

Direct Observation of the Zigzag Edge States of a Supramolecular Diatomic Kagome Lattice

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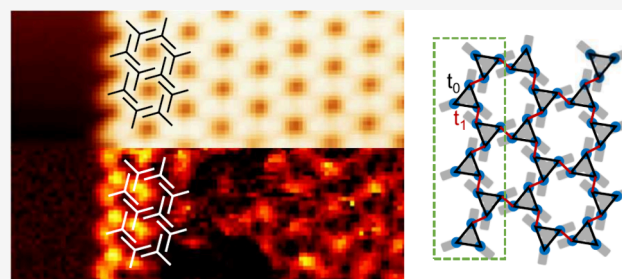
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Supporting Information

ABSTRACT: Lattice geometry plays a fundamental role in the behavior of Bloch electrons in a crystal. The diatomic Kagome lattice, an extension of the honeycomb and Kagome lattices, is predicted to give rise to emergent and topological phenomena, but its experimental investigation has been limited thus far. Here, we fabricate a diatomic Kagome lattice through self-assembly of a triptycene derivative with phenazine moieties (Trip-Phz)—a C_3 -symmetric, nonplanar π -conjugated molecule. Our scanning tunneling microscopy (STM) observations show that Trip-Phz forms a highly ordered diatomic Kagome lattice terminated by zigzag-type edges on the Pb(111) surface. Combined STM measurements and tight-binding calculations provide direct evidence for the existence of the edge states that correspond to those of graphene. These states are topological edge states dictated by the quantization of the Zak phase and the bulk-edge correspondence. This work reveals an ideal platform for exploring quantum materials with unique lattice geometries using supramolecular technology.

KEYWORDS: Diatomic-Kagome lattice, Edge states, Zak phase, Self-assembly, Nonplanar π -conjugated molecules, Scanning tunneling microscopy



Lattice geometry profoundly affects the behavior of itinerant electrons in a crystal and is central to the modern research on quantum materials and technologies.^{1–3} The honeycomb and Kagome lattices, the latter of which consists of corner-sharing triangles with enclosed hexagons, are two-dimensional (2D) lattices that have been studied the most intensively in the past decade.^{4–6} Tight-binding (TB) calculations predict the formation of linearly intersecting bands (Dirac bands) for both lattices and a nearly dispersionless band (flat band) originating from geometric frustration for the Kagome lattice.^{7,8} These remarkable band structures possess nontrivial topology and can be subject to strong electron correlation effects due to a vanishing kinetic energy, leading to rich emergent phenomena such as quantum anomalous Hall effect and superconductivity.^{9–16}

The honeycomb lattice can be extended in such a way that triangles with an internal coupling constant t_0 are placed at the lattice nodes while they are coupled to their nearest neighbors with t_1 (see Figure 1(a)). This can also be viewed as an extended Kagome lattice, where the vertices of the triangular units are connected by a diatomic pair (indicated by the dashed orange line in Figure 1(a)). This diatomic Kagome lattice, also called the star lattice because of its shape, can be regarded as a hybrid of the two basic lattices.^{17–19} TB

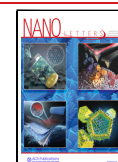
calculations predict the formation of four Dirac bands and two flat bands, the topology of which is switched by tuning the ratio t_0/t_1 .^{20–23} Recently, the diatomic Kagome lattice has attracted theoretical attention and is predicted to exhibit novel quantum states such as second-order topological states and excitonic insulators.^{21,22,24–26} However, its experimental investigation has been limited so far.^{22,27,28} Particularly, the one-dimensional edge states corresponding to those of graphene,^{29–33} which connect the projected Dirac points in momentum space and exhibit nanoscale magnetism, have not been observed yet. The diatomic Kagome lattice may have such edge states, but the very existence of them is unclear because there is no chiral symmetry that protects the edge states of graphene.^{21,22,31,34} Here, we report direct observations of the edge states of a diatomic Kagome lattice, which is made of supramolecular assembly of a triptycene derivative with

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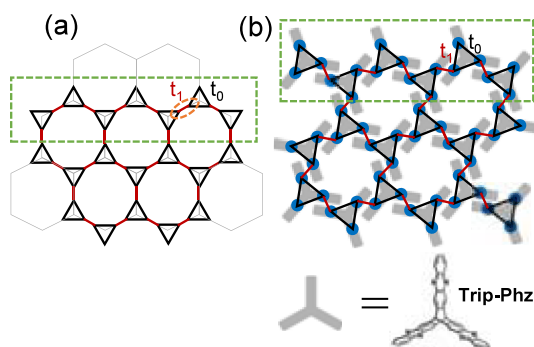


Figure 1. Diagram of the diatomic Kagome lattice. (a) Mathematical model with intracorner coupling t_0 and intercorner coupling t_1 . The lattice can be regarded as an extension of the honeycomb and Kagome lattices. The dashed orange line indicates a diatomic pair coupled with t_1 . (b) Materialization of the diatomic Kagome lattice using Trip-Phz molecules, where t_0 and t_1 represent intra- and intermolecular couplings, respectively. The gray symbols represent the C_3 -symmetric frame of Trip-Phz molecules. Left-handed chirality is chosen for this display. The green rectangles indicate the zigzag-type edge corresponding to that of graphene.

phenazine moieties (Trip-Phz) on the Pb(111) surface. Our scanning tunneling microscopy (STM) observations reveal that Trip-Phz forms well-ordered molecular lattices, terminated by straight boundaries that correspond to the graphene zigzag edge. The spectroscopic signatures of the Dirac and flat bands are confirmed using STM and TB calculations. Most importantly, we provide direct evidence for the existence of edge states that corresponds to those of graphene. These states are topological edge states dictated by the quantization of the Zak phase and the bulk-edge correspondence. This study provides solid experimental evidence for the edge states in the diatomic Kagome lattice and significantly expands the scope of quantum material research driven by lattice geometry.

