

Supplementary Information

Real-Space Imaging of Band Topology via Wavefunction Zeros

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S1. DARK SETS IN ALL 17 WALLPAPER GROUPS

Here we enumerate the dark sets for all irreps in the 17 wallpaper groups: $p1$, $p2$, pm , pg , cm , pmm , pmg , pgg , cmm , $p4$, $p4m$, $p4g$, $p3$, $p3m1$, $p31m$, $p6$, and $p6m$. We take the high-symmetry data from the Bilbao Crystallographic Server [1–4] and compute each dark set using the formula in the main text. We present tables for the 15 groups with non-vacuous dark sets. In Group No. 1 ($p1$), the only point stabiliser is C_1 , so no symmetry-enforced dark spot is possible. In Group No. 4 (pg), the only non-translation point operation is a fixed-point-free glide; it cannot produce a real-space stabiliser and likewise produces no dark set rule.

Column orthogonality of characters supplies a sharp consistency check on the tables: for each probe position $\mathbf{r}_*$, a sum rule holds:

$$\sum_{\rho} d_{\rho} m_{\mathbf{k}_*, \mathbf{r}_*}(\rho) = |\bar{G}_{\mathbf{k}_*}| / |H_{\mathbf{k}_*, \mathbf{r}_*}| \quad (\text{S1})$$

where $m_{\mathbf{k}_*, \mathbf{r}_*}(\rho)$ is the index of the main text Eq. (4) evaluated for irrep ρ , d_{ρ} is the irrep dimension, and $\bar{G}_{\mathbf{k}_*}$ is the little co-group. Each probe is bright in exactly as many irreps, weighted by dimension, as the index of its stabiliser allows. At a C_3 centre at K , for instance, the sum equals one: exactly one of the three C_3 irreps is bright per centre.

A fixed-point-free nonsymmorphic operation, such as a glide reflection, cannot belong to a real-space stabiliser. Consequently, one-point real-space probes cannot resolve character data carried only by such operations; they distinguish only irreps whose restrictions to the visible, fixed-point symmetries differ. Specifically, we identify the invisible nonsymmorphic sectors for all nonsymmorphic groups as follows. In Group No. 7 (pmg), despite the group being nonsymmorphic, all inequivalent irreps at Γ and Y have distinct dark sets, while at X and S there is only a single two-dimensional projective irrep, so no further ambiguity arises. In Group No. 8 (pgg), the Γ -point irreps A_1 and A_2 cannot be distinguished, nor can B_1 and B_2 , because the members of each pair differ only in their characters under the glide reflections. At X and Y there is only a single two-dimensional projective irrep, so no ambiguity arises at those high-symmetry momenta. At M , the four one-dimensional projective irreps form two complex-conjugate pairs, yet the two pairs have distinct dark sets, with one pair dark at the $2a$ centres and the other at the $2b$ centres. In Group No. 12 ($p4g$), all the Γ -point irreps are resolvable. At X and Y there is only a single two-dimensional projective irrep, while at M the four one-dimensional projective irreps form two complex-conjugate pairs and the remaining irrep is two-dimensional. These three physical classes have distinct dark sets, so the M -point irreps are resolvable up to the complex-conjugate pairing.

Within the visible sector, all irreps at all high-symmetry points in the wallpaper groups have a unique dark set, with one systematic exception: at time-reversal invariant momenta (TRIM) — i.e. $\mathbf{k}_*$ for which $2\mathbf{k}_*$ is a reciprocal lattice vector — complex-conjugate irrep pairs have identical dark sets. Examples include $E_{\pm}$ of the little groups C_3 , C_4 , C_6 . The collision of their dark sets can be understood physically: at such momenta, every realisable local phase is ± 1 , and the pair $(\rho, \bar{\rho})$ consists of time-reversal partners with pointwise identical charge density, which no density measurement can distinguish (SM Sec. S9). However, we note that in systems with time-reversal symmetry, complex-conjugate irreps are properly thought of as two components of a single irreducible corepresentation, and therefore this ambiguity is only meaningful in systems with broken time-reversal symmetry.

The figures and tables below use a common member-resolution convention. Colours identify complete wallpaper-group Wyckoff families. The pale-grey polygon marks the central primitive Wigner–Seitz cell. Repeated markers or line segments outside the grey cell are lattice-related copies included to make the periodic geometry visible. Nearby mathematical labels identify individual members only when a high-symmetry momentum splits a full Wyckoff orbit into subsets with different dark sets. Correspondingly, a table uses the unsplit family label whenever all members of that family have the same dark status, and uses member-resolved labels only when a proper subset must be distinguished. The meaning of solid and dashed symmetry lines is stated in each figure caption.

TABLE I. *p2* (**No. 2**) **Dark sets**. Probe positions are Wyckoff centres $1a = (0, 0)$, $1b = (0, \frac{1}{2})$, $1c = (\frac{1}{2}, 0)$, and $1d = (\frac{1}{2}, \frac{1}{2})$, all with site symmetry 2. High-symmetry momenta are $\Gamma = (0, 0)$, $X = (\pi, 0)$, $Y = (0, \pi)$, and $M = (\pi, \pi)$. Entries list the Wyckoff centres that are *symmetry-forbidden (dark)* by the local projector for each little-group irrep. All little groups are C_2 , with one-dimensional irreps A (even) and B (odd).

	Irrep	Dark set
$\Gamma; C_2$	A	$\emptyset$
	B	$\{1a, 1b, 1c, 1d\}$
$X; C_2$	A	$\{1c, 1d\}$
	B	$\{1a, 1b\}$
$Y; C_2$	A	$\{1b, 1d\}$
	B	$\{1a, 1c\}$
$M; C_2$	A	$\{1b, 1c\}$
	B	$\{1a, 1d\}$

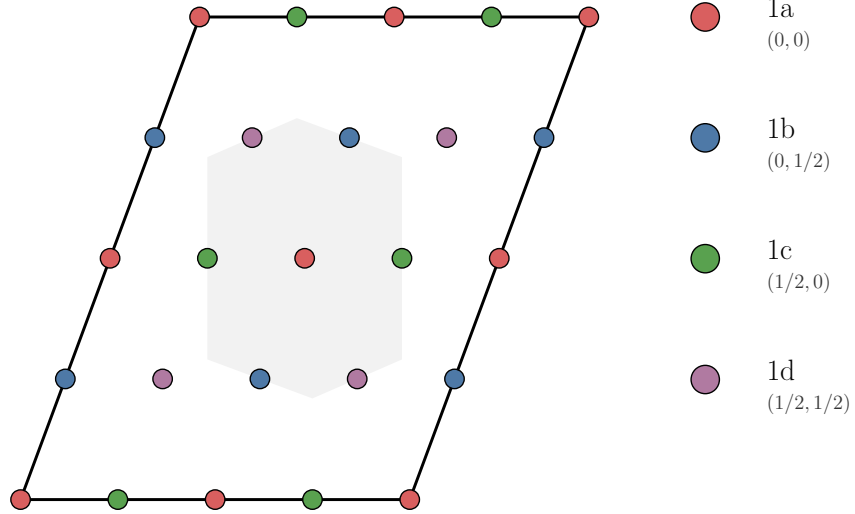


FIG. S1. **Unit cell and Wyckoff positions for $p2$** . Colours distinguish the four inequivalent C_2 -centre families $1a$ – $1d$, with representative coordinates given in the legend. The black parallelogram bounds the displayed periodic patch, while the pale-grey polygon marks the central primitive Wigner–Seitz cell; repeated boundary markers are lattice translates of the same Wyckoff positions.

