Remote control of spin-polarized topological corner states by a local electric potential

Yinong Zhou\textsuperscript{1} and Ruqian Wu\textsuperscript{1}\textsuperscript{a}

\textsuperscript{1}Department of Physics and Astronomy, University of California, Irvine, California 92697-4575, USA

(Dated: March 15, 2022)

In higher-order topological insulators, the lower-dimensional boundary states are separated by a non-negligible distance. Interestingly, the crystalline symmetries protect the robustness of their higher-order corner or hinge states with long-range entanglement. Here, we demonstrate the possibility of direct control of the topological corner states by introducing the spin degree of freedom in a two-dimensional rhombus-shaped Kekulé nanostructure with local magnetization and electric potential. By applying a local electric potential on one corner, the spin polarization can be reversed on both corners, along with a phase transition from the antiferromagnetic to ferromagnetic order. We also propose a material realization using a $\gamma$-graphyne nanostructure with the first-principles calculations. Our studies give a showcase of the remote correlation of quantum states in higher-order topological materials and open a door for the development of spintronic and quantum applications.

Research interest in topological insulators (TIs) \textsuperscript{1} has been extremely high as they host gapless edge or surface states, which are robust against defects and disorders \textsuperscript{2–5}. Recently, the proposal of the electric multipole insulators \textsuperscript{6} led to a new class of topological materials, so-called higher-order topological insulators (HOTIs) \textsuperscript{7–13}, which show lower-dimensional corner or hinge states within the edge or surface gap. Several 2D lattices have been proposed for the realization of the HOTI phase, including square lattice \textsuperscript{14–16}, breathing Kagome lattice \textsuperscript{14, 15}, Kekulé lattice \textsuperscript{16–22}, and non-periodic quasicrystals \textsuperscript{23}. The difference between the intercell and intracell hopping parameters drives these systems into a higher-order topological phase by opening a topological gap for edge or surface states and generating more localized corner or hinge states. Unlike the conventional bulk-edge correspondences \textsuperscript{24} in 2D TIs, the higher-order corner states manifest the bulk-corner correspondence \textsuperscript{1, 25} or the edge-corner correspondence \textsuperscript{26–27}. The robustness of corner states is protected by certain crystalline symmetries so that the higher-order topology is preserved in the presence of disorders \textsuperscript{28–31}.

In 2D TIs, the topological edge states lead to the quantum spin Hall effect (QSHE) \textsuperscript{32–34} or the quantum anomalous Hall effect (QAHE) \textsuperscript{35–38}, both are promising for applications in quantum computing and spintronic devices \textsuperscript{33, 34}. Comparatively, the potential use of the corner states in 2D HOTls has rarely been discussed. In this regard, it is essential to establish a more profound understanding of HOTI and to design possible conceptual devices for benefiting from the discovery of this new topological phase. As an attempt, the valley degrees of freedom in HOTls were discussed in sonic crystals, for which the topological corner states become valley-selective by rotating the scatterers \textsuperscript{43}. As one of the most important factors in all topological phases, it is natural to perceive that the spin degree of freedom of the topological corner states is essential for fundamental and applicational studies. The spin polarization (SP) of electrons in TIs generates chiral edge or surface states with spin-momentum interlock, leading to the QAHE \textsuperscript{35–38}. In HOTls, pseudospin-polarized corner states have been considered by introducing the artificial pseudospin degree of freedom \textsuperscript{10}. However, the study of the real-spin degree of freedom of topological corner states is still barren.

In this letter, we propose a possibility of making remote magnetoelectric control in rhombus-shaped Kekulé nanostructure, through theoretical studies using the tight-binding (TB) method with tunable local magnetization ($\lambda_z$) and local electric potential ($V$). The topological corner states of this HOTI can be magnetized by a local magnetic field, dopant, or adsorbate. Without electric manipulation, the SP at the two corners is large for the antiferromagnetic (AFM) order but is extremely small for the ferromagnetic (FM) order. By increasing $V$ at one corner, the SP is gradually enhanced at both corners for FM order and a phase transition occurs as the exchange coupling between two corners changes from AFM to FM, even the two corners are far apart. The sign of the SP is also inversed during the phase transition. Furthermore, we demonstrate the material realization using a $\gamma$-graphyne nanostructure with the first-principles calculations. The corner states are obtained, and they show identical responses to the manipulations of small $\lambda_z$ and $V$ as predicted by the TB model. When $V$ is enhanced, a large SP can also be realized. This study extends the understanding of HOTI and gives a showcase of using the topological corner states in quantum and spintronic devices.

