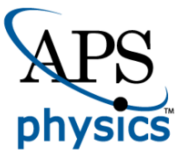

Topological superconducting phase and Majorana fermions in half-metal/superconductor heterostructures

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Topological superconductivity and Majorana fermions in half-metal / superconductor heterostructure

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As a half-metal is spin-polarized at its Fermi level by definition, it was conventionally thought to have little proximity effect to an s-wave superconductor. Here we show that with interface spin-orbit coupling $p_x + ip_y$ superconductivity without spin degeneracy is induced on the half-metal, and we give an estimate of its bulk energy gap. Therefore a single-band half-metal can give us a topological superconductor with a single chiral Majorana edge state. Our band calculation shows that two atomic layers of VTe or CrO_2 is a single-band half-metal for a wide range ($\sim$0.1eV) of Fermi energy and thus is a suitable candidate material.

Introduction: Possibility of Majorana fermions arising out of condensed matter system has aroused great interest in recent years[1]. One class of systems where Majorana fermions can appear is the two-dimensional (2D) chiral superconductor which has a full pairing gap in the bulk, and $\mathcal{N}$ gapless chiral one-dimensional (1D) states, which consists of Majorana fermions[2,3], at the edge. In a $\mathcal{N} = 1$ chiral topological superconductor (TSC), a single Majorana zero mode is bound to a vortex core[3–5], giving rise to non-Abelian statistics which can be potentially useful for topological quantum computation[6]. The most straightforward way to realize such a chiral TSC is the intrinsic $p_x + ip_y$ superconductivity in spinless fermions[3]. The strongest candidate material for this superconductivity, albeit a spinful version, is Sr_2RuO_4[7], but the experimental situation is not definitive[8]. Recently, there has been alternative proposals involving inducing s-wave superconductivity in material with strong spin-orbit coupling through proximity effect[9–17]. It was pointed out in one of the proposals[11] that spin polarized $p_x + ip_y$ superconductor can be obtained in a ferromagnetic film through proximity to a superconductor. In this Rapid Communication, we further develop this line of approach and demonstrate through explicit calculations the feasibility of creating Majorana fermions in a half metal / conventional s-wave superconductor heterostructure.

We consider the pair formation on a half-metal (HM) that is in proximity contact to an s-wave superconductor (SC). A HM, by definition, is spin-polarized at the Fermi surface[18], *i.e.* it is a metal for the majority-spin and an insulator for the minority-spin. Our proposal has two major advantages over other current proposals. One is that our proposal does not require any fine-tuning of the Fermi level. The other is that, due to better Fermi surface matching, we expect more robust proximity effect between SC and HM than between SC and semiconductor. It has been known that at the normal metal to s-wave SC interface, p-wave pairing can be induced due to broken inversion symmetry[19]. Eschrig *et al.* showed that when normal metal is HM, even frequency pairing would be mostly p-wave[20]. Furthermore, there are experimental indications of strong proximity effect between a HM and an s-wave superconductor[21,22]. Here we will show how we can obtain $p_x + ip_y$ pairing symmetry in a 2D HM when it is coupled to an s-wave superconductor only through electron hopping across the interface. If the 2D HM has a single Fermi pocket without spin degeneracy, such $p_x + ip_y$ pairing will give us the TSC with $\mathcal{N} = 1$. We will show band calculation for thin film material that is HM and has a single Fermi pocket. We will also discuss the suitable superconductor for optimizing this proximity effect and the method we can use for detecting the $p_x + ip_y$ pairing in the HM.

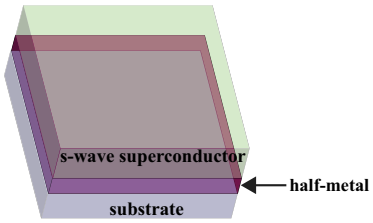

FIG. 1. The heterostructure for obtaining $p_x + ip_y$ superconductivity. The half-metal layer has a 2D electronic structure with a single Fermi surface without spin degeneracy. It is coupled to the s-wave superconductor through hopping. The substrate stabilizes the half-metal crystal structure without affecting qualitatively its electronic structure.