TABLE II. *pm* (No. 3) **Dark sets**. Probe positions are Wyckoff families $1a = (0, y)$ and $1b = (\frac{1}{2}, y)$, both on vertical mirrors with site symmetry m , and the general family $2c = (x, y), (-x, y)$ with site symmetry 1. High-symmetry momenta are $\Gamma = (0, 0)$, $X = (\pi, 0)$, $Y = (0, \pi)$, and $S = (\pi, \pi)$. Entries list the Wyckoff families that are *symmetry-forbidden (dark)* by the local projector for each little-group irrep. At all four momenta the little co-group is $C_s = \{E, \sigma_x\}$, with one-dimensional irreps A' and A'' satisfying $\chi(\sigma_x) = +1$ and -1 , respectively. The general family $2c$ never yields a symmetry-forced node.

	Irrep	Dark set
$\Gamma; C_s$	A'	$\emptyset$
	A''	$\{1a, 1b\}$
$X; C_s$	A'	$\{1b\}$
	A''	$\{1a\}$
$Y; C_s$	A'	$\emptyset$
	A''	$\{1a, 1b\}$
$S; C_s$	A'	$\{1b\}$
	A''	$\{1a\}$

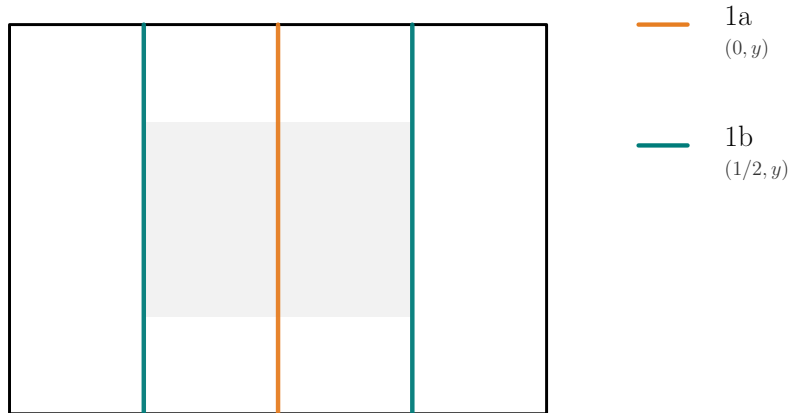


FIG. S2. **Unit cell and Wyckoff positions for *pm***. The orange and teal vertical lines are the mirror families $1a$ and $1b$, respectively. Translated affine copies of a given colour belong to the same Wyckoff family and carry the same table label. The pale-grey rectangle marks the central primitive Wigner-Seitz cell.

TABLE III. *cm* (No. 5) **Dark sets**. The mirror Wyckoff family is $2a = \{(0, y), (\frac{1}{2}, y + \frac{1}{2})\}$ in the conventional centred cell; the two displayed representatives differ by the centring translation and therefore have identical dark status. The general family $4b$ has site symmetry 1 and never yields a symmetry-forced node. The momentum coordinates $\Gamma = (0, 0)$, $X = (\pi, 0)$, $Y = (0, \pi)$, and $S = (\pi, \pi)$. The little co-group is C_s at Γ and S , and C_1 at X and Y .

	Irrep	Dark set
$\Gamma; C_s$	A'	$\emptyset$
	A''	$\{2a\}$
$X; C_1$	A	$\emptyset$
$Y; C_1$	A	$\emptyset$
$S; C_s$	A'	$\emptyset$
	A''	$\{2a\}$

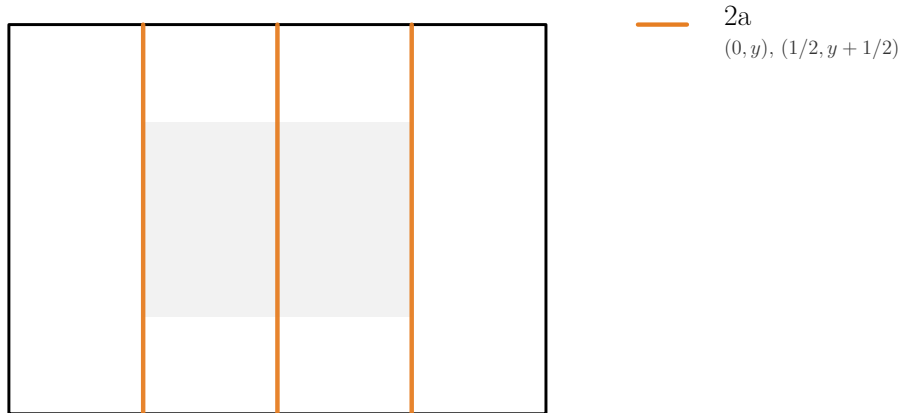


FIG. S3. **Unit cell and Wyckoff positions for *cm***. All orange lines are solid members of the single centred mirror orbit $2a$. They are related by centring or lattice translations and have identical dark status. Accordingly, every table entry labelled $2a$ applies to all shown members.

TABLE IV. *pmm* (No. 6) **Dark sets**. Probe positions are the Wyckoff families $1a = (0,0)$, $1b = (0, \frac{1}{2})$, $1c = (\frac{1}{2}, 0)$, and $1d = (\frac{1}{2}, \frac{1}{2})$, all with site symmetry $2mm$; the horizontal-mirror families $2e = (x, 0)$ and $2f = (x, \frac{1}{2})$; and the vertical-mirror families $2g = (0, y)$ and $2h = (\frac{1}{2}, y)$. High-symmetry momenta are $\Gamma = (0,0)$, $X = (\pi, 0)$, $Y = (0, \pi)$, and $M = (\pi, \pi)$; each little co-group is C_{2v} . We choose B_1 odd under the horizontal mirror and B_2 odd under the vertical mirror. Entries list the Wyckoff families that are *symmetry-forbidden* (*dark*) by the local projector.