We start from the TB model Hamiltonian for the Kekulé lattice:

$$H_0 = t_0 \sum_{\langle ij \rangle} c_i^\dagger c_j + t_1 \sum_{\langle i'j' \rangle} c_{i'}^\dagger c_{j'}.$$

Here, $c_i^\dagger$ is the operator of the electron creation on-site $i$. $\langle ij \rangle$ and $\langle i'j' \rangle$ represent the nearest-neighbor hopping for intracell ($t_0$) and intercell ($t_1$), respectively, as shown in the inset of Fig. 1(a). In order to show the topological corner states, we construct a rhombus-shaped nanostructure with an $11 \times 11$ Kekulé lattice [Fig 1(a)]. As
reported in previous studies \[10\]–\[22\], a HOTI phase is created on the Kekulé lattice when \( t_1 > t_0 \). Here, we choose \( t_1/t_0 = 1.25 \) in the following discussions. The gapped edge states and parity calculations shown in Fig. S1 and Table S1 \[44\] confirm the higher-order topology with \( Z_2 = 1 \). Discrete energy levels of the nanostructure are shown in Fig. 1(b). There is a pair of states located in the gap of the bulk and edge bands around the Fermi level, representing the bonding and antibonding corner states. The wavefunctions are evenly distributed at two corners, as shown in Fig. 1(c,d). Next, we consider the interplay between \( \lambda_z \) and \( V \) at the two 120° corner hexagons. The total Hamiltonian appears as:

\[
H_{\text{tot}} = H_0 + \lambda_z \sum_{\sigma} c_{\alpha \sigma}^\dagger (\sigma \otimes \tau_{1,2}) c_{\alpha \sigma} + V \sum_{\alpha} c_{\alpha \uparrow}^\dagger (I_2 \otimes \tau_3) c_{\alpha \uparrow},
\]

where \( \lambda_z \) represents exchange splitting, \( V \) represents electric potential, \( \sigma \) is the spin index, \( \tau_{1,2} \) is the Pauli matrix and \( I_2 \) stands for a 2×2 identity matrix. \( \tau_i \) \((i=1, 2, 3)\) represents 2×2 matrices acting on the bottom right and top left corners [Fig. 1(e,i)], where \( \tau_{1,2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \) represents FM and AFM orders and \( \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \) means that \( V \) only applies on the bottom-right corner. The SP of the corner states is defined as \( SP = | \langle \alpha_{\uparrow} | \psi \rangle |^2 - | \langle \alpha_{\downarrow} | \psi \rangle |^2 \), where \( \psi \) is the wavefunction of the corner states. We first choose parameters \( \lambda_z = 0.3t_0 \) and \( V = 0.4t_0 \) to establish the primary findings.

When \( \lambda_z \neq 0 \) and \( V = 0 \), the spin degeneracy is broken for both FM and AFM orders, as shown in Fig. 1(f). The AFM order is more stable as it has smaller total energy than the FM order. Here the total energy is calculated as the summation of all occupied states. Comparing Fig. 1(g) and (h), the SP for FM order is much smaller than the AFM order. Interestingly, when \( V > \lambda_z \) is applied on one corner, the FM order becomes more stable than the AFM one. The SP for the FM order becomes much larger than that for the AFM order, as shown in Fig. 1(k) and (l). The sign of the SP is also reversed on both corners. This offers a convenient way to control the magnetization and spin transport properties of HOTI flakes.