Our strategy for creating the diatomic Kagome lattice in Figure 1(a) is based on supramolecular chemistry using Trip-Phz.^{35,36} This type of triptycene derivative molecule comprises three π -conjugated planes as moieties assembled in a nonplanar configuration, featuring a rigid Y-shape with the strict C_3 symmetry. They can form a highly ordered 2D lattice by π - π pancake bonding between the moieties in a solution and on a substrate surface.^{20,35–41} With the centers of molecules located at the honeycomb nodes and the orbitals of the moieties arranged in a triangular form around them, it can form an ideal diatomic Kagome lattice (Figure 1(b)). This molecular assembly is chiral when formed on a surface; the chirality here is referred to as left-handed, while its mirror-symmetric counterpart as right-handed, in this work.³⁶ We note that the chirality mentioned here is geometrical and should not be confused with the chiral symmetry of graphene, which is determined by the structure of the Hamiltonian¹⁸ (see Supporting Note 1). Figure 1 panels (a) and (b) also show basic edge structures of the diatomic Kagome and Trip-Phz lattices, respectively (green rectangles). This type of edge is referred to as zigzag edge here because it matches that of the honeycomb lattice in the limit of $t_0 \rightarrow \infty$ (i.e., when the triangles are reduced to points).

We first study the structure of self-assembled molecules using STM (for details, see Supporting Information, Methods). Figure 2(a) shows a representative, large-scale, constant-current image of Trip-Phz molecules with an average coverage

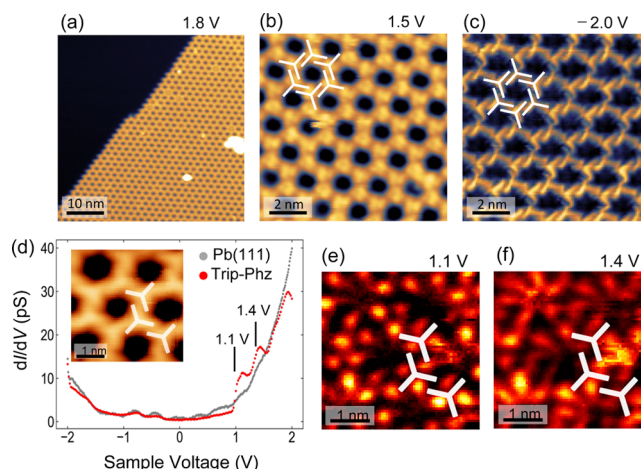


Figure 2. STM observations of the diatomic Kagome lattice of Trip-Phz on Pb(111). (a) Large-area STM topographs recorded using $I = 10$ pA and $V = 1.8$ V. (b, c) Detailed topographs acquired using (b) $V = 1.5$ V and (c) -2.0 V. (d) dI/dV spectrum averaged over the molecular network of Trip-Phz (red dots) and a reference spectrum on a bare Pb(111) (gray dots). Inset: STM topograph of the relevant area recorded using $V = 2.0$ V, $I = 50$ pA. (e, f) dI/dV images taken over the same area as in (d) using (e) $V = 1.1$ V and (f) 1.4 V. For the images in (b–f), the molecular adsorption geometries are denoted by white Y-shaped lines.

of ~ 0.3 monolayers (ML) on a Pb(111) surface. We find a monolayer molecular island (100×80 nm²) consisting of a single well-ordered domain. Its boundaries are predominantly straight. Figure 2 panels (b) and (c) present more detailed topographs of the same island, acquired at $V = 1.5$ and -2.0 V, respectively. These STM images reflect the real-space distribution of the LUMO+1 orbital and the shape of the Trip-Phz molecular framework, respectively; the LUMO+1 states are located at $V = 1.5$ V while there exist no HOMO states at $V = -2.0$ V, as will be revealed below. The overlaid white Y-shaped lines indicate the molecular frames. Evidently, Trip-Phz molecules are arranged in the form of the diatomic Kagome lattice with left-handed chirality, as in Figure 1(b). The lattice parameter of the island was determined to be 1.92 ± 0.04 nm, and the azimuthal rotation angle of the lattice relative to the principal orientations of the Pb(111) surface $51.3 \pm 2^\circ$. Assuming a commensurate epitaxy on the Pb(111) lattice, the only possible superstructure is Pb(111)-($\sqrt{31} \times \sqrt{31}$)R51°, with a lattice constant of $\sqrt{31} a_0 = 1.95$ nm, where $a_0 = 0.350$ nm is the nearest-neighbor distance of the Pb(111) surface. We also found a molecular arrangement with the right-handed chirality, which can be denoted as Pb(111)-($\sqrt{31} \times \sqrt{31}$)R9° (see Supporting Information, Figure S1).