	Irrep	Dark set
$\Gamma; C_{2v}$	A_1	$\emptyset$
	A_2	$\{1a, 1b, 1c, 1d, 2e, 2f, 2g, 2h\}$
	B_1	$\{1a, 1b, 1c, 1d, 2e, 2f\}$
	B_2	$\{1a, 1b, 1c, 1d, 2g, 2h\}$
$X; C_{2v}$	A_1	$\{1c, 1d, 2h\}$
	A_2	$\{1a, 1b, 1c, 1d, 2e, 2f, 2g\}$
	B_1	$\{1a, 1b, 1c, 1d, 2e, 2f, 2h\}$
	B_2	$\{1a, 1b, 2g\}$
$Y; C_{2v}$	A_1	$\{1b, 1d, 2f\}$
	A_2	$\{1a, 1b, 1c, 1d, 2e, 2g, 2h\}$
	B_1	$\{1a, 1c, 2e\}$
	B_2	$\{1a, 1b, 1c, 1d, 2f, 2g, 2h\}$
$M; C_{2v}$	A_1	$\{1b, 1c, 1d, 2f, 2h\}$
	A_2	$\{1a, 1b, 1c, 2e, 2g\}$
	B_1	$\{1a, 1c, 1d, 2e, 2h\}$
	B_2	$\{1a, 1b, 1d, 2f, 2g\}$

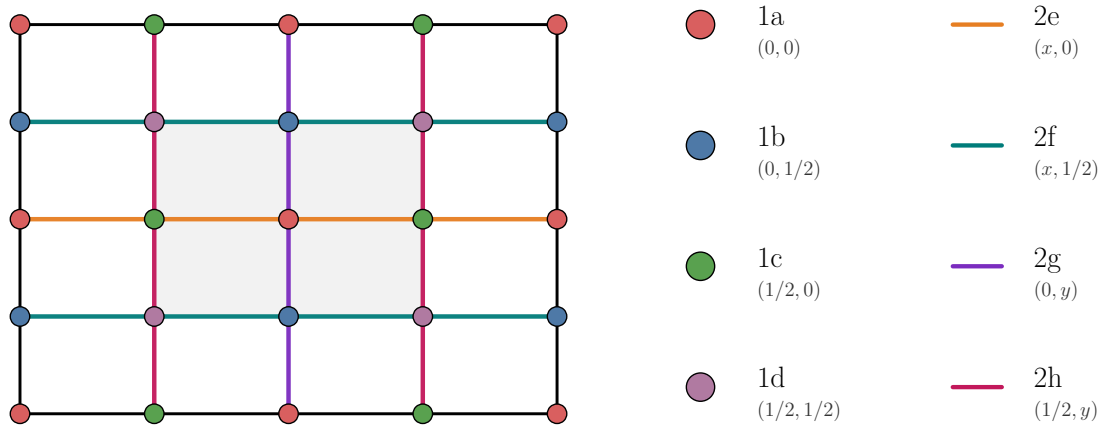


FIG. S4. **Unit cell and Wyckoff positions for *pmm***. Marker colours distinguish the four $2mm$ centres $1a$ – $1d$. The coloured horizontal and vertical lines identify the mirror families $2e$ – $2h$ listed in the legend. Translated copies of a given colour belong to the same family.

TABLE V. *pmg* (No. 7) **Dark sets**. Probe positions are Wyckoff families $2a$ with C_2 centres at $(0,0)$ and $(\frac{1}{2},0)$, $2b$ with C_2 centres at $(0,\frac{1}{2})$ and $(\frac{1}{2},\frac{1}{2})$, and $2c$ on the vertical mirrors with site symmetry m . High-symmetry momenta are $\Gamma = (0,0)$, $X = (\pi,0)$, $Y = (0,\pi)$, and $S = (\pi,\pi)$. At X and S the unique small irrep is two-dimensional and projective; its local projector has positive rank at every listed probe.

	Irrep	Dark set
$\Gamma; C_{2v}$	A_1	$\emptyset$
	A_2	$\{2c\}$
	B_1	$\{2a, 2b\}$
	B_2	$\{2a, 2b, 2c\}$
X	X_5 (2D projective)	$\emptyset$
$Y; C_{2v}$	A_1	$\{2b\}$
	A_2	$\{2b, 2c\}$
	B_1	$\{2a\}$
	B_2	$\{2a, 2c\}$
S	S_5 (2D projective)	$\emptyset$

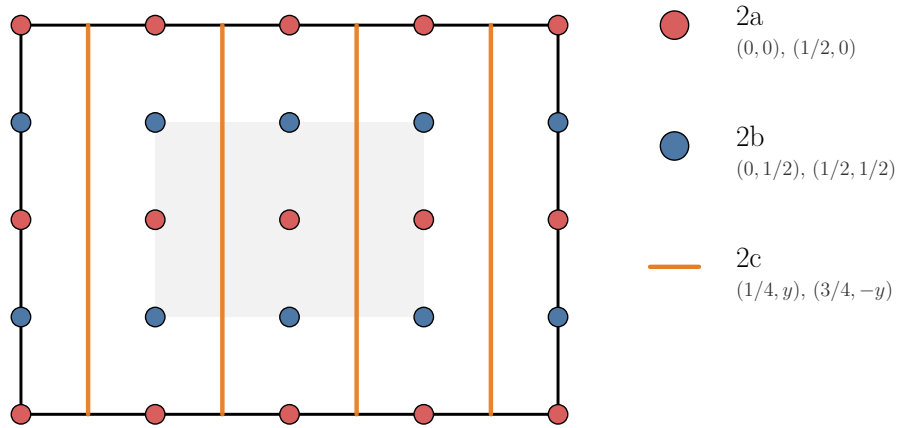


FIG. S5. **Unit cell and Wyckoff positions for *pmg***. Red and blue markers show the C_2 families $2a$ and $2b$. All orange vertical lines are solid affine members of the mirror orbit $2c$.

TABLE VI. *pgg* (**No. 8**) **Dark sets**. Probe positions are the C_2 Wyckoff families $2a = \{(0, 0), (\frac{1}{2}, \frac{1}{2})\}$ and $2b = \{(\frac{1}{2}, 0), (0, \frac{1}{2})\}$. The general family $4c$ has site symmetry 1 and never yields a symmetry-forced node. At X and Y there is one two-dimensional projective small irrep, denoted X_5 and Y_5 . At M there are four one-dimensional projective small irreps; in the ordering (E, C_2, g_x, g_y) their character signatures are $\rho_1 = (1, -1, -i, i)$, $\rho_2 = (1, -1, i, -i)$, $\rho_3 = (1, 1, -i, -i)$, and $\rho_4 = (1, 1, i, i)$.