To understand these important findings, we investigate the evolvement of the corner states with \( \lambda_z \) and \( V \), respectively. First, let's consider the change of \( \lambda_z \) and fix \( V = 0 \). As shown in Fig. 2(a), when \( \lambda_z \) is small (about \( \lambda_z < 0.01t_0 \)), the corner states locate at two corner tips, as the left four inserts shown in Fig. 2(a). The wavefunction of the corner states are evenly distributed for the FM order but unevenly distributed for AFM order, leading to a small or large SP, respectively. With the increase of \( \lambda_z \), the energy between bonding and antibonding states are
unchanged, but the spin splittings are increased. When $V \sim 0.01t_0$, the spin-down (spin-up) states merge into the lower (upper) boundary of the edge states. Spontaneously, the edge states adjacent to the corners become more localized and generate new corner states in a concave shape, as seen in the right four inserts in Fig. 2(a). This is because that large $\lambda_z$ lifts the energy level of corner hexagons away from their neighbors. The further increase of $\lambda_z$ reduces the coupling between the magnetized corner hexagons and the adjacent atoms. As a result, the induced spin splitting of the new corner states decreases when $\lambda_z > 0.01t_0$. Since the new corner states are not located at the magnetized corner hexagons, the spin splitting is less sensitive to $\lambda_z$ than the corner states at the onset (Fig. S2 and S3). The system appears to favor the AFM order in the whole range of $\lambda_z$ (Fig. S4). More results of SPs and WDs are shown in Supplemental Material, Fig. S5 44.

Next, we set $\lambda_z = 0$ and focus on the influence of $V$. As shown in Fig. 2(b), the gap between bonding and antibonding corner states is quickly enlarged by small $V$ (about $V < 0.01t_0$). The distribution of the corner states becomes uneven at two corners with the addition of $V$, as shown in the two left inserts in Fig. 2(b). When $V > 0.01t_0$, the bonding corner states merge into the edge states and new corner states are formed. Since we only add $V$ on the bottom-right corner, the distribution at that corner becomes a concave shape for the new corner states, as shown in the two right inserts in Fig. 2(b). Again, larger $V$ weakens the coupling between the bottom-right corner hexagon and adjacent atoms so that the energy separation between bonding and antibonding corner states decreases with further increasing $V$. It is important to note that the persistence of having the corner states in our model against either electric or magnetic manipulation is another clear indicative of its HOTI nature.

Now, we investigate the response of these topological corner states to the interplay of $\lambda_z$ and $V$. where we set $\lambda_z = 0.3t_0$ as an example. As shown in Fig. 3(a), the magnetic phase transition from the AFM to FM order happens when $V \sim \lambda_z$. To understand the origin of this transition, we plot the energy levels of the corner states around the transition point in Fig. 3(b). With increasing $V$, the energy of spin-up corner states remains almost the same, but spin-down corner states are lifted until the upper state merges into the boundary of edge states. After the transition, a new spin-down corner state is formed at the bottom boundary of edge states and then is gradually lifted with increasing $V$. In Fig. 3(c), we plot a schematic figure with one corner state to further illustrate these changes. When $\lambda_z = 0$ and $V = 0$, the corner state is located within the gap with spin degeneracy. With small $\lambda_z$, the spin splitting occurs for both corner and edge states, but the former has much larger splitting than the latter. With large $\lambda_z$, the original corner states merge into the boundary of edge states. Meanwhile, the original edge states become more localized and form new corner states with opposite spins. After applying $V$, all of the levels are lifted so that the bottom spin-down edge states have stronger coupling with the spin-down corner
TABLE I. The table of wavefunction distribution (WD) and spin polarization (SP) for typical values of $V$ in Fig. 3(a) with FM and AFM orders, respectively.

| $V/(t_0)$ | 0   | 0.2 | 0.25 | 0.35 | 0.4 |
|-----------|-----|-----|------|------|-----|
| **WD**    |     |     |      |      |     |
| FM        | = 4 | = 4 | = 4  | = 4  | = 4 |
| AFM       |     |     |      |      |     |
| **SP**    |     |     |      |      |     |
| FM        | = 1 | = 1 | = 1  | = 1  | = 1 |
| AFM       |     |     |      |      |     |

state while the top spin-up edge states have weaker coupling with the spin-up corner state. Consequently, the energy of the spin-up corner state is unchanged, but the spin-down corner state merges into the edge state boundary and hence drives the transition from AFM to FM.