Next, we investigate the spectroscopic features of the “bulk” region of an island, sufficiently away from the edges (Figure 2(d)). The STM topograph of this area is shown in the inset, where the locations of the molecules are indicated by Y-shaped lines. The dI/dV spectrum averaged over the Trip-Phz lattice (excluding the pore sites) is displayed in red, while a spectrum averaged over a bare Pb(111) surface is plotted in gray as a reference. On the positive energy side, two peaks are clearly visible at $V = 1.1$ and 1.4 V (indicated by solid lines). Since the lowest unoccupied molecular orbital (LUMO) and LUMO+1 of Trip-Phz are located at -2.57 and -2.16 eV below the vacuum level, respectively (Supporting Information, Figure

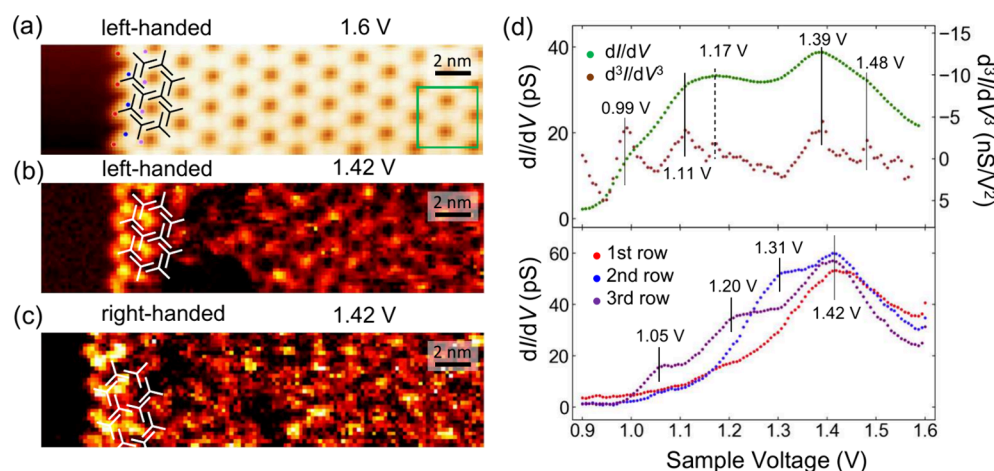


Figure 3. Spectroscopic evidence of the zigzag edge states and the Dirac and flat bands of the diatomic Kagome lattice of Trip-Phz. (a) Topograph of the zigzag edge structure with left-handed chirality, recorded using $V = 1.6$ V, $I = 50$ pA. (b) dI/dV image taken at $V = 1.42$ V over the area shown in (a). (c) dI/dV image obtained under the same conditions from a Trip-Phz lattice with right-handed chirality. (d) Upper panel: dI/dV spectrum acquired within the green square in (a) (green dots). The positions of the peak and shoulders were determined from d^3I/dV^3 (brown dots), which was obtained by taking the second derivative of dI/dV with respect to V . Lower panel: dI/dV spectra acquired near the edge. The colors of the dots correspond to those in (a); red for the first row (closest to the edge), blue for the second row, and purple for the third row.