	Irrep	Dark set
$\Gamma; C_{2v}$	A_1	$\emptyset$
	A_2	$\emptyset$
	B_1	$\{2a, 2b\}$
	B_2	$\{2a, 2b\}$
X	X_5 (2D projective)	$\emptyset$
Y	Y_5 (2D projective)	$\emptyset$
M	ρ_1	$\{2a\}$
	ρ_2	$\{2a\}$
	ρ_3	$\{2b\}$
	ρ_4	$\{2b\}$

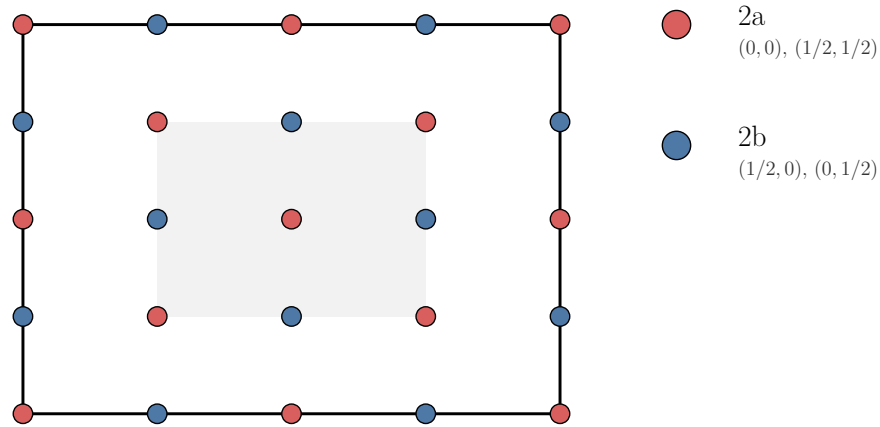


FIG. S6. **Unit cell and Wyckoff positions for *pgg***. Red and blue markers distinguish the two C_2 Wyckoff families $2a$ and $2b$; repeated markers are lattice translates. The general family $4c$ is omitted because its site symmetry is trivial and it never contributes a symmetry-enforced one-point zero.

TABLE VII. *cm*m (No. 9, *c2mm*) **Dark sets**. The figure uses the standard families $2a = \{(0, 0), (\frac{1}{2}, \frac{1}{2})\}$, $2b = \{(0, \frac{1}{2}), (\frac{1}{2}, 0)\}$, the C_2 family $4c$, horizontal-mirror family $4d$, and vertical-mirror family $4e$; the general family is $8f$. At X, Y , we resolve $4c$ into the centring-related pairs $4c^{(1)} = \{(\frac{1}{4}, \frac{1}{4}), (\frac{3}{4}, \frac{3}{4})\}$ and $4c^{(2)} = \{(\frac{3}{4}, \frac{1}{4}), (\frac{1}{4}, \frac{3}{4})\}$. At Γ, M , the label $4c$ denotes the complete four-point family. The momentum coordinates $\Gamma = (0, 0)$, $X = (\pi, 0)$, $Y = (0, \pi)$, and $M = (\pi, \pi)$ are quoted in the reciprocal basis dual to primitive translations. The little co-group is C_{2v} at Γ, M and C_2 at X, Y . We choose B_1 odd under the horizontal mirror and B_2 odd under the vertical mirror.

	Irrep	Dark set
$\Gamma; C_{2v}$	A_1	$\emptyset$
	A_2	$\{2a, 2b, 4d, 4e\}$
	B_1	$\{2a, 2b, 4c, 4d\}$
	B_2	$\{2a, 2b, 4c, 4e\}$
$X; C_2$	A	$\{2b, 4c^{(1)}\}$
	B	$\{2a, 4c^{(2)}\}$
$Y; C_2$	A	$\{2b, 4c^{(2)}\}$
	B	$\{2a, 4c^{(1)}\}$
$M; C_{2v}$	A_1	$\{4c\}$
	A_2	$\{2a, 2b, 4c, 4d, 4e\}$
	B_1	$\{2a, 2b, 4d\}$
	B_2	$\{2a, 2b, 4e\}$

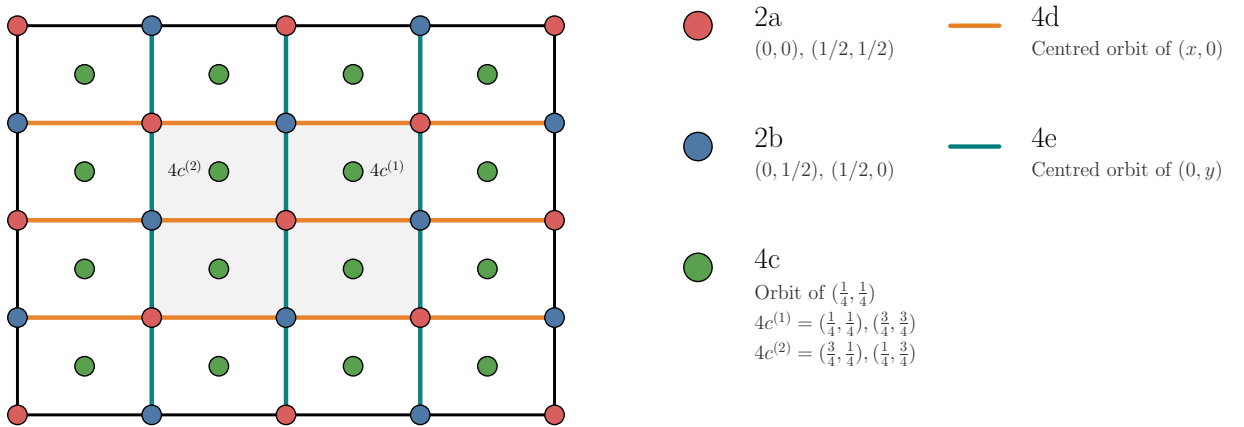


FIG. S7. **Unit cell and Wyckoff positions for *cm̄m***. Colours identify the full families $2a$, $2b$, and $4c$, while orange and teal lines show the horizontal $4d$ and vertical $4e$ mirror families. The nearby labels $4c^{(1)}$ and $4c^{(2)}$ identify the two centring-related pairs required at X, Y ; at Γ, M the table uses the unsplit label $4c$. All displayed $4d$ and $4e$ mirrors form a single member-resolved family.

TABLE VIII. *p4* (**No. 10**) **Dark sets**. Probe positions are $1a = (0, 0)$ and $1b = (\frac{1}{2}, \frac{1}{2})$, with site symmetry 4, and the two members $2c_x = (\frac{1}{2}, 0)$ and $2c_y = (0, \frac{1}{2})$ of the $2c$ family, with site symmetry 2. The general family $4d$ has site symmetry 1 and never yields a symmetry-forced node. High-symmetry momenta are $\Gamma = (0, 0)$, $X = (\pi, 0)$, $Y = (0, \pi)$, and $M = (\pi, \pi)$; the little co-groups are C_4 at Γ, M and C_2 at X, Y . At Γ, M , the label $2c$ denotes both members; the resolved labels $2c_x, 2c_y$ are used at X, Y .