Basic Model: We consider the model with a bulk s-wave superconductor and a 2D half-metal coupled by a weak hopping between two systems:

$$\mathcal{H} = \mathcal{H}_{SC} + \mathcal{H}_{HM} + \mathcal{H}_t \tag{1}$$

where

$$\begin{aligned}\mathcal{H}_{SC} &= \sum_{\mathbf{k},\sigma}(\epsilon'_{\mathbf{k}} - \mu')c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}}(\Delta'_{\mathbf{k}}c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow} + \text{h.c.}),\\ \mathcal{H}_{HM} &= \sum_{\mathbf{k}_\parallel}(\epsilon_{\mathbf{k}_\parallel} - \mu)f^\dagger_{\mathbf{k}_\parallel\uparrow}f_{\mathbf{k}_\parallel\uparrow},\\ \mathcal{H}_t &= \sum_{\mathbf{k}\sigma}(t_{\mathbf{k},\uparrow\sigma}f^\dagger_{\mathbf{k}_\parallel\uparrow}c_{\mathbf{k}\sigma} + \text{h.c.});\end{aligned} \tag{2}$$

note that $\mathbf{k}_\parallel$ is the in-plane projection of $\mathbf{k}$ and the spin quantization axis is along the normal direction. This model provides a general mechanism for SC proximity effect in the clean interface limit, where $\mathbf{k}_\parallel$ is conserved in the hopping process. This model allows for both spin-conserving and spin-flip hopping.

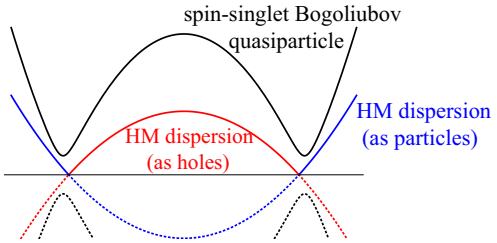

FIG. 2. A schematic representation of the HM and SC bands for weak hopping. Two HM bands are due to the artificial doubling of degrees of freedom in the Bogoliubov-de Gennes formalism. In this formalism, the pairing amplitude and gap require hybridization of the 'particle' and 'hole' bands, which is due to the interface hopping in our model.

In this model, the symmetry of the pairing correlation on the half-metal side, $\langle f_{-\mathbf{k}_\parallel\uparrow} f_{\mathbf{k}_\parallel\uparrow}\rangle$, is determined entirely by $t_{\mathbf{k},\uparrow\sigma}$. In this model, the only channel for this Cooper pair formation is to have the HM electrons with momenta $\mathbf{k}_\parallel$ and $-\mathbf{k}_\parallel$ hop to the SC to form a pair there. This process requires that hopping flips the spin of either one of the $\mathbf{k}_\parallel$ and $-\mathbf{k}_\parallel$ electrons. Since the Cooper pair on the SC side is in the spin-singlet s-wave state, the two processes interfere destructively, giving us

$$\langle f_{-\mathbf{k}_\parallel\uparrow} f_{\mathbf{k}_\parallel\uparrow}\rangle \propto t_{\mathbf{k}_\parallel,\uparrow\uparrow} t_{-\mathbf{k}_\parallel,\uparrow\downarrow} - t_{-\mathbf{k}_\parallel,\uparrow\uparrow} t_{\mathbf{k}_\parallel,\uparrow\downarrow} \tag{3}$$

with an s-wave multiplicative factor when there is no $k_\perp$ dependence; note the odd spatial parity. In the limit of weak hopping, $|t_{\mathbf{k},\uparrow\sigma}| \ll |\Delta'_{\mathbf{k}}|$, we find the pairing amplitude at the HM Fermi surface (where $\epsilon_{\mathbf{k}_\parallel} = \mu$) to be[23]

$$\langle f_{-\mathbf{k}_\parallel\uparrow} f_{\mathbf{k}_\parallel\uparrow}\rangle \approx \frac{1}{2}\left\langle \frac{\eta_{\mathbf{k}}}{\sqrt{|\eta_{\mathbf{k}}|^2 + |\zeta_{\mathbf{k}}|^2}} \right\rangle_{k_\perp}, \tag{4}$$

where $\mathbf{k} = (\mathbf{k}_\parallel, k_\perp)$, $\langle\cdots\rangle_{k_\perp}$ is averaging over $k_\perp$, and