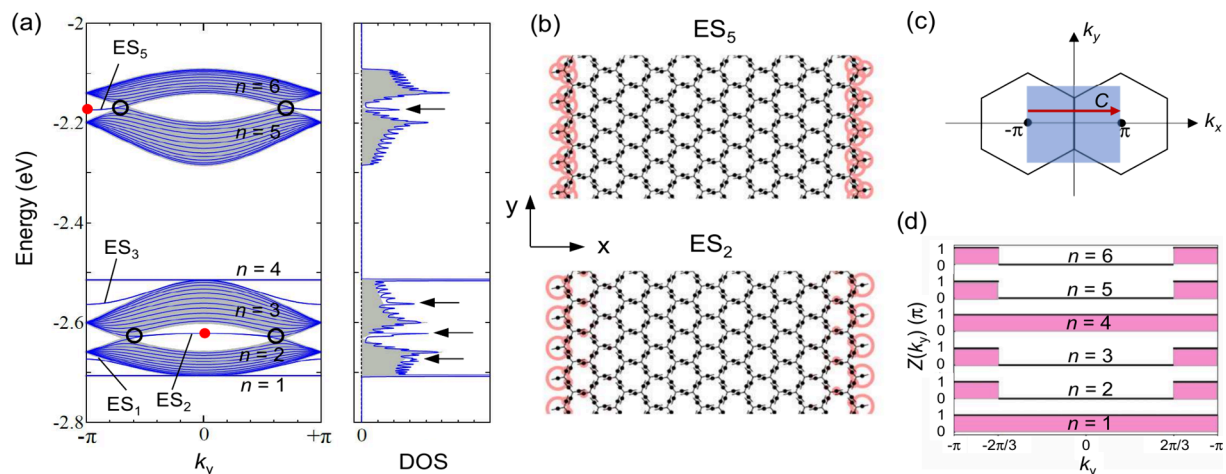


Figure 4. Results of tight-binding (TB) calculations for the diatomic Kagome lattice of Trip-Phz. (a) Band structure in the k_y direction (left panel, blue lines) and the corresponding density of states (DOS) (right panel, blue lines). The edge states located between the bulk bands n and $n + 1$ are denoted as ES_n . The projected band structure and the corresponding DOS of TB-calculated bulk states are shown by the gray regions. The arrows indicate peaks due to the edge states. (b) Spatial distributions of the edge states of ES_5 at $k_y = -\pi$ (top panel) and ES_2 at $k_y = 0$ (bottom panel) indicated by red dots in (a). Red circles mark the locations of the edge states. The diameter of each circle is proportional to the local DOS of the corresponding states. (c) Illustration of the Brillouin zones of the diatomic Kagome lattice, where the Zak phase is defined along the path C . (d) The Zak phases calculated for the individual bulk bands $n = 1, 2, \dots, 6$ as a function of k_y .

$S2$),³⁵ those peaks can be attributed to molecular bands derived from them. By contrast, on the negative energy side of the spectrum, no HOMO states are discernible down to $V = -2.0$ V. Figure 2 panels (e) and (f) display dI/dV maps acquired at $V = 1.1$ and 1.4 V, respectively, in the same area. For both voltages, the bright spots are located between the three arms of the molecules. These spots can be interpreted as the LUMOs of Trip-Phz, since the LUMOs protrude from the π -conjugated planes of the molecular moieties in the normal direction (Supporting Information, Figure S2). These states should hardly overlap with those of the Pb(111) surface because they are oriented parallel to the surface.³⁶ This is advantageous for observing the intrinsic molecular states. For discussions on the molecule–substrate interaction, see Supporting Note 2.

We now focus on an area including the edge of the Trip-Phz lattice. The topograph of Figure 3(a) reveals that this edge belongs to the zigzag edge defined above, as is evident from the overlaid black Y-shaped markers. The image also shows that the chirality is left-handed. Repeated STM observations of a boundary region confirmed that it was dominated by the zigzag type. This is in striking contrast to the honeycomb lattice of graphene, for which armchair edges are predominantly formed.³² Figure 3(d) shows dI/dV spectra taken at selected sites within the area of Figure 3(a). The green dots represent the data averaged over an area far from the edge (green square in Figure 3(a)). They reveal that the two peaks identified in Figure 2(d) actually include four features, as indicated by the solid lines. Their positions were determined from d^3I/dV^3 (brown dots), which was obtained by taking the second

derivative of dI/dV with respect to V : $V = 0.99$ and 1.11 V for one and $V = 1.39$ and 1.48 V for the other. An additional weak peak may also exist at $V = 1.17$ V (dotted line). These features were repeatedly observed at locations far from the edge (see Supporting Information, Figure S3). By contrast, the spectra acquired near the edge (red, first row; blue, second row; purple, third row; see also Figure 3(a)) all exhibit pronounced peaks at $V = 1.42$ V. This strongly suggests the presence of edge states centered at $V = 1.42$ V. Indeed, a dI/dV image taken at this voltage reveals bright spots localized on the first three rows of the edge, clarifying the spatial distribution of the zigzag edge states (Figure 3(b)). They are observable only around $V = 1.42$ V, in agreement with the pronounced peaks of the dI/dV spectra at this voltage. As expected from the symmetry, molecular lattices with right-handed chirality also exhibit edge states, as revealed in the dI/dV image in Figure 3(c). The weaker appearance of the edge states for this chirality can be attributed to larger spatial fluctuations in the dI/dV signal caused by disorder. The presence of the edge states at $V = 1.42$ V can also be confirmed in a wider area (see Supporting Information, Figure S3(c)). A line profile taken in the normal direction shows that the dI/dV intensities at the edge region are significantly larger, on average, than those in the inner bulk area (Figure S3(d)). We note that the dI/dV spectra acquired on the second and third rows include shoulders at $V = 1.05$, 1.20 , and 1.31 V (solid lines). Furthermore, dI/dV images acquired around $V = 1.20$ V reveal higher intensities near these rows (see Supporting Information, Figure S4 and Movie S1). They suggest the presence of edge states at these voltages, although they are not as conspicuous as those observed around $V = 1.42$ V.

To interpret our experimental results, we performed TB calculations. The model is based on the diatomic Kagome lattice depicted in Figure 1, where the intramolecular coupling t_0 and intermolecular coupling t_1 represent the mutual overlap of the LUMOs of the phenazine moieties. Although the substrate is not included in the calculations, it gives only a minor effect on the molecular band structure.³⁶ The absence of the Shockley surface states on Pb(111) within the relevant energy region also rationalizes this treatment (see Supporting Information, Figure S5). The molecular lattice was terminated by zigzag edges in the x direction, while a periodic boundary condition was imposed in the y direction. The transfer integrals $t_0 = -0.141$ eV and $t_1 = -0.096$ eV were determined from the LUMO level splitting of Trip-Phz and a pair of phenazine moieties, respectively, through density functional theory (DFT) calculations (see Supporting Information, Methods).