We also investigate the evolutions of WDs and SPs in Table 1. When $V = 0$, the wavefunctions are evenly distributed at two corners for the FM order, but unevenly distributed for the AFM order, leading to a small or large SP, respectively. Before the transition, the increase of $V$ enhances the uneven distribution for both FM and AFM orders. Comparing $V = 0$, $0.2t_0$, and $0.25t_0$ in Table 1, the WD for spin-up corner state remains almost the same, but the spin-down state becomes more localized at the top-left corner, leading to the enhance of SP for both FM and AFM cases. After the transition, a new spin-down corner state is formed at the bottom edge-state-boundary, as we discussed in Fig. 3(b). The new spin-down corner state is localized at the bottom-right corner, as shown under the $V = 0.35t_0$ column in Table 1. The change of the wavefunction localization induces the reverse of the sign of SP at both corners. With further increase $V$, the wavefunction become delocalized, leading to the decrease of SP, comparing $V = 0.35t_0$ and $0.4t_0$ in Table 1.

From discussions above, there are three key messages from our systematic studies for the control of spin-polarized corner states: 1), the $V$ on one corner can influence the WDs of other corners separated by a significant distance; 2), the SP of corners of HOTI can be remotely controlled by $V$; 3), the manipulation of $V$ can induce a magnetic phase transition between AFM and FM orders. The negative $V$ shows the same conclusions (see more details in Fig. S6) [44].

Last but not least, we discuss the possible realizations and advantages of our model. Using the first-principles calculations, we find the FM features of our model can be achieved in the $\gamma$-graphyne nanostructures [45], which are known as the HOTI [18]. In order to introduce the magnetization, we build an isosceles-trapezoid-shaped nanostructure with zigzag edges, as shown in the inset in Fig. 4(a). The ground-state of this nanostructure shows FM order at two $60^\circ$ corners due to Lieb’s theorem [46, 47].

There are three sets of spin-split corner states close to the Fermi level, as shown in Fig. 4(a). The charge densities of these corner states are shown in Fig. 4(c). While corner states 1,2,4, and 5 are evenly distributed at two $60^\circ$ corners, states 3 and 6 are created due to the size limit. The calculation method and more detailed discussions can be found in Supplemental Material [44].

To mimic the $V$ in DFT, we replace one C atom with Si to lift the on-site potential for both spin-up and spin-down states at the bottom right corner, as the WDs shown in Fig. 4(b). The energy levels of the corner states 2 and 5 are lifted. The charge densities become unevenly distributed at two corners [Fig. 4(d)]. We find that the Si-doped system can be a good analog to the TB model in cases of small $\lambda_z$ and $V$. Comparing Fig. 4(a,c) and (b,f), we can see similar manifestations between DFT and

FIG. 4. Material realization of the $\gamma$-graphyne nanostructures. (a,b) Energy levels (a) without and (b) with Si dopant at the bottom-right corner. Six corner states are labeled in 1-6. The inserts at the bottom-right show the lattice structures. (c,d) The partial charge density for spin-up (yellow) and spin-down (blue) corner states correspond to the levels labeled in (a,b). Isovalue = 0.0002/Å. (e,f,g) The energy levels of TB model with $\lambda_z = -0.003t_0$, (e) $V = 0$, (f) $V = 0.002t_0$, and (g) $V = 0.1t_0$. The insets are WDs of corner states. (e) and (f) are comparable with DFT results in (a) and (b). (h) The SPs for the bonding corner states in (e) with $V = 0$ and (g) with $V = 0.1t_0$. 
TB results, i.e., the small $V$ lifts the energy levels for the antibonding states and induces a strongly uneven distribution for all the corner states. If we can enlarge $V$ by gating, a new set of concave-shaped corner states can be generated, as the WDs shown in Fig. 4(g). Consequently, a large SP can be obtained for the bonding corner states when $V$ is large [Fig. 4(h)]. Compared with the SP without $V$, the SP is dramatically enlarged with the opposite sign at two corners, which shows similar manifestations as we discussed in Fig. 1(g,k).