$$\begin{aligned}\eta_{\mathbf{k}} =& (t_{\mathbf{k},\uparrow\uparrow} t_{-\mathbf{k},\uparrow\downarrow} - t_{\mathbf{k},\uparrow\downarrow} t_{-\mathbf{k},\uparrow\uparrow})\langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}\rangle|_{\epsilon_{\mathbf{k}_\parallel}=\mu},\\ \zeta_{\mathbf{k}} =& \frac{|t_{\mathbf{k},\uparrow\uparrow}|^2 + |t_{\mathbf{k},\uparrow\downarrow}|^2}{2}[(\epsilon'_{\mathbf{k}} - \mu')/E'_{\mathbf{k}}]_{\epsilon_{\mathbf{k}_\parallel}=\mu}\end{aligned} \tag{5}$$

with $E'_{\mathbf{k}} = \sqrt{(\epsilon'_{\mathbf{k}} - \mu')^2 + |\Delta'_{\mathbf{k}}|^2}$ ($|t_{\mathbf{k},\uparrow\sigma}|^2 = |t_{-\mathbf{k},\uparrow\sigma}|^2$ assumed). Eqs. (4) and (5) tell us that if the Fermi surfaces of the HM and the SC match exactly for all values of $k_\perp$ (*i.e.* $\epsilon'_{\mathbf{k}} = \mu'$ when $\epsilon_{\mathbf{k}_\parallel} = \mu$), we have $\langle f_{-\mathbf{k}_\parallel\uparrow} f_{\mathbf{k}_\parallel\uparrow}\rangle = e^{i\phi_{\mathbf{k}}}\langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}\rangle$ at the HM Fermi surface, with $e^{i\phi_{\mathbf{k}}}$ being the phase factor of $t_{\mathbf{k},\uparrow\uparrow} t_{-\mathbf{k},\uparrow\downarrow} - t_{\mathbf{k},\uparrow\downarrow} t_{-\mathbf{k},\uparrow\uparrow}$, . Physically, $\eta_{\mathbf{k}}$ is proportional to the amplitude that the $\mathbf{k}_\parallel$ and $-\mathbf{k}_\parallel$ HM electrons hop to the s-wave SC with opposite spins and form a Cooper pair, while $\zeta_{\mathbf{k}}$ is proportional to the amplitude that these electrons hop to the SC with their spins aligned and do not form a Cooper pair.

Our model gives us not only the pairing amplitude but also the pairing gap on the HM side. In the weak hopping limit we have been discussing, we obtain

$$\Delta^{HM}_{\mathbf{k}} = \left\langle \frac{\eta_{\mathbf{k}}}{E'_{\mathbf{k}}} \right\rangle_{k_\perp} = \left\langle \frac{t_{\mathbf{k},\uparrow\uparrow} t_{-\mathbf{k},\uparrow\downarrow} - t_{\mathbf{k},\uparrow\downarrow} t_{-\mathbf{k},\uparrow\uparrow}}{2E'^2_{\mathbf{k}}} \Delta'_{\mathbf{k}} \right\rangle_{k_\perp} \tag{6}$$

at the HM Fermi surface[23]. Note here that $|\Delta'_{\mathbf{k}}|$ is maximized when we have a perfect Fermi surface matching between the HM and the SC. Eq.(6) tells us that we have an energy gap in the HM due to the proximity induced electron pairing of Eq.(4) because the HM is in the 2D limit[24,25]. Therefore, the topological property of SC induced in the HM is determined entirely by $t_{\mathbf{k},\uparrow\sigma}$.

In the limit of strong hopping, we obtain a much larger pairing gap while Eq.(3) still holds. Our strong hopping limit requires at the HM Fermi surface, the energetics is dominated by the spin-conserving hopping $t_{\mathbf{k},\uparrow\uparrow}$, *i.e.* $|t_{\mathbf{k},\uparrow\uparrow}| \gg E'_{\mathbf{k}}$ and $|t_{\mathbf{k},\uparrow\uparrow}| \gg |t_{\mathbf{k},\uparrow\downarrow}|$. Within this model, at the HM Fermi surface, the pairing amplitude is still given by Eq.(4), while the pairing gap now[23]

$$\Delta^{HM}_{\mathbf{k}} = \left\langle \frac{\eta_{\mathbf{k}} E'_{\mathbf{k}}}{|t_{\mathbf{k},\uparrow\uparrow}|^2} \right\rangle_{k_\perp} = \left\langle \frac{t_{\mathbf{k},\uparrow\uparrow} t_{-\mathbf{k},\uparrow\downarrow} - t_{\mathbf{k},\uparrow\downarrow} t_{-\mathbf{k},\uparrow\uparrow}}{2|t_{\mathbf{k},\uparrow\uparrow}|^2} \Delta'_{\mathbf{k}} \right\rangle_{k_\perp} \tag{7}$$

The above HM pairing gap is much larger than that of Eq.(6); note that in Eq.(7), Δ^{HM} is proportional to $t_{\uparrow\downarrow}/t_{\uparrow\uparrow}$, while in Eq.(6), it is proportional to $t_{\uparrow\downarrow} t_{\uparrow\uparrow}/E'^2$.

