hat{v}_N^*(\mathbf{p}, 0)] + \sum_{k=1}^{N-1} \text{Tr}[\hat{u}_N(\mathbf{p}, k) \hat{v}_N^*(\mathbf{p}, k)] \right\}. \quad (17)$$

All the bulk states with $p > p_{\text{FB}}$ are normalized to the sample width $W = dN$ (i.e., $u^*(z) \sim 1/\sqrt{W}$). According to Eq. (5), $E \sim v_F p > t$ in Eq. (17). Therefore,

$$\Delta_B \approx \frac{V p_c^2}{4\pi\hbar^2} \frac{N}{W} \left[\frac{\Delta}{v_F p_c} - O\left(\frac{\Delta}{v_F p_c}\right)^3 \right].$$

If there was only the bulk contribution ($\Delta \equiv \Delta_B = \Delta_N$), the gap equation would have a nonzero solution only for a potential strength higher than a certain critical value $V p_c / (4\pi\hbar^2 v_F d) > 1$, as is the case in the usual single-layer graphene with zero doping.^{15,16}

The surface states for $p < p_{\text{FB}}$ are normalized according to Eq. (14). We find from Eq. (16):

$$\Delta_S = 2V \int_{p < p_{\text{FB}}} \frac{d^2 p}{(2\pi\hbar)^2} |C|^2 uv \tanh \frac{E}{2k_B T}. \quad (18)$$

For simplicity we assume that V is constant up to the cutoff momentum p_c . Here, u and v are determined by Eqs. (13) and (14). In the case of a flat band $uv = 1/2$ while $E = \Delta(1 - v_F^2 p^2/t^2)$. For $T = 0$ it gives

$$\Delta_S = \Delta_0 \equiv g/(8\pi), \quad (19)$$

where $g = \tilde{V} p_{\text{FB}}^2/\hbar^2$ is the characteristic pairing energy and $\tilde{V} = V/d$ is the two-dimensional pairing potential.

The ratio of the order parameter in the bulk to that on surface is of the order $(\Delta/t)(v_F p_c/t)$. Since $\Delta \ll t$, the contribution from the bulk states with $E > t$ can be neglected if the cutoff momentum of the interaction p_c does not considerably exceed t/v_F . We thus arrive at the central result of our paper, namely that the surface superconductivity in the presence of a flat band dominates over the bulk superconductivity. This follows from an infinitely large density of states associated with the flat band. The critical temperature is determined by Eq. (19) with $\Delta \rightarrow 0$, which gives $\Delta_0 = 3k_B T_c$. Due to its linear dependence on the interaction strength, the critical temperature is proportional to the area of the flat band and can be essentially higher than that in the bulk.

For a flat band $\xi_p = 0$, with $p_c = p_{\text{FB}}$, the only characteristic values in the superconducting surface state are the energy Δ and the momentum p_{FB} . Therefore, the coherence length should be of the order of the only available length scale, $\xi_0 \sim \hbar/p_{\text{FB}}$. It is much larger than the interatomic distance, $\xi_0 \gg a$, since $p_{\text{FB}} \ll p_0 \sim \hbar/a$.

Doping destroys the surface superconductivity. This can be seen from Eq. (18) with $uv = \Delta/(2\tilde{E}_+)$ and $E = (1 - v_F^2 p^2/t^2)\tilde{E}_+$ where \tilde{E}_+ is taken from Eq. (15). The critical temperature is found by putting $\Delta = 0$. For example, if μ and μ_N have the same sign, both Δ_0 and T_c vanish at the critical doping level that satisfies

$$1 = \frac{\tilde{V}}{4\pi\hbar^2 |\mu_N - \mu|} \left| \frac{1}{2} - \frac{\mu}{\mu_N - \mu} + \frac{\mu^2}{(\mu_N - \mu)^2} \ln \frac{\mu_N}{\mu} \right|.$$

If $\mu_N = \mu$ the critical doping is $|\mu| = 2k_B T_c$.