The left panel of Figure 4(a) displays the obtained band structures in the k_y direction, which shows the energy dispersions parallel to the edges (blue lines). In agreement with previous work, two pairs of Dirac bands ($n = 2, 3, 5, 6$) are formed, with the projected Dirac points located at $E = -2.63$ and -2.17 eV (indicated by open circles).^{20–22,36} The lower Dirac bands accompany two flat bands ($n = 1, 4$) at the top and bottom ends. These are characteristic of the diatomic Kagome lattice with $t_0/t_1 > 2/3$, $t_0, t_1 < 0$. Importantly, because of the termination in the x direction, edge states emerge within some of the band gaps; the states located between the bulk bands n and $n + 1$ are denoted as ES_n . While ES_5 located around $k_y = \pm\pi$ corresponds to the edge states of graphene, ES_1 , ES_2 , and ES_3 are distinct because they span different momentum spaces. The right panel of Figure 4(a) shows the corresponding density of states (DOS). The edge states appear

as sharp peaks (indicated by black arrows) in addition to those due to the van Hove singularity (vHS) within the bulk bands. Figure 4(b) shows the spatial distributions of the edge states ES_5 at $k_y = -\pi$ (top panel) and ES_2 at $k_y = 0$ (bottom panel) indicated by red dots in Figure 4(a). The diameter of the red circles on the molecular sites is proportional to the local DOS. Their spatial dependence shows that ES_5 are localized to the first through third rows of the zigzag edges. By contrast, ES_2 extend slightly deeper into the interior.

Our spectroscopic data can largely be explained by these theoretical predictions. We note that the bands obtained through the TB calculations can be shifted rigidly for comparison to experimental data. Regarding the dI/dV spectrum in the central region of the Trip-Phz lattice (Figure 3(d), green dots), the shoulders at $V = 0.99$ and 1.11 V can be assigned to the two vHS peaks of the lower Dirac bands ($n = 2, 3$) and the two flat bands ($n = 1, 4$). Only two peaks out of the four are visible, probably because of the proximity of the flat bands to the neighboring vHS peaks and level broadening due to disorder. Indeed, the weak feature at $V = 1.17$ V may be assigned to one of the four DOS peaks. The peak and shoulder at $V = 1.39$ and 1.48 V are attributed to the two vHS peaks in the upper Dirac bands ($n = 5, 6$). Regarding the spectra in the first through third rows (Figure 3(d), red, blue, and purple dots), the peaks at $V = 1.42$ V are assigned to the edge state ES_5 . The bright features along the zigzag edges in the dI/dV images (Figure 3(b),(c)) also correspond well to the spatial distribution of ES_5 (Figure 4(b), top panel). By contrast, the assignment of the spectroscopic features observed in the second and third rows at V values of 1.05 , 1.20 , and 1.31 V is not straightforward. We speculate that multiple contributions from the edge states ES_1 , ES_2 , and ES_3 as well as Dirac and flat bands form the observed spectra.

Here, we show that the edge states found above have a topological origin associated with the Zak phase. The Zak phase is a Berry phase across an appropriately chosen one-dimensional Brillouin zone.^{42,43} For an intuitive picture of the Zak phase, refer to Supporting Note 3. In the present case, a path C is chosen at a constant k_y within the 2D Brillouin zone as shown by the red arrow in Figure 4(c). The Zak phase $Z_n(k_y)$ for a band n is given by the following equations:

$$Z_n(k_y) = \int_{-\pi}^{\pi} A_n(k_x, k_y) dk_x \quad (1)$$

$$A_n(k_x, k_y) = -i \left\langle u_n(k_x, k_y) \left| \frac{\partial}{\partial k_x} u_n(k_x, k_y) \right. \right\rangle \quad (2)$$

where $A_n(k_x, k_y)$ is the Berry connection and $|u_n(k_x, k_y)\rangle$ is the Bloch wave function. In the presence of inversion symmetry, $Z_n(k_y)$ is quantized to 0 or π (mod 2π), which is valid for the diatomic Kagome lattice. The presence of the edge states is dictated through the bulk-edge correspondence by the summation of $Z_n(k_y)$ over n

$$Z(k_y) = \sum_{n=1}^N Z_n(k_y) \quad (3)$$

where N refers to the number of bands below a relevant energy gap. If $Z(k_y) = \pi$ (mod 2π), the system is topologically nontrivial and the edge states appear in this gap. Otherwise, i.e., if $Z(k_y) = 0$ (mod 2π), the edge states are absent. Figure 4(d) shows the Zak phase calculated for the diatomic Kagome lattice with $t_0 = -0.141$ eV and $t_1 = 0.096$ eV, demonstrating

the quantization to 0 or π . The summation over $n = 1, 2, \dots, 5$ leads to $Z(k_y) = \pi \pmod{2\pi}$ for $2\pi/3 < |k_y| < \pi$ and 0 for elsewhere. This exactly corresponds to the presence of the edge states ES_5 within $2\pi/3 < |k_y| < \pi$. The other edge states can also be dictated in the same manner. Thus, the edge states found here have a topological origin associated with the quantization of the Zak phase, which dictates their existence through the bulk-edge correspondence. They can be regarded as a generalization of the zigzag edge states of graphene in a system without the chiral symmetry.