To this end, we perceive that not only $\gamma$-graphyne but also any 2D HOTIs should manifest the topological features revealed in our model. The $\Lambda_2$ can be applied by adding magnetic atoms near the corners, e.g., Mn, Cr, or Mo $^{48\, \text{[50]}}$, and $V$ can be easily controlled by the gate electrode $^{51\, \text{[52]}}$ or STM tips $^{53\, \text{[55]}}$ in experiments. Besides, the shape of the nanostructure is not constrained as the higher-order topology ensures the robustness of the corner states due to the bulk-boundary correspondence. The robust and remotely tunable spin-polarized corner states provide great advantages for diverse applications such as spin filtering, quantum gates, and information storage.

In summary, the interplay of magnetization and electric potential at the corners of 2D HOTI may strongly alter their spin degree of freedom, such as inducing a phase transition from AFM to FM order and remotely controlling the strength and sign of SP at corners. In particular, despite a significant distance between the corners, applying an electric potential on one corner can influence the charge distribution and SP at other corners due to the robust bulk-boundary correspondence. Our model sheds light on the understanding and manipulation of topological corner states. As the switch of SP can be detected by spin transport and quantum dynamics, remote control without the energy loss in such a HOTI nanostructure is imperative for applications in spintronics and quantum technologies.

We thank Prof. Feng Liu at University Utah for helpful discussions. Work was supported by DOE-BES (Grant No. DE-FG02-05ER46237). Computer simulations were partially performed at the U.S. Department of Energy Supercomputer Facility (NERSC).

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1. M. Z. Hasan and C. L. Kane, Reviews of modern physics 82, 3045 (2010).
2. S. Jia, H. Beidenkopf, I. Drozdov, M. Fucillo, J. Seo, J. Xiong, N. P. Ong, A. Yazdani, and R. J. Cava, Physical Review B 86, 165119 (2012).
3. Z. Hu, J. Gao, S. Zhang, J. Zhao, W. Zhou, and H. Zeng, Physical Review Materials 3, 074005 (2019).
4. X. Ni, H. Huang, and F. Liu, Physical Review B 101, 125114 (2020).
5. Z. Zhang, P. Delplace, and R. Fleury, Nature 598, 293 (2021).
6. W. A. Benalcazar, B. A. Bernevig, and T. L. Hughes, Science 357, 61 (2017).
7. F. Zhang, C. L. Kane, and E. J. Mele, Physical Review Letters 110, 046404 (2013).
8. Y. Peng, Y. Bao, and F. von Oppen, Physical Review B 95, 235143 (2017).
9. J. Langbehn, Y. Peng, L. Trifunovic, F. von Oppen, and P. W. Brouwer, Physical review letters 119, 246401 (2017).
10. Z. Song, Z. Fang, and C. Fang, Physical review letters 119, 246402 (2017).
11. W. A. Benalcazar, B. A. Bernevig, and T. L. Hughes, Physical Review B 96, 245151 (2017).
12. F. Schindler, A. M. Cook, M. G. Vergniory, Z. Wang, S. S. Parkin, B. A. Bernevig, and T. Neupert, Science advances 4, eaat0346 (2018).
13. F. Schindler, Z. Wang, M. G. Vergniory, A. M. Cook, A. Murani, S. Sengupta, A. Y. Kasumov, R. Debloch, S. Jeon, I. Drozdov, et al., Nature physics 14, 918 (2018).
14. M. Ezawa, Physical review letters 120, 026801 (2018).
15. H. Xue, Y. Yang, F. Gao, Y. Chong, and B. Zhang, Nature materials 18, 108 (2019).
16. L.-H. Wu and X. Hu, Scientific reports 6, 1 (2016).
17. Y. Liu, C.-S. Liu, Y. Li, Y. Xu, and W. Duan, Physical Review B 110, 255901 (2017).
18. B. Liu, G. Zhao, Z. Liu, and Z. Wang, Nano Letters 19, 6492 (2019).
19. F. Liu, H.-Y. Deng, and K. Wakabayashi, Physical review letters 122, 086804 (2019).
20. T. Mizoguchi, H. Araki, and Y. Hatsugai, Journal of the Physical Society of Japan 88, 104703 (2019).
21. F. Zangeneh-Nejad and R. Fleury, Physical Review Letters 123, 053902 (2019).
22. E. Lee, A. Furusaki, and B.-J. Yang, Physical Review B 101, 241109 (2020).
23. H. Huang, J. Fan, D. Li, and F. Liu, Nano Letters 21, 7056 (2021).
24. B. A. Bernevig, Topological insulators and topological superconductors (Princeton university press, 2013).
25. X.-L. Qi and S.-C. Zhang, Reviews of Modern Physics 83, 1057 (2011).
26. M. Ezawa, Physical Review B 102, 124105 (2020).
27. E. Khalaf, W. A. Benalcazar, T. L. Hughes, and R. Queiroz, Physical Review Research 3, 013239 (2021).
28. M. Proctor, P. A. Huidobro, B. Bradlyn, M. B. De Paz, M. G. Vergniory, D. Bercioux, and A. García-Etxarri, Physical Review Research 2, 042038 (2020).
29. A. Coutant, V. Achilleos, O. Richoux, G. Theocaris, and V. Pagneux, Physical Review B 102, 214204 (2020).
30. X. Xie, J. Dang, S. Yan, W. Zhang, H. Hao, S. Xiao, S. Shi, Z. Zuo, H. Ni, Z. Niu, et al., Optics Express 29, 30735 (2021).
31. Y.-S. Hu, Y.-R. Ding, J. Zhang, Z.-Q. Zhang, and C.-Z. Chen, Physical Review B 104, 094201 (2021).
32. C. L. Kane and E. J. Mele, Physical review letters 95, 226801 (2005).
33. B. A. Bernevig, T. L. Hughes, and S.-C. Zhang, science 314, 1757 (2006).
34. M. König, S. Wiedmann, C. Brune, A. Roth, H. Buhmann, L. W. Molenkamp, X.-L. Qi, and S.-C. Zhang, Science 318, 766 (2007).
35. F. D. M. Haldane, Physical review letters 61, 2015.
[36] C.-X. Liu, X.-L. Qi, X. Dai, Z. Fang, and S.-C. Zhang, Physical review letters 101, 146802 (2008).