d. Surface superconductivity in a finite array. Since the normal-state DOS defined as

$$v(\xi_p) = \frac{p}{2\pi\hbar^2} \frac{dp}{d\xi_p} = \frac{t(\xi_p/t)^{\frac{2-N}{N}}}{2\pi\hbar^2 N v_F^2} \quad (20)$$

has a low-energy singularity for $N > 2$, the surface superconductivity is favorable already for a system with a finite number of layers $N \geq 3$. A simple expression for the zero-temperature gap can be obtained if $N \geq 5$. For a finite N , the value ξ_p can reach values larger than Δ . We use Eqs. (12)–(14) for zero doping in Eq. (18), where the upper limit of integration p_c is now such that $\xi_c = t(v_F p_c/t)^N \gg \Delta$. Transforming to the energy integral with the normal-state DOS [Eq. (20)] we see that, for $N > 4$, the integral converges at $\xi_p \sim \Delta$ or $p \sim p_\Delta = p_{\text{FB}}(\Delta/t)^{1/N}$. The zero-temperature gap is

$$\Delta_0 = t \left(\frac{g}{4\pi t} \left[\alpha(N) - \frac{1}{2} (\Delta_0/t)^{\frac{2}{N}} \alpha(N/2) \right] \right)^{\frac{N}{N-2}}, \quad (21)$$

where

$$\alpha(N) = \int_0^\infty \frac{x^{\frac{N+2}{N}} dx}{(\sqrt{x^2+1})^3} = \frac{1}{\sqrt{\pi}} \Gamma\left(\frac{N-2}{2N}\right) \Gamma\left(\frac{N+1}{N}\right).$$

For $N \gg 1$ we have $\alpha_N = 1$. The flat-band result, Eq. (19), is recovered if the number of layers is $N \gg 2 \ln(t/\Delta_0)$.

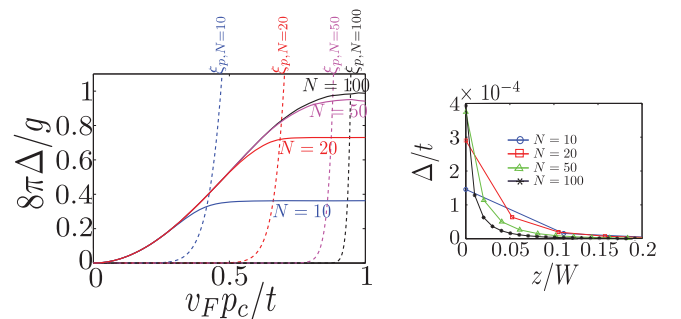


FIG. 2. (Color online) Zero-temperature gap self-consistently calculated from Eq. (16) for $g = 0.01t$. Left panel: Δ as a function of p_c for various N (solid lines). For $p_c \sim p_\Delta$ the gap saturates at the values given by Eq. (21) which approach Eq. (19) for $N \rightarrow \infty$. The dashed lines show the dispersion ξ_p for each N . Right panel: $\Delta(z)$ profile, $z = nd$. $\Delta(z)$ is symmetric with respect to $z \rightarrow W - z$.

The coherence length for a finite system is $\xi_0 \sim \hbar/p_\Delta$. It approaches \hbar/p_{FB} for $N \rightarrow \infty$.

Results of numerical integration of the self-consistency equation (16) with a cutoff p_c are plotted in Fig. 2, left panel. The right panel shows the order parameter as a function of the transverse coordinate. It extends into the bulk only over a few interlayer distances due to a decay of the wave functions. This supports the model of Eqs. (3)–(7) in which Δ is nonzero only on the outermost layers.

e. Conclusion. The flat band with infinite DOS emerges in semimetals with topologically protected nodal lines. The flat band promotes surface superconductivity with T_c proportional to the pairing interaction strength and to the area of the flat band in the momentum space determined by the projection of the nodal line onto the surface. The critical temperature can thus be considerably higher than an exponentially small bulk T_c . Formation of surface superconductivity is enhanced already for a system with $N \geq 3$ layers where the normal DOS has a

singularity at zero energy. Topologically protected flat bands may also appear on interfaces and on twin or grain boundaries in bulk topological materials leading to an enhanced bulk T_c . Indications toward surface superconductivity proving the existence of proper pairing interaction have been seen in graphite.^{20,21} Enhanced superconductivity was reported on twin boundaries in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$.²² These observations agree with our theory. Our predictions may be used to search for or fabricate layered and/or twinned systems with high-temperature and even room-temperature superconductivity.

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