Recently, Hu et al. predicted through TB calculations that edge states exist within an energy gap for certain types of diatomic Kagome lattice.^{21,22} They also showed the existence of corner states as second-order topological states in the same energy gap. Both of them were observed by dI/dV imaging using STM. Our TB parameters $t_0/t_1 > 2/3$, $t_0, t_1 < 0$ preclude such states, but nevertheless, it will be worth searching for them by tuning molecular parameters. Indeed, the ratio t_0/t_1 is sensitive to the molecular lattice constant, which in turn is tunable by choosing an appropriate substrate.³⁶ Telychko et al. and Yin et al. reported the formation of diatomic Kagome lattices by confining the Shockley surface states of noble metals using molecular templates.^{27,28} The latter authors also observed edge states around the boundary of a molecular island in the gap region of a breathing Kagome lattice. The edge states observed in the present work are derived from molecular orbitals that form an intrinsic tight-binding lattice. They are connected to the projected Dirac points and therefore have a different origin.

Finally, we remark on the prospects of the present study. Recently, Kagome-related materials have been one of the hottest topics in condensed-matter physics.^{9–16} For this purpose, various layered inorganic materials have been synthesized, but it still remains challenging to design and find appropriate systems. This is because the complicated interactions between multiple atomic sites and orbitals often destroy the electronic properties predicted by theoretical models.⁴⁴ By contrast, as demonstrated here, it is possible to fabricate a nearly ideal 2D lattice using chemically designed nonplanar π -conjugated molecules as building blocks. The upright configuration of the moiety planes enhances intralayer coupling while suppressing coupling with the substrate and neighboring stacking layers. The use of other nonplanar π -conjugated molecules also appears promising; for example, triptycene trithianthrene (TTA) forms a layered crystal with a breathing Kagome lattice in a solution.^{23,45} This will be the subject of a forthcoming study.

In summary, we successfully fabricated a highly ordered diatomic Kagome lattice through the self-assembly of Trip-Phz on Pb(111), which was predominantly terminated by zigzag-type edges. Our STM measurements and TB calculations provided direct evidence of the zigzag edge states that correspond to those of graphene within a pair of Dirac bands. They are topological states given by the quantization of the Zak phase and bulk-edge correspondence. This work offers a new platform based on supramolecular technology for exploring quantum materials with unique lattice geometries.

■ ASSOCIATED CONTENT

SI Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.nanolett.6c03195>.

Bias voltage dependence of dI/dV images (MP4)

Preparation and purification of Trip-Phz, sample preparation and STM measurements, tight-binding and DFT calculations, and references (Methods); the bias voltage dependence of high-resolution STM topographs of a Trip-Phz island (Figure S1), the energy levels and spatial distributions of the LUMOs (Figure S2), dI/dV spectra obtained in a bulk region of a Trip-Phz lattice (Figure S3), the edge states of Trip-Phz lattices observed in the same area as in Figures 3(a) and 3(b) (Figure S4), and electronic band structure of Pb(111) (Figure S5); Supporting Note 1: Chiral symmetry of graphene; honeycomb lattice of graphene (Figure S6); Supporting Note 2: Molecule-substrate interaction and the effect of spin-orbit interaction; Supporting Note 3: An intuitive picture of the Zak phase; Intuitive picture of the Zak phase and the bulk-edge correspondence (Figure S7) (PDF)

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Notes

The authors declare no competing financial interest.