	Irrep	Dark set
$\Gamma; C_4$	A	$\emptyset$
	B	$\{1a, 1b\}$
	E_+	$\{1a, 1b, 2c\}$
	E_-	$\{1a, 1b, 2c\}$
$X; C_2$	A	$\{1b, 2c_x\}$
	B	$\{1a, 2c_y\}$
$Y; C_2$	A	$\{1b, 2c_y\}$
	B	$\{1a, 2c_x\}$
$M; C_4$	A	$\{1b, 2c\}$
	B	$\{1a, 2c\}$
	E_+	$\{1a, 1b\}$
	E_-	$\{1a, 1b\}$

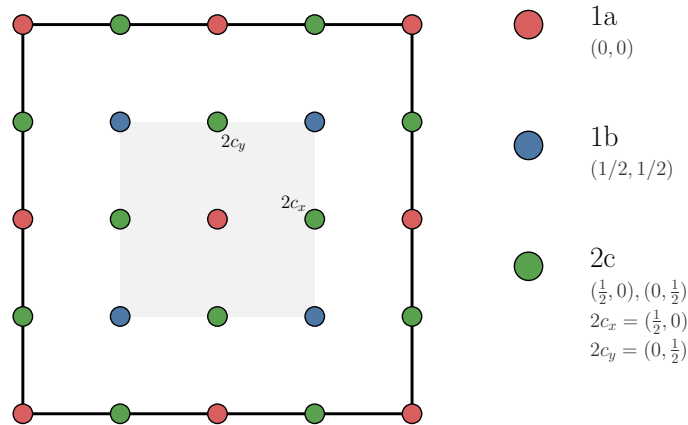


FIG. S8. **Unit cell and Wyckoff positions for *p4***. Colours identify $1a$, $1b$, and the complete $2c$ orbit. The nearby labels $2c_x = (\frac{1}{2}, 0)$ and $2c_y = (0, \frac{1}{2})$ mark the two central-cell members used separately at X, Y . At Γ, M , where the two members have the same dark status, the table uses the unsplit label $2c$.

TABLE IX. $p4m$ (**No. 11**, $p4mm$) **Dark sets**. Probe families are $1a = (0, 0)$ and $1b = (\frac{1}{2}, \frac{1}{2})$ with site symmetry $4mm$; the two members $2c_x = (\frac{1}{2}, 0)$ and $2c_y = (0, \frac{1}{2})$ of the $2c$ family, with site symmetry $2mm$; axis mirrors $4d$; shifted axis mirrors $4e$; and diagonal mirrors $4f$. At X, Y we resolve the axis families as $4d_h : y = 0$, $4d_v : x = 0$, $4e_h : y = \frac{1}{2}$, and $4e_v : x = \frac{1}{2}$. At Γ, M , the unsplit labels $2c$, $4d$, and $4e$ denote the complete corresponding families. The general family $8g$ has site symmetry 1. The little co-groups are C_{4v} at Γ, M and C_{2v} at X, Y . At Γ, M we use the standard convention in which B_1 is even under the axis mirrors and odd under the diagonal mirrors; at X, Y , B_1 is even under the horizontal mirror and B_2 is odd under it.

	Irrep	Dark set
$\Gamma; C_{4v}$	A_1	$\emptyset$
	A_2	$\{1a, 1b, 2c, 4d, 4e, 4f\}$
	B_1	$\{1a, 1b, 4f\}$
	B_2	$\{1a, 1b, 2c, 4d, 4e\}$
	E	$\{1a, 1b, 2c\}$
$X; C_{2v}$	A_1	$\{1b, 2c_x, 4e_v\}$
	A_2	$\{1a, 1b, 2c, 4d, 4e_h\}$
	B_1	$\{1a, 2c_y, 4d_v\}$
	B_2	$\{1a, 1b, 2c, 4d_h, 4e\}$
$Y; C_{2v}$	A_1	$\{1b, 2c_y, 4e_h\}$
	A_2	$\{1a, 1b, 2c, 4d, 4e_v\}$
	B_1	$\{1a, 1b, 2c, 4d_v, 4e\}$
	B_2	$\{1a, 2c_x, 4d_h\}$
$M; C_{4v}$	A_1	$\{1b, 2c, 4e\}$
	A_2	$\{1a, 1b, 2c, 4d, 4f\}$
	B_1	$\{1a, 1b, 2c, 4e, 4f\}$
	B_2	$\{1a, 2c, 4d\}$
	E	$\{1a, 1b\}$

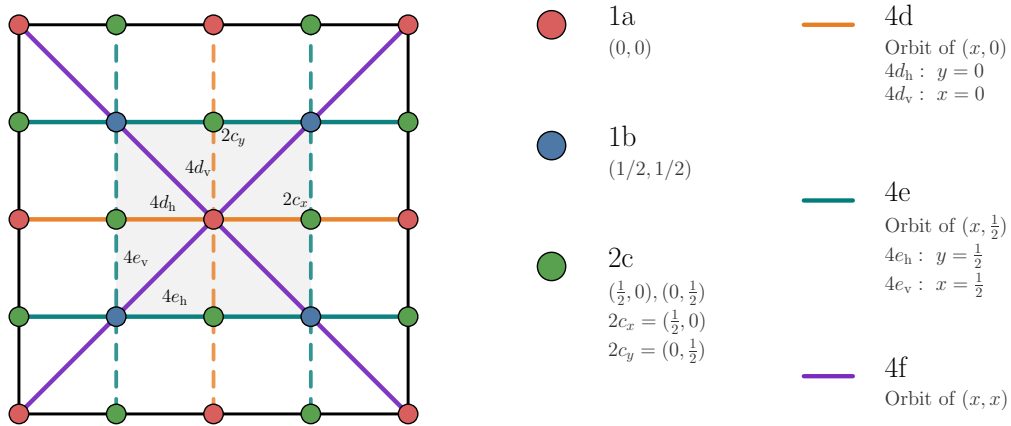


FIG. S9. **Unit cell and Wyckoff positions for $p4m$** . Marker colours identify $1a$, $1b$, and the full $2c$ orbit; nearby labels distinguish $2c_x$ and $2c_y$. For the axis-mirror families, solid orange horizontal segments are $4d_h$ and dashed orange vertical segments are $4d_v$, while solid teal horizontal segments are $4e_h$ and dashed teal vertical segments are $4e_v$. The two solid purple diagonals through the origin together form the unsplit family $4f$. The resolved labels are used at X, Y , whereas Γ, M use the complete-family labels $2c$, $4d$, and $4e$.