Interface hopping: To show how the $p_x + ip_y$ pairing arises in this proximity effect, we first discuss the interface spin-orbit coupling (SOC) giving chiral $\mathbf{k}_\parallel$-odd contribution to $t_{\mathbf{k},\uparrow\downarrow}$. We note that, at the bulk HM / bulk SC interface, there is Rashba SOC due to broken inversion symmetry[11,19]: $\mathcal{H}_{SOC} = \hbar\alpha(\boldsymbol{\sigma}\times\mathbf{k})\cdot\hat{\mathbf{n}}\delta(\hat{\mathbf{n}}\cdot\mathbf{r})$, where $\hat{\mathbf{n}}$ is the interface normal. The analogue of this SOC in our model should be contained in $\mathcal{H}_t$, as it affects only electrons whose wave functions extends across the interface. Also, it should contribute to spin-flip hopping for nonzero $\mathbf{k}_\parallel$, as the HM is spin-polarized along the interface normal. Such a hopping term, with the symmetry of the Rashba SOC, needs to be in the form

$$\mathcal{H}_{t-SOC} = t_{SOC}\sum_{\mathbf{k}} F^\dagger_{\mathbf{k}_\parallel}(\sigma^x \sin k_y a - \sigma^y \sin k_x a) C_{\mathbf{k}} + \text{h.c.}, \tag{8}$$

where $F_{\mathbf{k}} = (f_{\mathbf{k}_\parallel\uparrow}, f_{\mathbf{k}_\parallel\downarrow})^T$ and $C_{\mathbf{k}} = (c_{\mathbf{k}\uparrow}, c_{\mathbf{k}\downarrow})^T$. However, the terms involving $f_{\mathbf{k}_\parallel\downarrow}$ can be projected out due to the HM minority-spin gap, leaving only the $t_{\mathbf{k},\uparrow\downarrow}$ term.

We can now show explicitly how we obtain the $p_x + ip_y$ pairing from $t_{\mathbf{k},\uparrow\sigma}$. For this we take the $t_{\mathbf{k},\uparrow\downarrow}$ obtained above and set $t_{\mathbf{k},\uparrow\uparrow}$ to be momentum-independent:

$$\begin{aligned} t_{\mathbf{k},\uparrow\uparrow} =& t_0\\ t_{\mathbf{k},\uparrow\downarrow} =& t_{SOC}(i\sin k_x a + \sin k_y a).\end{aligned} \tag{9}$$

Inserting this into Eq.(3) gives us the chiral p-wave pairing on the HM side:

$$\begin{aligned}\langle f_{-\mathbf{k}_\parallel\uparrow} f_{\mathbf{k}_\parallel\uparrow}\rangle &\propto t_{\mathbf{k}_\parallel,\uparrow\uparrow} t_{-\mathbf{k}_\parallel,\uparrow\downarrow} - t_{-\mathbf{k}_\parallel,\uparrow\uparrow} t_{\mathbf{k}_\parallel,\uparrow\downarrow}\\ &= -2it_0 t_{SOC}(\sin k_x a - i\sin k_y a).\end{aligned} \tag{10}$$

We can see from the real space representation that Eq.(9) is a physically reasonable hopping. Assuming that the HM electrons can hop only to the top layer of the SC and we have a square lattice, the dominant hopping is the $t_{\mathbf{k},\uparrow\uparrow}$ of Eq.(9) - $t_0\sum_i f^\dagger_{i\uparrow} c_{i\uparrow}$ + h.c. Therefore the pairing symmetry Eq.(3) will be determined by