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REFERENCES

- (1) Leykam, D.; Andreanov, A.; Flach, S. Artificial flat band systems: from lattice models to experiments. *Adv. Phys. X* **2018**, *3*, 1473052.
- (2) Springer, M. A.; Liu, T.-J.; Kuc, A.; Heine, T. Topological two-dimensional polymers. *Chem. Soc. Rev.* **2020**, *49*, 2007.
- (3) Smirnova, D.; Leykam, D.; Chong, Y.; Kivshar, Y. Nonlinear topological photonics. *Appl. Phys. Rev.* **2020**, *7*, 021306.
- (4) Geim, A. K. Graphene: Status and Prospects. *Science* **2009**, *324*, 1530.
- (5) Polini, M.; Guinea, F.; Lewenstein, M.; Manoharan, H. C.; Pellegrini, V. Artificial honeycomb lattices for electrons, atoms and photons. *Nat. Nanotechnol.* **2013**, *8*, 625.
- (6) Yin, J.-X.; Lian, B.; Hasan, M. Z. Topological kagome magnets and superconductors. *Nature* **2022**, *612*, 647.
- (7) Ando, T. Theory of Electronic States and Transport in Carbon Nanotubes. *J. Phys. Soc. Jpn.* **2005**, *74*, 777.
- (8) Guo, H. M.; Franz, M. Topological insulator on the kagome lattice. *Phys. Rev. B* **2009**, *80*, 113102.
- (9) Haldane, F. D. M. Model for a Quantum Hall Effect without Landau Levels: Condensed-Matter Realization of the “Parity Anomaly”. *Phys. Rev. Lett.* **1988**, *61*, 2015.
- (10) Kane, C. L.; Mele, E. J. Z_2 Topological Order and the Quantum Spin Hall Effect. *Phys. Rev. Lett.* **2005**, *95*, 146802.
- (11) Novoselov, K. S.; Geim, A. K.; Morozov, S. V.; Jiang, D.; Katsnelson, M. I.; Grigorieva, I. V.; Dubonos, S. V.; Firsov, A. A. Two-dimensional gas of massless Dirac fermions in graphene. *Nature* **2005**, *438*, 197.
- (12) Tang, E.; Mei, J.-W.; Wen, X.-G. High-Temperature Fractional Quantum Hall States. *Phys. Rev. Lett.* **2011**, *106*, 236802.
- (13) Ye, L.; Kang, M.; Liu, J.; von Cube, F.; Wicker, C. R.; Suzuki, T.; Jozwiak, C.; Bostwick, A.; Rotenberg, E.; Bell, D. C.; Fu, L.; Comin, R.; Checkelsky, J. G. Massive Dirac fermions in a ferromagnetic kagome metal. *Nature* **2018**, *555*, 638.
- (14) Li, Z.; Zhuang, J.; Wang, L.; Feng, H.; Gao, Q.; Xu, X.; Hao, W.; Wang, X.; Zhang, C.; Wu, K.; Dou, S. X.; Chen, L.; Hu, Z.; Du, Y. Realization of flat band with possible nontrivial topology in electronic Kagome lattice. *Sci. Adv.* **2018**, *4*, No. eaau4511.
- (15) Ortiz, B. R.; Teicher, S. M. L.; Hu, Y.; Zuo, J. L.; Sarte, P. M.; Schueller, E. C.; Abeykoon, A. M. M.; Krogstad, M. J.; Rosenkranz, S.; Osborn, R.; Seshadri, R.; Balents, L.; He, J.; Wilson, S. D. CsV_3Sb_5 : A AZ_2 Topological Kagome Metal with a Superconducting Ground State. *Phys. Rev. Lett.* **2020**, *125*, 247002.
- (16) Jiang, Y.-X.; et al. Unconventional chiral charge order in kagome superconductor KV_3Sb_5 . *Nat. Mater.* **2021**, *20*, 1353.
- (17) Zheng, Y.-Z.; Tong, M.-L.; Xue, W.; Zhang, W.-X.; Chen, X.-M.; Grandjean, F.; Long, G. A. “Star” Antiferromagnet: A Polymeric Iron(III) Acetate That Exhibits Both Spin Frustration and Long-Range Magnetic Ordering. *Angew. Chem. Int.* **2007**, *46*, 6076.
- (18) Mizoguchi, T.; Maruyama, M.; Okada, S.; Hatsugai, Y. Flat bands and higher-order topology in polymerized triptycene: Tight-binding analysis on decorated star lattices. *Phys. Rev. Mater.* **2019**, *3*, 114201.
- (19) Jiang, W.; Ni, X.; Liu, F. Exotic Topological Bands and Quantum States in Metal-Organic and Covalent-Organic Frameworks. *Acc. Chem. Res.* **2021**, *54*, 416.
- (20) Shuku, Y.; Mizuno, A.; Ushiroguchi, R.; Hyun, C. S.; Ryu, Y. J.; An, B. K.; Kwon, J. E.; Park, S. Y.; Tsuchiizu, M.; Awaga, K. An exotic band structure of a supramolecular honeycomb lattice formed by a pancake π - π interaction between triradical trianions of triptycene tribenzoquinone. *Chem. Commun.* **2018**, *54*, 3815.
- (21) Hu, T. Y.; Zhang, T. F.; Mu, H. M.; Wang, Z. F. Intrinsic Second-Order Topological Insulator in Two-Dimensional Covalent Organic Frameworks. *J. Phys. Chem. Lett.* **2022**, *13*, 10905.
- (22) Hu, T.; Zhong, W.; Zhang, T.; Wang, W.; Wang, Z. F. Identifying topological corner states in two-dimensional metal-organic frameworks. *Nat. Commun.* **2023**, *14*, 7092.
- (23) Shuku, Y.; Suizu, R.; Nakano, S.; Tsuchiizu, M.; Awaga, K. Engineering Dirac cones and topological flat bands with organic molecules. *Phys. Rev. B* **2023**, *107*, 155123.
- (24) Guo, X.; Liu, Z.; Liu, B.; Li, Q. X.; Wang, Z. F. Non-Collinear Orbital-induced Planar Quantum Anomalous Hall Effect. *Nano Lett.* **2020**, *20*, 7606.
- (25) Sethi, G.; Zhou, Y.; Zhu, L.; Yang, L.; Liu, F. Flat-Band-Enabled Triplet Excitonic Insulator in a Diatomic Kagome Lattice. *Phys. Rev. Lett.* **2021**, *126*, 196403.
- (26) Sethi, G.; Cuma, M.; Liu, F. Excitonic Condensate in Flat Valence and Conduction Bands of Opposite Chirality. *Phys. Rev. Lett.* **2023**, *130*, 186401.
- (27) Telychko, M.; Li, G.; Mutombo, P.; Soler-Polo, D.; Peng, X.; Su, J.; Song, S.; Koh, M. J.; Edmonds, M.; Jelinek, P.; Wu, J.; Lu, J. Ultrahigh-yield on-surface synthesis and assembly of circumcoronene into a chiral electronic Kagome-honeycomb lattice. *Sci. Adv.* **2021**, *7*, No. eabf0269.
- (28) Yin, R.; et al. Artificial kagome lattices of Shockley surface states patterned by halogen hydrogen-bonded organic frameworks. *Nat. Commun.* **2024**, *15*, 2969.
- (29) Fujita, M.; Wakabayashi, K.; Nakada, K.; Kusakabe, K. Peculiar Localized State at Zigzag Graphite Edge. *J. Phys. Soc. Jpn.* **1996**, *65*, 1920.
- (30) Nakada, K.; Fujita, M.; Dresselhaus, G.; Dresselhaus, M. S. Edge state in graphene ribbons: Nanometer size effect and edge shape dependence. *Phys. Rev. B* **1996**, *54*, 17954.
- (31) Ryu, S.; Hatsugai, Y. Topological Origin of Zero-Energy Edge States in Particle-Hole Symmetric Systems. *Phys. Rev. Lett.* **2002**, *89*, 077002.
- (32) Kobayashi, Y.; Ichi Fukui, K.; Enoki, T.; Kusakabe, K.; Kaburagi, Y. Observation of zigzag and armchair edges of graphite using scanning tunneling microscopy and spectroscopy. *Phys. Rev. B* **2005**, *71*, 193406.
- (33) Li, J.; Sanz, S.; Merino-Diez, N.; Vilas-Varela, M.; Garcia-Lekue, A.; Corso, M.; de Oteyza, D. G.; Frederiksen, T.; Pena, D.; Pascual, J. I. Topological phase transition in chiral graphene nanoribbons: from edge bands to end states. *Nat. Commun.* **2021**, *12*, 5538.

