Unconventional superconductivity in a doped quantum spin Hall insulator

Xianxin Wu,1 Mario Fink,1 Werner Hanke,1 Ronny Thomale,1 and Domenico Di Sante1

1Institut für Theoretische Physik und Astrophysik, Universität Würzburg,
Am Hubland Campus Süd, Würzburg 97074, Germany

(Dated: Tuesday 6th November, 2018)

A monolayer of jacutingaite (Pt\textsubscript{3}HgSe\textsubscript{3}) has recently been identified as a novel quantum spin Hall insulator. By first-principles calculations, we study its Fermiology in the doped regime and unveil a type-I and type-II van Hove singularity for hole and electron doping, respectively. We find that the common link between the propensity for a topological band gap at pristine filling and unconventional superconductivity at finite doping roots in the longer ranged hybridization integrals on the honeycomb lattice. In a combined effort of random phase approximation and functional renormalization group, we find chiral $d$-wave order for the type-I and odd-parity $f$-wave order for the type-II regime.

Introduction – Quantum spin Hall effect and unconventional superconductivity are among the most intensely studied fields of contemporary condensed matter research [1-3]. At a superficial level, both topical areas do not seem to be particularly intertwined: in the pursuit of a quantum spin Hall insulator with most preferable properties, essential parameters of optimization include spin-orbit coupling and other single-particle properties to enhance the topological bulk gap; in order to accomplish a high-$T_c$ unconventional superconductor as a quantum many-body state of matter, tuning the electronic interaction strength and profile appears as the most relevant guiding principle.

Still, superconductivity and topological band insulators or semimetals have previously faced each other in several contexts. Most prominently, this holds for the principal topological classification of single-particle scenarios where the emergent particle-hole symmetry in superconductors plays a pivotal role [1], and for the case of superconducting proximity effect imposed on a topologically non-trivial band structure [5-8]. All these instances, however, do not include the joint avenue of a superconductor and a topological band insulator in the same material at only different doping. Ideally, such a setting might allow for the synthesis of a high-quality domain boundary between a superconductor and a topological insulator with identical lattice structures, under the assumption that it were possible to impose distinct gating in both domains. Until today, there are only few reports of materials that are believed to be both topological insulators and superconductors. Half-Heusler semimetals [9], Cu-doped Bi\textsubscript{2}Se\textsubscript{3} [10], doped BaBiO\textsubscript{3} [11, 12], and monolayer WTe\textsubscript{2} [13] are such remarkable exceptions, where a conventional, i.e., phonon-driven mechanism for superconductivity is likely to dominate.

In this Letter, we propose a monolayer of jacutingaite (Pt\textsubscript{3}HgSe\textsubscript{3}) to host, besides a quantum spin Hall insulator at pristine filling [14], different phases of unconventional superconductivity for finite hole and electron doping. The central overarching motif that enables both the realization of quantum spin Hall effect and unconventional superconductivity is a specific longer ranged hybridization profile which roots in the extended Wannier functions of jacutingaite (Fig. 1). The multi-orbital composition and the honeycomb monolayer buckling conspire to yield an effective tight-binding description which not only provides for a large topological band gap, but also gives rise to van Hove singularities (vHs) close by pristine filling, with type-I profile for hole and type-II profile for electron doping. For type-I, the saddle points locate at the time-reversal invariant momenta (TRIM) $M$ of the hexagonal lattice. For type-II, the saddle points appear along the $K-M$ lines in the Brillouin zone, and hence do not coincide with TRIMs [15, 16]. As such, while the van Hove induced enhancement of Fermi level density of states promotes unconventional superconductivity in general, the nature of the unconventional superconducting state sensitively depends on the type-I vs. type-II regime, which we analyze through random phase approximation (RPA) and functional renormalization group (FRG). We find a $d$-wave instability for the type-I setting which yields spontaneous time-reversal symmetry breaking according to a chiral $d$-wave state. For the type-II setting, the ferromagnetic fluctuations dominate and promote an odd-parity $f$-wave state.