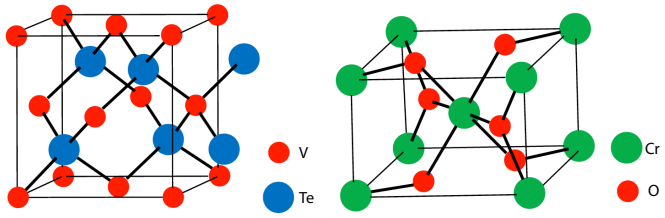

FIG. 3. Crystal structures of two candidate materials, VTe and CrO_2.The left shows the zinc blende crystal structure of bulk VTe. Here, both V and Te forms body-centered cubic with the lattice constant of $a = 0.6271$nm ($a = 0.6202$nm for zb-CrTe). The left shows the rutile crystal structure of bulk CrO_2, where $a = 0.4421$nm, $c = 0.2916$nm. The distance between the nearest O and Cr on the same layer is 0.1817nm.

the largest spin-flip hopping with odd spatial symmetry, and that should of the 'nearest neighbor' type, *i.e.* $\sum_{\delta\mathbf{r}_\parallel/a=\pm\hat{\mathbf{x}},\pm\hat{\mathbf{y}}} t_{\delta\mathbf{r}_\parallel} f^\dagger_{i\uparrow} c_{i+\delta\mathbf{r}_\parallel,\downarrow} + \text{h.c.}$, where $t_{-\delta\mathbf{r}} = -t_{\delta\mathbf{r}}$. This hopping can be expressed as a sum of the Rashba-like $t_{\mathbf{k},\uparrow\downarrow}$ of Eq.(9), and of a Dresselhaus-like term; however, the chirality of Eq.(10) is maintained unless the Dresselhaus-like and the Rashba-like terms are equal in magnitude. Therefore, the topological property of this p-wave pairing is robust against any small modification to the hopping term. Eq.(9) gives us the $\mathcal{N} = 1$ TSC in the strong hopping limit as well as the weak hopping limit[23]. We also note that the $p_x + ip_y$ is considered to be the likely pairing symmetry for intrinsic SC in a HM[26].

From the origin of the interface SOC, we can estimate of the HM pairing gap to be

$$|\Delta^{HM}| \sim |\Delta'|(\alpha_{SOC}/W), \tag{11}$$

where α_{SOC} is the Rashba SOC of the s-wave SC and W is the bandwidth. Physically, when SOC is strong for the s-wave SC but weak for the HM, we can expect to have the interface SOC. This situation is experimentally relevant because s-wave SC can exist in materials with strong SOC, while the spin-polarized ARPES indicates complete spin polarization for the HM, as in CrO_2[27]. Assuming that we have zero effective SOC on the HM, we will effectively have the spin-orbit coupling hopping $t_{SOC} \sim (\alpha_{SOC}/W)t_0$ induced through second order perturbation. This is sufficient for estimating $|\Delta^{HM}|$, because, in the strong hopping limit, we find $\Delta^{HM} \sim (t_{SOC}/t_0)\Delta'$ by inserting Eq.(10) into Eq.(7).

We also point out that this HM/SC proximity effect can provide us with a means to obtain a multi-domain chiral p-wave SC. Eqs.(8) and (9) show us that if we reverse the HM spin polarization, than we will also reverse the chirality of the induced SC. Therefore in a HM, a domain boundary between opposite spin polarization will also be the domain boundary between the $p_x + ip_y$ and $p_x - ip_y$ domain when SC is induced.

Candidate material: We note that the spin-polarized (or single-spin) $p_x + ip_y$ SC with a single Fermi pocket gives us the $\mathcal{N} = 1$ TSC[3], but the same cannot be said for the $p_x + ip_y$ SC with multiple Fermi pockets[28,29]. Therefore to obtain the $\mathcal{N} = 1$ TSC, it is important that we