- (34) Sun, Y.-L.; Chen, G.-H.; Du, S.-C.; Chen, Z.-B.; Zhou, Y.-W.; Ye, E.-J. Spin-valley polarized edge states in quasi-one-dimensional asymmetric kagome lattice. *Front. Phys.* **2022**, *10*, 1033836.
- (35) Ushiroguchi, R.; Shuku, Y.; Suizu, R.; Awaga, K. Variable Host-Guest Charge-Transfer Interactions in 1D Channels Formed in a Molecule-Based Honeycomb Lattice of Phenazine Analogue of Triptycene. *Cryst. Growth Des.* **2020**, *20*, 7593.
- (36) Nemoto, R.; Arafune, R.; Nakano, S.; Tsuchiizu, M.; Takagi, N.; Suizu, R.; Uchihashi, T.; Awaga, K. Chiral Honeycomb Lattices of Nonplanar π -Conjugated Supramolecules with Protected Dirac and Flat Bands. *ACS Nano* **2024**, *18*, 19663.
- (37) Bhola, R.; Payamya, P.; Murray, D. J.; Kumar, B.; Teator, A. J.; Schmidt, M. U.; Hammer, S. M.; Saha, A.; Sakamoto, J.; Schluter, A. D.; King, B. T. A Two-Dimensional Polymer from the Anthracene Dimer and Triptycene Motifs. *J. Am. Chem. Soc.* **2013**, *135*, 14134.
- (38) Kissel, P.; Murray, D. J.; Wulftange, W. J.; Catalano, V. J.; King, B. T. A nanoporous two-dimensional polymer by single-crystal-to-single-crystal photopolymerization. *Nat. Chem.* **2014**, *6*, 774.
- (39) Kohl, B.; Bohnwagner, M. V.; Rominger, F.; Wadepohl, H.; Dreuw, A.; Mastalerz, M. Attractive Dispersion Interactions Versus Steric Repulsion of tert-Butyl groups in the Crystal Packing of a D_{3h} -Symmetric Tris(quinoxalinophenanthrophenazine). *Chem.—Eur. J.* **2016**, *22*, 646.
- (40) Das, S.; Nascimbeni, G.; de la Morena, R. O.; Ishiwari, F.; Shoji, Y.; Fukushima, T.; Buck, M.; Zojer, E.; Zharnikov, M. Porous Honeycomb Self-Assembled Monolayers: Tripodal Adsorption and Hidden Chirality of Carboxylate Anchored Triptycenes on Ag. *ACS Nano* **2021**, *15*, 11168.
- (41) Grossmann, L.; King, B. T.; Reichlmaier, S.; Hartmann, N.; Rosen, J.; Heckl, W. M.; Bjork, J.; Lackinger, M. On-surface photopolymerization of two-dimensional polymers ordered on the mesoscale. *Nat. Chem.* **2021**, *13*, 730.
- (42) Zak, J. Berry's phase for energy bands in solids. *Phys. Rev. Lett.* **1989**, *62*, 2747.
- (43) Delplace, P.; Ullmo, D.; Montambaux, G. Zak phase and the existence of edge states in graphene. *Phys. Rev. B* **2011**, *84*, 195452.
- (44) Jovanovic, M.; Schoop, L. M. Simple Chemical Rules for Predicting Band Structures of Kagome Materials. *J. Am. Chem. Soc.* **2022**, *144*, 10978.
- (45) Tang, S.; Ruan, H.; Hu, Z.; Zhao, Y.; Song, Y.; Wang, X. A cationic sulfur-hydrocarbon triradical with an excited quartet state. *Chem. Commun.* **2022**, 58, 1986.