TABLE X. $p4g$ (No. 12, $p4gm$) **Dark sets.** Probe families are $2a = \{(0,0), (\frac{1}{2}, \frac{1}{2})\}$ with site symmetry 4, $2b = \{(\frac{1}{2}, 0), (0, \frac{1}{2})\}$ with site symmetry $2mm$, and the diagonal-mirror family $4c$; the general family $8d$ has site symmetry 1. At Γ the small representations are the ordinary C_{4v} irreps. At X, Y there is one two-dimensional projective small irrep, denoted X_5, Y_5 . At M the projective irreps have character signatures in the ordering $(E, C_2, C_4, C_4^{-1}, g_x, g_y, m_d, m_{d'})$: $\rho_1 = (1, -1, -i, i, -i, i, -1, 1)$, $\rho_2 = (1, -1, i, -i, -i, -1, 1)$, $\rho_3 = (1, -1, -i, i, i, -1, -1)$, $\rho_4 = (1, -1, i, -i, -i, i, 1, -1)$, and $\rho_5 = (2, 2, 0, 0, 0, 0, 0, 0)$.

	Irrep	Dark set
$\Gamma; C_{4v}$	A_1	$\emptyset$
	A_2	$\{2b, 4c\}$
	B_1	$\{2a, 2b, 4c\}$
	B_2	$\{2a\}$
	E	$\{2a, 2b\}$
X	X_5 (2D projective)	$\emptyset$
Y	Y_5 (2D projective)	$\emptyset$
M	ρ_1	$\{2a, 2b, 4c\}$
	ρ_2	$\{2a, 2b, 4c\}$
	ρ_3	$\{2a\}$
	ρ_4	$\{2a\}$
	ρ_5	$\{2b\}$

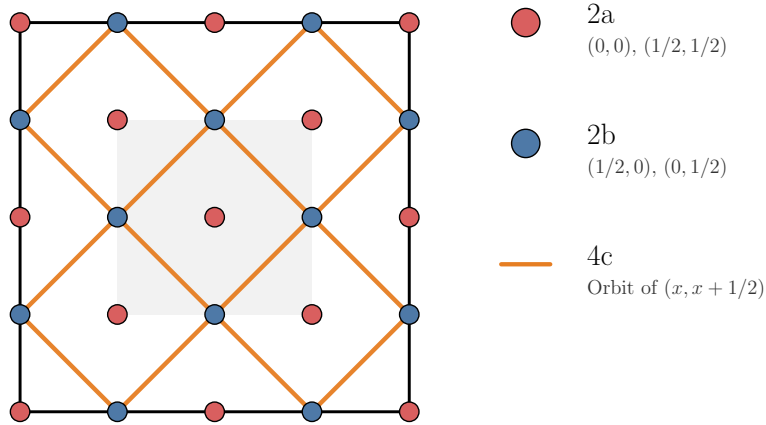


FIG. S10. **Unit cell and Wyckoff positions for $p4g$.** Red and blue markers identify the $2a$ and $2b$ families. All orange diagonal lines are solid members of the mirror orbit $4c$, related by wallpaper-group symmetries and translations. No member split of $4c$ is required in the table.

TABLE XI. *p3* (No. 13) **Dark sets**. Probe families are $1a = (0, 0)$, $1b = (\frac{1}{3}, \frac{2}{3})$, and $1c = (\frac{2}{3}, \frac{1}{3})$, all with site symmetry 3. The general family $3d$ has site symmetry 1. The little co-group is C_3 at Γ, K, K' and C_1 at the edge-centre momenta, which therefore give no nontrivial selection rule. In the Cartesian axes used in Fig. S11, the primitive reciprocal vectors are $\mathbf{b}_1 = (0, 2\pi)$ and $\mathbf{b}_2 = (\sqrt{3}\pi, \pi)$, so $K = \frac{1}{3}(\mathbf{b}_1 + \mathbf{b}_2) = (\pi/\sqrt{3}, \pi)$ and $K' = -K$.

	Irrep	Dark set
$\Gamma; C_3$	A	$\emptyset$
	E_+	$\{1a, 1b, 1c\}$
	E_-	$\{1a, 1b, 1c\}$
$K; C_3$	A	$\{1b, 1c\}$
	E_+	$\{1a, 1b\}$
	E_-	$\{1a, 1c\}$
$K'; C_3$	A	$\{1b, 1c\}$
	E_+	$\{1a, 1c\}$
	E_-	$\{1a, 1b\}$

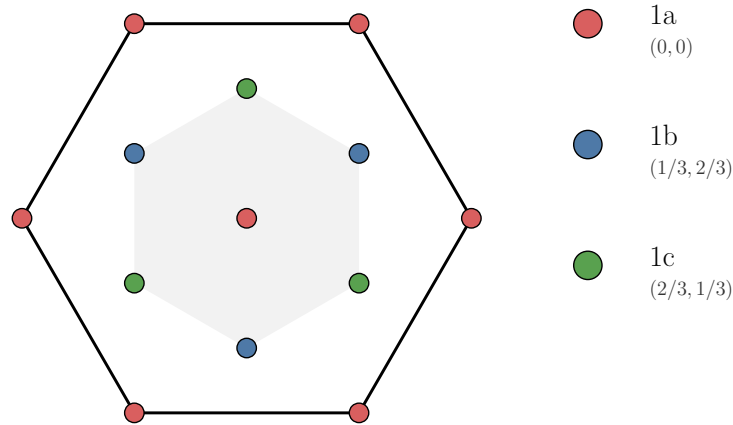


FIG. S11. **Unit cell and Wyckoff positions for $p3$** . The three colours distinguish the inequivalent C_3 centres $1a$, $1b$, and $1c$, with coordinates listed in the legend. In the Cartesian reciprocal convention associated with these axes, $\mathbf{b}_1 = (0, 2\pi)$ and $\mathbf{b}_2 = (\sqrt{3}\pi, \pi)$, hence $K = (\pi/\sqrt{3}, \pi)$ and $K' = -K$. The black hexagon bounds the periodic patch and the pale-grey hexagon is the central primitive Wigner-Seitz cell.