Effective model – Monolayer jacutingaite crystallizes in the spacegroup $P\bar{3}m1$ (164), where the Hg atoms form a buckled honeycomb lattice surrounded by triangles of Pt and Se (Fig. 1b). As first pointed out by Marrazzo et al. [14], the low-energy bandstructure of jacutingaite can be reduced to an effective tight-binding description that shares several terms with the Kane-Mele model for a quantum spin Hall insulator in graphene [1]. Anticipating its relevance for jacutingaite at finite doping, we further add hybridization integrals up to 4th nearest neighbor which yields

$$H_0^\lambda = \sum_{\langle ij \rangle} t_n \sum_{\langle ij \rangle} c_{i\sigma}^\dagger c_j + i\lambda_{SO} \sum_{\langle ij \rangle} \mu_{ij} c_{i\sigma}^\dagger c_j + i\lambda_{R} \sum_{\langle ij \rangle} \mu_{ij} c_{i\sigma}^\dagger (\sigma \times \hat{d}_{ij}) \cdot c_j. \quad (1)$$
Such a long range hybridization character originates from the delocalized nature of Hg 6s and Pt 5d orbitals, which mix to form the hermaphrodite Wannier functions shown in Fig. 1b).

The parameters $t_n$, $\lambda_{SO}$, and $\lambda_R$ are real, where $t_n$ denotes the $n$th nearest neighbor hopping, $\lambda_{SO}$ is the spin-orbit coupling (SOC) induced second nearest neighbor hopping, and $\lambda_R$ describes the Rashba SOC. The absence of a Semenoff mass is due to the centrosymmetric structure of jacutingaite, i.e., the two Wannier functions composing the low-energy model have the same on-site energy. The imaginary parts of nearest and 3rd nearest neighbor hopping vanish due to mirror (with respect to the Hg-Hg bonds) and time-reversal symmetries. Note that $t_2$ connects equal sublattices on the honeycomb lattice, and as such breaks the chiral symmetry. The chiral symmetry operator is $S = \sum_i c_{i,x}^\dagger \tau_z s_{s'} c_{i,x'}$ where $s(s')$ represents the sublattice index. Since $S^{-1} H_0^1 S \neq -H_0^1$ when a real $t_2$ hopping is included, the resulting energy spectrum ceases to be chiral symmetric in the presence of finite $t_2$. The parameters extracted by projecting the density functional theory Hamiltonian onto a set of maximally localized Wannier orbitals at different levels of sophistication [17], as shown in Fig. 2, for the HSE(+SOC) cases, are summarized in Table I.

The topological bulk gap yields $E_g \sim 6\sqrt{3} \lambda_{SO}$. Note that $\lambda_{SO}$ in a Kane-Mele single-orbital scenario describes an effective SOC which, starting from the local atomic term, also considers a downscaling due to the higher-order perturbative effect via second nearest neighbor hybridization. In a QSH material candidate such as graphene, this leads to a significant reduction of $\lambda_{SO}$ because the longer range hybridization is small [18], whereas for jacutingaite, this rescaling is much weaker, combined with the enhanced atomic SOC of Hg in comparison to C. An alternative path to enhance $E_g$ is to realize a two-orbital model per site, as such allowing for local atomic SOC to affect the low-energy effective model and to avoid the rescaling due to longer range hybridization. This is accomplished for bismuthene on SiC [19, 20].

Aside from the large gap, further relevant aspects of the resulting band structure are visible as we analyze the precise dispersion of the bands in the two-dimensional Brillouin zone. By looking at the DOS in Fig. 2a, vHs peaks arise at the M point for the valence band and along the K–M line for the conduction band, respectively. The Fermi surface at the former vHs (Fig. 2a) shows a hexagonal profile, with triangular hole pockets around the K points. The Fermi surface at the latter vHs (Fig. 2c), on the other hand, shows a different shape, with small pockets touching at the saddle points. We refer to this vHs as type-II [15, 16], to distinguish it from the type-I vHs where the saddle points locate at TRIMs. A necessary condition for a coexistence of both type-I and type-II vHs in jacutingaite is a sizable real hopping parameter $t_2$ in [1]. This contribution is not contained in the Kane-Mele model [1], but indispensable to account for a realistic setting such as the buckled honeycomb lattice of monolayer jacutingaite. To reproduce the band dispersion given by first-principles calculations, and in particular to obtain the type-II vHs we find in jacutingaite, longer range hoppings $t_3$ and $t_4$ need to be taken into consideration (Table I). While these new terms do not change the principal topological nature of the bulk band gap [14], they are of primary importance for an accurate study of pairing states nearby van Hove filling [17].