[37] C.-Z. Chang, J. Zhang, X. Feng, J. Shen, Z. Zhang, M. Guo, K. Li, Y. Ou, P. Wei, L.-L. Wang, et al., Science 340, 167 (2013).

[38] R. B. Laughlin, Physical Review Letters 50, 1395 (1983).

[39] C. Nayak, S. H. Simon, A. Stern, M. Freedman, and S. D. Sarma, Reviews of Modern Physics 80, 1083 (2008).

[40] T. Yokoyama, Y. Tanaka, and N. Nagaosa, Physical review letters 102, 166801 (2009).

[41] L. Zhang, K. Chang, X. Xie, H. Buhmann, and L. Molenkamp, New Journal of Physics 12, 083058 (2010).

[42] O. Breunig and Y. Ando, Nature Reviews Physics, 1 (2021).

[43] X. Zhang, L. Liu, M.-H. Lu, and Y.-F. Chen, Physical Review Letters 126, 156401 (2021).

[44] See Supplemental Material at http://link.aps.org/supplemental/xxx for more details which include Refs. [32–47].

[45] Q. Li, Y. Li, Y. Chen, L. Wu, C. Yang, and X. Cui, Carbon 136, 248 (2018).

[46] E. H. Lieb, Physical review letters 62, 1201 (1989).

[47] D. Yu, E. M. Lupton, H. Gao, C. Zhang, and F. Liu, Nano Research 1, 497 (2008).

[48] M. Wu, E.-Z. Liu, M. Ge, and J. Jiang, Applied Physics Letters 94, 102505 (2009).

[49] M. Wu, C. Cao, and J. Jiang, New Journal of Physics 12, 063020 (2010).

[50] J. Thakur, H. S. Saini, M. Singh, A. Reshak, and M. K. Kashyap, Physica E: Low-dimensional Systems and Nanostructures 78, 35 (2016).

[51] Y.-J. Yu, Y. Zhao, S. Ryu, L. E. Brus, K. S. Kim, and P. Kim, Nano letters 9, 3430 (2009).

[52] J. Wang, B. Lian, and S.-C. Zhang, Physical review letters 115, 036805 (2015).

[53] C. Girard, C. Joachim, C. Chavy, and P. Sautet, Surface science 282, 400 (1993).