TABLE XII. $p3m1$ (No. 14) **Dark sets**. Probe families are $1a = (0, 0)$, $1b = (\frac{1}{3}, \frac{2}{3})$, and $1c = (\frac{2}{3}, \frac{1}{3})$ with site symmetry $3m$, and $3d$ on the three mirror orientations with site symmetry m . The general family $6e$ has site symmetry 1. In the Cartesian axes used in Fig. S12, take $\mathbf{b}_1 = (0, 2\pi)$ and $\mathbf{b}_2 = (\sqrt{3}\pi, \pi)$, so $K = (\pi/\sqrt{3}, \pi)$, $K' = -K$, and $M_1 = \frac{1}{2}\mathbf{b}_1 = (0, \pi)$. The little co-groups are C_{3v} at Γ , C_3 at K, K' , and C_s at M_1 . The vector M_1 points along the positive Cartesian y direction, and so $3d_{\parallel}$ denotes the member on the vertical mirror $x = 0$, parallel to M_1 ; the other two edge-centre momenta follow by C_3 rotation.

	Irrep	Dark set
$\Gamma; C_{3v}$	A_1	$\emptyset$
	A_2	$\{1a, 1b, 1c, 3d\}$
	E	$\{1a, 1b, 1c\}$
$K; C_3$	A	$\{1b, 1c\}$
	E_+	$\{1a, 1b\}$
	E_-	$\{1a, 1c\}$
$K'; C_3$	A	$\{1b, 1c\}$
	E_+	$\{1a, 1c\}$
	E_-	$\{1a, 1b\}$
$M_1; C_s$	A'	$\emptyset$
	A''	$\{1a, 1b, 1c, 3d_{\parallel}\}$

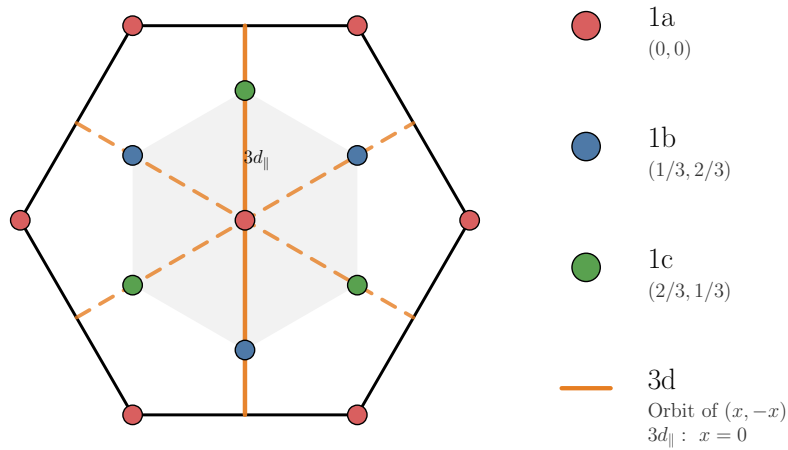


FIG. S12. **Unit cell and Wyckoff positions for $p3m1$** . Orange lines show the three mirror orientations of the $3d$ orbit. In the Cartesian reciprocal convention $\mathbf{b}_1 = (0, 2\pi)$ and $\mathbf{b}_2 = (\sqrt{3}\pi, \pi)$, the selected edge-centre momentum is $M_1 = \frac{1}{2}\mathbf{b}_1 = (0, \pi)$ and therefore points vertically. The solid mirror $x = 0$ is the member $3d_{\parallel}$, parallel to M_1 ; the two dashed mirrors are the other C_3 -related members. At Γ the table uses the unsplit family $3d$, and the other two edge-centre momenta follow by C_3 rotation.

TABLE XIII. $p31m$ (No. 15) **Dark sets**. Probe families are $1a = (0, 0)$ with site symmetry $3m$, $2b = \{(\frac{1}{3}, \frac{2}{3}), (\frac{2}{3}, \frac{1}{3})\}$ with site symmetry 3, and the mirror family $3c$ with site symmetry m . The general family $6d$ has site symmetry 1. In the Cartesian axes used in Fig. S13, take $\mathbf{b}_1 = (0, 2\pi)$ and $\mathbf{b}_2 = (\sqrt{3}\pi, \pi)$, so $K = (\pi/\sqrt{3}, \pi)$, $K' = -K$, and $M_1 = \frac{1}{2}\mathbf{b}_1 = (0, \pi)$. The little co-groups are C_{3v} at Γ, K, K' and C_s at M_1 . Because M_1 points along the positive Cartesian y direction, $3c_\perp$ denotes the member on the horizontal mirror $y = 0$, perpendicular to M_1 ; the other two edge-centre momenta follow by C_3 rotation.

	Irrep	Dark set
$\Gamma; C_{3v}$	A_1	$\emptyset$
	A_2	$\{1a, 3c\}$
	E	$\{1a, 2b\}$
$K; C_{3v}$	A_1	$\{2b\}$
	A_2	$\{1a, 2b, 3c\}$
	E	$\{1a\}$
$K'; C_{3v}$	A_1	$\{2b\}$
	A_2	$\{1a, 2b, 3c\}$
	E	$\{1a\}$
$M_1; C_s$	A'	$\emptyset$
	A''	$\{1a, 3c_\perp\}$

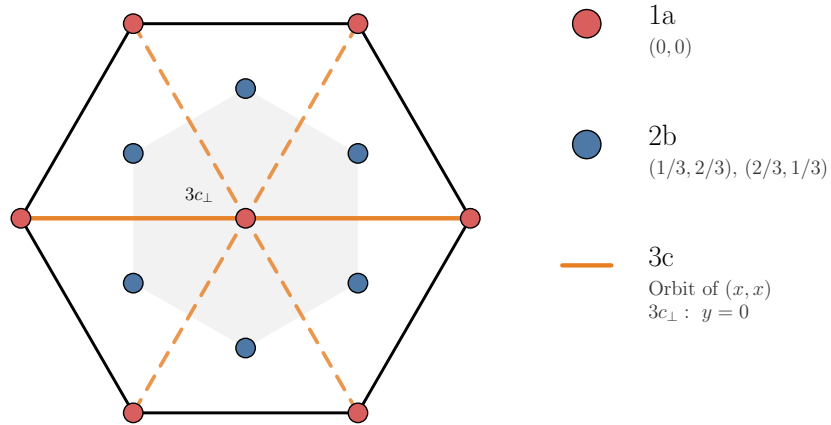


FIG. S13. **Unit cell and Wyckoff positions for $p31m$** . Orange lines show the three mirror orientations of the $3c$ orbit. In the Cartesian reciprocal convention $\mathbf{b}_1 = (0, 2\pi)$ and $\mathbf{b}_2 = (\sqrt{3}\pi, \pi)$, the selected edge-centre momentum is $M_1 = \frac{1}{2}\mathbf{b}_1 = (0, \pi)$ and therefore points vertically. The solid mirror $y = 0$ is the member $3c_\perp$, perpendicular to M_1 ; the two dashed mirrors are the other C_3 -related members. At Γ, K, K' the table uses the unsplit family $3c$.