Supercconducting instabilities – In order to account for electronic interactions, we consider the onsite Hubbard model on the 2D hexagonal lattice, with the non-interacting single particle Hamiltonian given by [1], and $U$ parametrizing the Hubbard coupling strength. The full Hamiltonian reads

$$H^1 = H^1_0 + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i,\sigma},$$

### TABLE I. Model parameters extracted by projecting the low-energy states onto two hermaphrodite Wannier orbitals, that map onto each other under inversion. One of the two is shown in Fig. 1b). All the parameters are given in meV.

| Method          | $t_1$  | $t_2$  | $\lambda_{SO}$ | $\lambda_R$ | $t_3$  | $t_4$  |
|-----------------|--------|--------|-----------------|-------------|--------|--------|
| PBE+SOC         | 178    | 18     | 22              | 28          | 11     | 15     |
| HSE+SOC         | 267    | 28     | 21              | 27          | -0.4   | -28    |
| PBE             | 178    | 31     | 18              | 28          | 16     | 24     |
| HSE             | 267    | 35     | 21              | 27          | 4      | 32     |
where $\mu$ is the chemical potential tuned to access the two vH regimes. The combination of Fermi level density of states and finite $U$ triggers superconducting instabilities, which we analyze in the following. At the simplified RPA level, where the electronic two-particle vertex function is replaced by the bare interaction $U$, an effective attractive interaction can emerge through the exchange of charge and magnetic fluctuations. These are governed by the respective charge and magnetic susceptibilities $\chi_{c/m}^{ph}(q) = [1 \pm U\chi_0^{ph}(q)]^{-1}\chi_0^{ph}(q)$. The zero-frequency component of the bare susceptibility matrix in the particle-hole channel is defined as

$$[\chi_0^{ph}(q)]_{lm}^{ij} = -\frac{1}{N_k} \sum_{k, nm} a_{l}^{i}(k)a_{n}^{j*}(k)a_{m}^{l}(k + q)$$

$$a_{n}^{j*}(k + q)f(\varepsilon_{nk}) - f(\varepsilon_{mk+q})\varepsilon_{nk} - \varepsilon_{mk+q},$$

where $l = 1, 2$ is the sublattice index and $a_{n}^{j}(k)$ is the $l,i$th component of the $n$th eigenvector. This quantity reveals the distribution of momentum transfer $q$ implied by spin and charge fluctuations.

In Fig. 3 we show the susceptibility $\chi_0^{ph}(q)$ at the type-I vHs. Significant intensity close to the $M$ point suggests dominant antiferromagnetic spin fluctuations in the system, and is a consequence of the high degree of nesting of the Fermi surface at the type-I vHs, as evident from Fig. 2b. Such a setting for spin fluctuations has been found to trigger an even-parity chiral superconducting instability [21–23]. At the type-II vHs, on the other hand, there is no Fermi surface nesting, and $\chi_0^{ph}(q)$ is solely peaked around the $\Gamma$ point, suggesting that in this case, the dominant magnetic fluctuations involve a long range modulation (i.e., ferromagnetic fluctuations in the limit $q \to 0$). General arguments based on analytical weak coupling renormalization group applied to saddle points located not at TRIM, close to type-II vHs, point to a spin-triplet odd-parity superconducting state [15, 16].

In order to provide a most substantiated analysis of the superconducting instabilities, we apply a combined effort of RPA and FRG. For the problem at hand, we find that all approaches we have used reach the same conclusion on the nature of the superconducting state. Since the FRG tracks vertex corrections and treats all instability channels on equal footing, we choose to discuss the FRG results in the main text, and defer the confirming evidence from RPA to the supplement [17]. Within FRG,
we formulate a set of coupled integro-differential equations which describes a two-particle vertex flow equation $V_\Lambda$ where the temperature flow parameter $\Lambda$ corresponds to the cutoff parameter that evolves from high energies towards the Fermi level [24, 25]. Within the patch-FRG we employ here, the two-particle vertex is projected to the Fermi level, and discretized into $N = 96$ patches. The initial condition for the $96^3 \sim 8.8 \times 10^5$-dimensional system of integro-differential equations is given by the many-body interaction $U$. In order to further improve the numerical performance, we consider the HSE ab-initio band structure without SOC in order to exploit full SU(2) symmetry, and obtain the spin triplet and singlet sectors by vertex antisymmetrization and symmetrization, respectively. This approximation is justified for the case of jacutingaite. As already hinted at in Fig. 2a and carefully checked by us, the SOC term predominantly serves to open a band gap, but hardly affects the Fermi surface dispersion and eigenstates at the electron and hole doped van Hove levels. A minor difference is given for the precise location of the saddle points along the $\textbf{K} - \textbf{M}$ lines for the type-II vHs, or the degree of warping for the type-I vHs. Facing the choice between enhanced radial resolution via more patches and tracking those minor differences in terms of SOC-inclusive Fermiology, we find it preferable to keep maximal radial resolution.