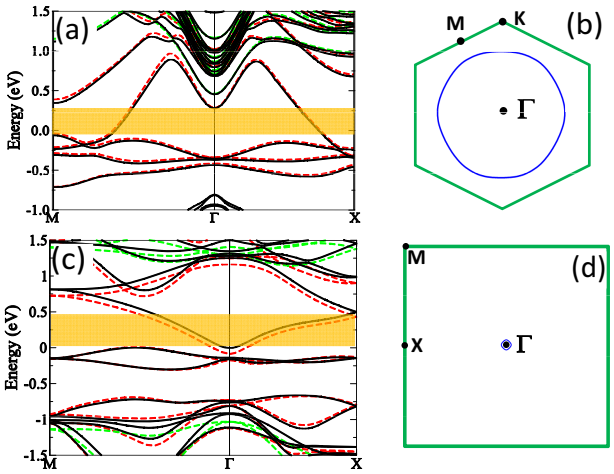

FIG. 4. (Color online) (a) The band structure of the VTe-ZnTe(111) model. There is no spin degeneracy in these bands; the red (darker gray) and the green (gray) dotted curve shows the spin-up and -down bands when SOC is absent. The region shaded in orange (lighter gray) shows the energy range for which we obtain a single Fermi pocket. (b) The single Fermi surface at the energy level 0.0eV for ZnTe-VTe(111) model. The green (gray) box shows the first Brillouin zone(BZ). (c) The band structure of the CrO_2 (001) model. (d) The single Fermi surface around the Γ point at the energy level 0.01eV for the CrO_2 (001) model, the green (gray) box showing the 1st BZ.

find a 2D HM with a single Fermi pocket, as we have in Eq.(2). That way, the HM / SC proximity effect we discussed will give us an equivalent of the single-spin $p_x + ip_y$ SC with a single Fermi pocket. However, applying the Luttinger's theorem to HM tells us that, in order to have a single Fermi pocket, we need a fractional number of electrons per unit cell.

One candidate material for a 2D HM with a single Fermi pocket is the zinc blende VTe or CrTe that is two atomic layers thick in the (111) direction. We identified candidate material through *ab-initio* band calculations performed in the frame of density-functional theory[30,31] with the plane-wave pseudopotential method[23]. Both VTe and CrTe in the zinc blende structure have been shown to be HM in band calculation[32]; a thin film of the zinc blende CrTe has been fabricated in thin films by molecular-beam epitaxy[33]. As we see in Fig. 4, two atomic layers of zinc blende VTe (111) on the zinc blende ZnTe substrate is a single Fermi pocket HM at 0eV. This is due to a charge transfer mechanism[23] that gives us one-half electrons per unit cell; there are analogous previous examples[34,35]. As we have a 0.3eV range for the Fermi level that gives us a single Fermi pocket, unlike in many of the previous proposals for obtaining the $\mathcal{N} = 1$ TSC[12] we do not require fine-tuning of the HM Fermi level. CrTe has a single Fermi pocket for a narrower Fermi level range (≈ 0.06eV).

We also point out that the CrO_2 film that is two atomic layers thick in the (001) direction comes close to fulfilling our requirement. Bulk CrO_2 has been experimentally

confirmed to be HM[27,36], and it was also shown in experiment to have a strong proximity effect to an s-wave SC - NbTiN - that has a relatively high T_c (~ 14K) and a spin-orbit coupling larger than the SC gap. Since the width of bands near Fermi level for NbN is about 7.2eV[37] and the atomic spin-orbit coupling of Nb is 0.1eV[38], a pairing gap up to $\sim$1K can be estimated from Eq.(11). The bulk CrO_2 crystal, as shown in Fig. 3, has a rutile structure[39]. The band calculation for two atomic layer of CrO_2 (001) in a perfect rutile structure gives us a single Fermi pocket HM when we raise the Fermi level by 0.01 eV (though at 0eV there are additional Fermi pockets)[23]. For a Fermi level range of $\sim$ 0.5eV, this material is a single Fermi pocket HM.

Detection: Detecting a single chiral Majorana edge state along with the fully gapped quasiparticle spectrum in the bulk of the HM will confirm that we have $\mathcal{N} = 1$ TSC in the HM. When a large enough $|\Delta^{HM}|$, one direct method would be detecting with STM a zero bias peak only at the edge or along the HM domain boundary[22,40]. The chiral Majorana state can also be detected from transport experiments[41,42].

In summary, we have shown that we can obtain the $\mathcal{N} = 1$ TSC in a HM through proximity effect with an s-wave SC. In a model where the HM is coupled to the SC through hopping, the symmetry of SC pairing induced in the HM is determined entirely by the hopping term. Due to the interface Rashba spin-orbit coupling, the hopping term will induce the pairing with $p + ip$ symmetry. In order for this $p_x + ip_y$ pairing to lead to the $\mathcal{N} = 1$ TSC, we need to have a HM with single Fermi surface, and our band calculation shows that this can be obtained for a very thin CrO_2 film. STM measurement can be used to verify that TSC is induced in the HM.

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