[54] F. Yin, R. Palmer, and Q. Guo, Physical Review B 73, 073405 (2006).

[55] M. Ohara, Y. Kim, and M. Kawai, Physical Review B 78, 201405 (2008).

[56] T. L. Hughes, E. Prodan, and B. A. Bernevig, Physical Review B 83, 245132 (2011).

[57] Z. Song, T. Zhang, and C. Fang, Physical Review X 8, 031069 (2018).

[58] L. Fu and C. L. Kane, Physical Review B 76, 045302 (2007).

[59] Y. Kim, B. J. Wieder, C. Kane, and A. M. Rappe, Physical review letters 115, 036806 (2015).

[60] A. M. Turner, Y. Zhang, R. S. Mong, and A. Vishwanath, Physical Review B 85, 165120 (2012).

[61] H. C. Po, A. Vishwanath, and H. Watanabe, Nature Communications 8, 50 (2017).

[62] P. E. Blöchl, Physical review B 50, 17953 (1994).

[63] G. Kresse and D. Joubert, Physical review b 59, 1758 (1999).

[64] J. P. Perdew, K. Burke, and M. Ernzerhof, Physical review letters 77, 3865 (1996).

[65] G. Kresse and J. Furthmüller, Physical review B 54, 11169 (1996).

[66] M. Methfessel and A. Paxton, Physical Review B 40, 3616 (1989).

[67] D. Hobbs, G. Kresse, and J. Hafner, Physical Review B 62, 11556 (2000).
Supplemental material for

Remote control of spin-polarized topological corner states by a local electric potential

Yinong Zhou\textsuperscript{1} and Ruqian Wu\textsuperscript{1,*}

\textsuperscript{1}Department of Physics and Astronomy, University of California, Irvine, California 92697-4575, USA

I. TOPOLOGICAL PROPERTIES OF KEKULÉ LATTICE

FIG. S1. (a) The unit cell band structure. (b) The gapped edge states of the ribbon system. $t_1/t_0 = 1.25$, local magnetization ($\lambda_z$) and local electric potential ($V$) equal to zero.

TABLE S1. The parity at time-reversal invariant momenta, $\Gamma$ and $M$ points for the six bands in Fig. S1(a). The 1 to 6 band index represents the bands from bottom to top.

| Band # | 1  | 2  | 3  | 4  | 5  | 6  |
|--------|----|----|----|----|----|----|
| $\Gamma$ | $+$ | $+$ | $+$ | $-$ | $-$ | $-$ |
| $M$      | $-$ | $+$ | $-$ | $+$ | $-$ | $+$ |

$Z_2$ number ($\nu$) can be calculated by using the parity eigenvalues at time-reversal invariant momenta:\textsuperscript{1,2}

$$-1^\nu = (-1)^{[N_{\text{occ}}(\Gamma)/2]} \times \left\{ (-1)^{[N_{\text{occ}}(M)/2]} \right\}^3,$$

(S1)

where $N_{\text{occ}}$ is the number of the occupied bands with odd parity, and the square bracket represents the integer part of the number inside. The $Z_2$ number for the half occupation of Table S1 is calculated as $\nu = 1$. 
II. MORE DETAILS WITH LOCAL MAGNETIZATION

FIG. S2. Discrete energy levels of the corner states as a function of $\lambda_z < 0.01$ and $V = 0$. The red (spin-up) and blue (spin-down) dashes (dots) represent the energy levels of the corner states with FM (AFM) order, and the green lines represent the gap of the edge states.

FIG. S3. The spin splitting gap as a function of $\lambda_z < 0.01$. The spin splitting of corner states is linear dependent and exceedingly sensitive to $\lambda_z$. The blue and orange dots represent the $\lambda_z$ located on the corner one atom and corner six atoms, respectively. The dashed lines are linear fitting lines.
FIG. S4. The energy difference between the FM and AFM orders as a function of $\lambda_z$ with $V = 0$.