Within FRG, the renormalized interaction $V_\Lambda$ starts to diverge in some channel as the infrared cutoff $\Lambda$ approaches the Fermi surface; this marks the onset of a leading instability, which we subsequently analyze within mean field theory [20]. The FRG procedure adjusted to Fermi surface instabilities of interacting fermions allows for an equal treatment of all possible 2-particle instabilities, which is an immediate advantage in comparison to RPA where the procedure is constrained to only a single 2-particle channel of interest, such as particle-particle or particle-hole. While the precise validity range of FRG in terms of interaction strength still cannot be rigorously specified, it provides numerical guidance to model interacting electron systems at intermediate coupling. Fig. 4 shows that when the chemical potential locates nearby the type-I vHs, the effective interaction $V_\Lambda$ diverges in the even-parity spin-singlet superconducting channel. Its two degenerate order parameters $d_{xy}$ and $d_{x^2-y^2}$ transform as the two-dimensional $E_g$ irreducible representation of $D_{3d}$, the point group of the buckled honeycomb structure. The gap functions $\Delta_{d_{xy}}$ and $\Delta_{d_{x^2-y^2}}$ both have line nodes along the Fermi surface (form factors depicted in Fig. 4). As evident from a subsequent mean field treatment, the system gains condensation energy below the instability level by removing the nodes via complex superposition $d_{xy} \pm id_{x^2-y^2}$ (inset of Fig. 4), a manifestation of spontaneous time reversal symmetry breaking. As a subleading pairing channel, $f$-wave pairing emerges, which is also observed within RPA [17].

When the chemical potential is shifted to the type-II vHs, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is dominated by ferromagnetic $\text{vH}_s$, the Fermi surface is marked by a wave state (Fig. 4b). Again, RPA calculations are consistent with FRG in this setting [17].

Conclusions – We have identified monolayer jacutingaite as a promising host not only for a quantum spin Hall phase at pristine filling [13], but also for unconventional superconductivity at van Hove level for electron and hole doping. The type-I vHs is reached upon doping by 0.39 holes, which corresponds to about 9.8% hole doping. For the type-II vHs, even only 4.0% electron doping ($\sim 0.16$ electrons) is needed, a value that in principle may even already be achieved by electrolytic gating. In addition to the interest generated due to its inherently exotic nature, the high experimental feasibility of possibly accomplishing a type-II van Hove level without chemical doping is a highly appealing feature of monolayer jacutingaite. Note that, for instance, several attempts were made to dope graphene to the vHs point by Ca and K adsorbates [27]. Notwithstanding the efforts, so far no evidence of superconductivity was reported. Conversely, the

![Figure 4.](image-url)
rather small amount of doping needed to reach the type-II vHs renders jacutingaita a promising material candidate to realistically achieve unconventional superconductivity in a doped quantum spin Hall insulator.

We thank A. Marrazzo and G. Sangiovanni for discussions. This work was supported by the DFG through SFB1170 "Tocotronics" (project B04) and by ERC-StG-336012-Thomale-TOPOLECTRICS. We gratefully acknowledge the Gauss Centre for Supercomputing e.V. (www.gauss-centre.eu) for funding this project by providing computing time on the GCS Supercomputer SuperMUC at Leibniz Supercomputing Centre (www.lrz.de).

[1] C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 146802 (2005).
[2] B. A. Bernevig, T. L. Hughes, and S.-C. Zhang, Science 314, 1757 (2006).
[3] M. Sigrist and K. Ueda, Rev. Mod. Phys. 63, 239 (1991).
[4] A. P. Schnyder, S. Ryu, A. Furusaki, and A. W. W. Ludwig, Phys. Rev. B 78, 195125 (2008).
[5] L. Fu and C. L. Kane, Phys. Rev. Lett. 100, 096407 (2008).
[6] J. D. Sau, R. M. Lutchyn, S. Tewari, and S. Das Sarma, Phys. Rev. Lett. 104, 040502 (2010).
[7] R. M. Lutchyn, J. D. Sau, and S. Das Sarma, Phys. Rev. Lett. 105, 077001 (2010).
[8] Y. Oreg, G. Refael, and F. von Oppen, Phys. Rev. Lett. 105, 177002 (2010).
[9] Y. Nakajima, R. Hu, K. Kirshenbaum, A. Hughes, P. Syers, X. Wang, K. Wang, R. Wang, S. R. Saha, D. Pratt, J. W. Lynn, and J. Paglione, Science Advances 1, e1500242 (2015).
[10] Y. S. Hor, A. J. Williams, J. G. Checkelsky, P. Roushan, J. Seo, Q. Xu, H. W. Zandbergen, A. Yazdani, N. P. Ong, and R. J. Cava, Phys. Rev. Lett. 104, 057001 (2010).
[11] B. Yan, M. Jansen, and C. Felser, Nat. Phys. 9, 709 (2013).
[12] G. Li, B. Yan, R. Thomale, and W. Hanke, Sci. Rep. 5, 10435 (2015).
[13] V. Fatemi, S. Wu, Y. Cao, L. Bretheau, Q. D. Gibson, K. Watanabe, T. Taniguchi, R. J. Cava, and P. Jarillo-Herrero, ArXiv:1809.04637 (2018).
Supplemental material for "Unconventional superconductivity in a doped quantum spin Hall insulator"

**TYPE I AND TYPE II VAN HOVE SINGULARITIES FROM LONG RANGE HOPPING**

Neglecting spin-orbit coupling and considering long range hopping terms, the Hamiltonian matrix of our effective model for the buckled honeycomb lattice is given by

\[
H_0^J = \begin{pmatrix} H_{AA} & H_{AB} \\ H_{BA} & H_{BB} \end{pmatrix},
\]

where \(A/B\) refers to the sublattice index. The matrix elements of the Hamiltonian with up to 4th nearest neighbor hopping are

\[
H_{AB} = t_1(e^{\frac{i k_x a_0}{\sqrt{3}} a_0} + 2e^{\frac{i k_y a_0}{\sqrt{3}} a_0} \cos \frac{2 k_y a_0}{2} + t_3(e^{\frac{-i k_x a_0}{\sqrt{3}} a_0} + 2e^{\frac{-i k_y a_0}{\sqrt{3}} a_0} \cos \frac{3 k_y a_0}{2}),
\]

\[
H_{BA} = H_{AB},
\]

\[
H_{AA} = t_2(2 \cos k_y a_0 + 4 \cos \frac{\sqrt{3}}{2} k_x a_0 \cos \frac{1}{2} k_y a_0).
\]

Here, \(t_2\) denotes an intra-sublattice and \(t_{1,3,4}\) inter-sublattice hopping integrals. As the \(t_2\) term breaks chiral symmetry, the spectrum is asymmetric with respect to half filling. If one were to consider only inter-sublattice hopping, the energy spectrum would exhibit a chiral symmetry; the \(t_2\) term, however, is diagonal in the sublattice space, and hence imposes a \(k\) dependent energy shift for the spectrum. As a consequence of such a shift, the spectrum becomes asymmetric with respect to half filling. When only the NN hopping is included, the Fermi surface develops a perfect hexagonal shape when the Fermi level is exactly at the van Hove singularity point. The saddle point is located at the time reversal invariant momentum, and the corresponding vHs point is dubbed type-I. If the saddle point is not at the time reversal invariant momentum, the corresponding vHs point is called type-II.