FIG. S5. Discrete energy levels of the corner states as a function of $\lambda_z$ with $V = 0$. The inserts show wavefunction distribution for spin-up (red) and spin-down (blue) corner states with $\lambda_z = 0.0005t_0$, $0.003t_0$, $0.05t_0$ and $0.3t_0$, respectively. The bottom two rows show spin polarization for each $\lambda_z$, which is small for FM order and large for AFM order in the whole regime.
III. NEGATIVE LOCAL ELECTRIC POTENTIALS

FIG. S6. Energy levels of corner states for both negative and positive electric potentials with $t_1/t_0 = 1.25$ and $\lambda_z = 0.3t_0$. Red and blue dashes (dots) represent spin-up and spin-down levels with FM (AFM) order. The wavefunction distributions for the valence levels labeled 1-4 for positive (right panel) and 1$^-$-4$^-$ for negative (left panel) from lower to higher energy for both small (inner panel) and large (outer panel) electric potentials. The spin polarization distributions are also plotted accordingly. The size of the red and blue circles is proportional to the local charge density of corner states. The sign of $V$ induces an inversion of the bonding and antibonding corner states.

IV. FIRST-PRINCIPLES CALCULATION METHOD

Our first-principles calculations are performed with the projector-augmented wave pseudopotentials [7, 8] and the generalized gradient approximation of Perdew-Burke-Ernzerhof [9] using Vienna Ab initio Simulation Package [10] code. An energy cutoff of 450 eV and a $1 \times 1 \times 1$ Monkhorst-Pack $k$-point grid is used [11]. The structure is optimized until the atomic forces are smaller than 0.03 eV/Å. The vacuum layer is larger than 15 Å to ensure decoupling between neighboring nanostructures. The magnetic moments are considered in the self-consistent calculation [12].

V. MATERIAL REALIZATION DETAILS

The $\gamma$-graphyne is a HOTI due to the different intra-cell C-C and inter-cell C=C\equivC-C bonds. The corner states without magnetization are shown in Fig. S7. Conceptually, because of the chiral charge cancellation at the corners, only the corners terminated by the same sublattice can generate corner states. In the isosceles-trapezoid-shaped $\gamma$-graphyne, only two 60° corners should appear corner states. But in Fig. S7, we can see three corner states at the Fermi level. The additional corner state is mainly distributed in the middle of the bottom edge, as shown in Fig. 4 and S7, which is due to the size limit of density-functional theory calculations. We build a relatively small nanostructure, which already contains 244 atoms. If the size of the nanostructure is large enough, there will only emerge two corner states. The spatial distribution of the spin density difference is shown in Fig. S8. The top edge shows the opposite spin to the other three edges so that the bottom two 60° corners are ferromagnetic ordered.
FIG. S7. Energy levels without magnetization. Three corner states are labeled in 1-3. The insert at the bottom right shows the lattice structure. (b) The partial charge density for each corner state corresponds to the labels in (a).

FIG. S8. The spatial distribution of the spin density difference for isosceles-trapezoid-shaped $\gamma$-graphyne with Si dopant on the right bottom corner (iso-value = 0.0005/Å).

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*wur@uci.edu*

[1] T. L. Hughes, E. Prodan, and B. A. Bernevig, Physical Review B 83, 245132 (2011).
[2] Z. Song, T. Zhang, and C. Fang, Physical Review X 8, 031069 (2018).
[3] L. Fu and C. L. Kane, Physical Review B 76, 045302 (2007).
[4] Y. Kim, B. J. Wieder, C. Kane, and A. M. Rappe, Physical review letters 115, 036806 (2015).
[5] A. M. Turner, Y. Zhang, R. S. Mong, and A. Vishwanath, Physical Review B 85, 165120 (2012).
[6] H. C. Po, A. Vishwanath, and H. Watanabe, Nature Communications 8, 50 (2017).
[7] P. E. Blöchl, Physical review B 50, 17953 (1994).
[8] G. Kresse and D. Joubert, Physical review b 59, 1758 (1999).
[9] J. P. Perdew, K. Burke, and M. Ernzerhof, Physical review letters 77, 3865 (1996).
[10] G. Kresse and J. Furthmüller, Physical review B 54, 11169 (1996).
[11] M. Methfessel and A. Paxton, Physical Review B 40, 3616 (1989).
[12] D. Hobbs, G. Kresse, and J. Hafner, Physical Review B 62, 11556 (2000).