Along the K-M line, i.e. for \(k_x = \frac{2 \pi}{\sqrt{3} a_0}\), the elements of the Hamiltonian are

\[
H_{AB} = h t_1 + h t_3 + h t_4,
\]

\[
H_{AA} = H_{BB} = h t_2,
\]

\[
h t_1 = t_1 e^{\frac{2i \pi}{3}} f_1(k) = t_1 e^{\frac{2i \pi}{3}} (1 - 2 \cos \frac{2 k_y a_0}{2}),
\]

\[
h t_2 = t_2 f_2(k) = t_2(2 \cos k_y a_0 - 4 \cos \frac{1}{2} k_y a_0),
\]

\[
h t_3 = t_3 e^{\frac{2i \pi}{3}} f_3(k) = t_3 e^{\frac{2i \pi}{3}} (2 \cos k_y a_0 + 1),
\]

\[
h t_4 = t_4 e^{-\frac{i \pi}{3}} f_4(k) = t_4 e^{-\frac{i \pi}{3}} (\cos \frac{3 k_y a_0}{2} - \cos k_y a_0 + \cos \frac{3 k_y a_0}{2}).
\]

At the M (\(\frac{2 \pi}{\sqrt{3} a_0},0\)) point, we have \(H_{AB} = (-t_1 + 3 t_3 - 2 t_4) e^{\frac{2i \pi}{3}}\) and \(H_{AA/BB} = -2 t_2\). At the K-\(\left(\frac{2 \pi}{\sqrt{3} a_0}, \frac{2 \pi}{\sqrt{3} a_0}\right)\) point instead, \(H_{AB} = 0\) and \(H_{AA/BB} = -3 t_2\). In a monolayer of jacutingaite, \(t_{1,3,4} > 0\) and \(t_4 < 0\), such that \(t_3/t_4\) will partly compensate \(t_1\) in \(H_{AB}\), generating a flat band along the KM line (as shown in Fig. S1(b)). With an eventual inclusion of the \(t_2\) term, we end up with a type-II VHS point in the conduction band and a type-I VHS point in the valence band, as shown in Fig. S1(c).

**FIRST-PRINCIPLES DFT CALCULATIONS**

First-principles calculations were performed by using the projector augmented plane wave method as implemented in the Vienna Ab-initio Simulation Package (VASP) [1]. We adopt both the PBE [2] as well as the Heyd-Scuseria-Emznerhof (HSE) hybrid functional [3] for the exchange-correlation part, while SOC has been included self-consistently in a scalar-relativistic scheme. We use a plane wave cutoff of 600 eV on a 12×12×1 Monkhorst-Pack k-point mesh. The projection onto maximally localized wannier functions was achieved via the WANNIER90 package [4].
Fig. S1. (color online) Band structures related to S1. (a) with only NN hopping $t_1$, (b) with hopping $t_1$, $t_3$ and $t_4$, (d) with all hoppings up to 4th NN.

Fig. S2. RPA pairing strengths as a function of $U$ at (a) type-I van Hove filling and (b) type-II van Hove filling.

RPA Calculations

We perform RPA calculations by following those described in Refs. [5, 6]. The pairing strengths of the dominant pairing states as a function of interaction at type-I and type-II VHS points are displayed in Fig. S2(a) and (b), respectively. At the type-I vHs point, $d + id$ pairing state is the most dominant one for $0.4 \leq U \leq 0.6$ eV due to the strong antiferromagnetic fluctuations from Fermi surface nesting, and competes strongly with the singlet $s-$wave and $f-$wave instabilities depending on the interaction strength. At the type-II vHs point, there is no Fermi surface nesting, and $f_{y^3-3yx^2}$ wave pairing state is the most dominant due to the ferromagnetic fluctuations. The gap functions of $E_{2g}$ and $A_{2u}$ states are shown in Fig. S3. The findings are consistent with the FRG results presented and discussed in the main text.

Fig. S3. RPA gap functions of the most dominant pairing states at type-I and type-II van Hove filling: (a) $E_{2g}(d_{x^2-y^2})$, (b) $E_{2g}(d_{xy})$; (c) $A_{2u}(f_{y^3-3yx^2})$. 

[1] G. Kresse and J. Furthmüller, Phys. Rev. B 54, 11169 (1996).
[2] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1996).
[3] J. Heyd, G. E. Scuseria, and M. Ernzerhof, J. Chem. Phys. 121, 1187 (2004).
[4] A. A. Mostofi et al., Comput. Phys. Commun. 178, 685 (2008).
[5] S. Graser, T. A. Maier, P. J. Hirschfeld and D. J. Scalapino, New J. Phys., 11, 025016 (2009)
[6] N. E. Bickers, D. J. Scalapino and S. R. White, Phys. Rev. Lett., 62 961 (1989)