TABLE XIV. *p6* (No. 16) **Dark sets**. Probe families are $1a = (0, 0)$ with site symmetry 6, $2b = \{(\frac{1}{3}, \frac{2}{3}), (\frac{2}{3}, \frac{1}{3})\}$ with site symmetry 3, and $3c = \{(\frac{1}{2}, 0), (0, \frac{1}{2}), (\frac{1}{2}, \frac{1}{2})\}$ with site symmetry 2. The general family $6d$ has site symmetry 1. In the Cartesian axes used in Fig. S14, take $\mathbf{b}_1 = (0, 2\pi)$ and $\mathbf{b}_2 = (\sqrt{3}\pi, \pi)$, so $K = (\pi/\sqrt{3}, \pi)$, $K' = -K$, and $M_1 = \frac{1}{2}\mathbf{b}_1 = (0, \pi)$; M_1 points vertically and the other two edge-centre momenta follow by C_3 rotation. At K, K' the two $2b$ members are denoted $2b^{(1)} = (\frac{1}{3}, \frac{2}{3})$ and $2b^{(2)} = (\frac{2}{3}, \frac{1}{3})$. At M_1 we write $3c_x = (\frac{1}{2}, 0)$, $3c_y = (0, \frac{1}{2})$, and $3c_d = (\frac{1}{2}, \frac{1}{2})$.

	Irrep	Dark set
$\Gamma; C_6$	A	$\emptyset$
	B	$\{1a, 3c\}$
	E_1^+	$\{1a, 2b, 3c\}$
	E_1^-	$\{1a, 2b, 3c\}$
	E_2^+	$\{1a, 2b\}$
	E_2^-	$\{1a, 2b\}$
$K; C_3$	A	$\{2b\}$
	E_+	$\{1a, 2b^{(1)}\}$
	E_-	$\{1a, 2b^{(2)}\}$
$K'; C_3$	A	$\{2b\}$
	E_+	$\{1a, 2b^{(2)}\}$
	E_-	$\{1a, 2b^{(1)}\}$
$M_1; C_2$	A	$\{3c_x, 3c_d\}$
	B	$\{1a, 3c_y\}$

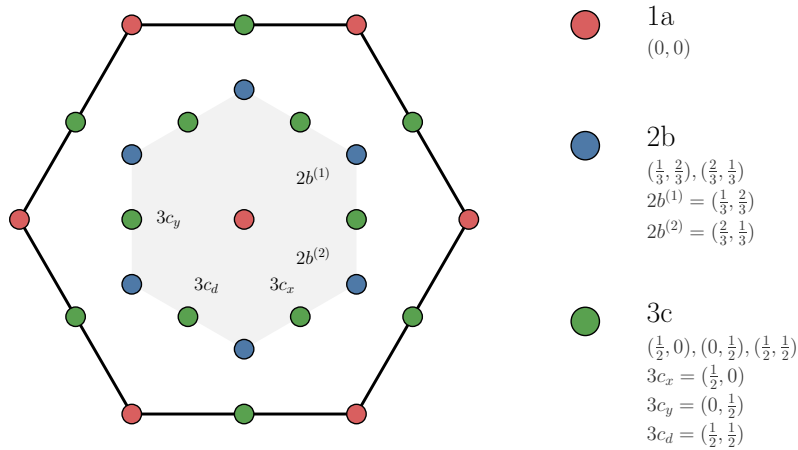


FIG. S14. **Unit cell and Wyckoff positions for *p6***. The legend gives the complete $1a$, $2b$, and $3c$ families. In the Cartesian reciprocal convention $\mathbf{b}_1 = (0, 2\pi)$ and $\mathbf{b}_2 = (\sqrt{3}\pi, \pi)$, one has $K = (\pi/\sqrt{3}, \pi)$, $K' = -K$, and $M_1 = (0, \pi)$, with M_1 directed vertically. Nearby labels identify $2b^{(1)}$ and $2b^{(2)}$, used separately at K, K' , and $3c_x, 3c_y$, and $3c_d$, used at M_1 . Complete-family labels are retained whenever all members have the same dark status; the other two edge-centre momenta follow by C_3 rotation.

TABLE XV. $p6m$ (No. 17, $p6mm$) **Dark sets.** The standard Wyckoff families are $1a = (0,0)$ with site symmetry $6mm$, $2b = \{(\frac{1}{3}, \frac{2}{3}), (\frac{2}{3}, \frac{1}{3})\}$ with site symmetry $3m$, $3c = \{(\frac{1}{2}, 0), (0, \frac{1}{2}), (\frac{1}{2}, \frac{1}{2})\}$ with site symmetry $2mm$, and the two mirror families $6d$ and $6e$; the general family is $12f$. In the Cartesian axes used in Fig. S15, take $\mathbf{b}_1 = (0, 2\pi)$ and $\mathbf{b}_2 = (\sqrt{3}\pi, \pi)$, so $K = (\pi/\sqrt{3}, \pi)$, $K' = -K$, and $M_1 = \frac{1}{2}\mathbf{b}_1 = (0, \pi)$. At M_1 we write $3c_x = (\frac{1}{2}, 0)$, $3c_y = (0, \frac{1}{2})$, and $3c_d = (\frac{1}{2}, \frac{1}{2})$. The vector M_1 points vertically, and so the two mirror-orbit subsets fixed by the M_1 little group are denoted $6d_\perp$ for the horizontal mirror pair and $6e_\parallel$ for the vertical mirror pair; in fractional real-space coordinates they may be represented as $6d_\perp = \{(0, x), (0, -x)\}$ and $6e_\parallel = \{(2x, x), (-2x, -x)\}$. The other two edge-centre momenta follow by C_3 rotation. We choose B_1 odd on the $6d$ mirrors and B_2 odd on the $6e$ mirrors.

	Irrep	Dark set
$\Gamma; C_{6v}$	A_1	$\emptyset$
	A_2	$\{1a, 2b, 3c, 6d, 6e\}$
	B_1	$\{1a, 3c, 6d\}$
	B_2	$\{1a, 2b, 3c, 6e\}$
	E_1	$\{1a, 2b, 3c\}$
	E_2	$\{1a, 2b\}$
$K; C_{3v}$	A_1	$\{2b\}$
	A_2	$\{1a, 2b, 3c, 6d\}$
	E	$\{1a\}$
$K'; C_{3v}$	A_1	$\{2b\}$
	A_2	$\{1a, 2b, 3c, 6d\}$
	E	$\{1a\}$
$M_1; C_{2v}$	A_1	$\{3c_x, 3c_d\}$
	A_2	$\{1a, 2b, 3c, 6d_\perp, 6e_\parallel\}$
	B_1	$\{1a, 3c_y, 6d_\perp\}$
	B_2	$\{1a, 2b, 3c_y, 6e_\parallel\}$

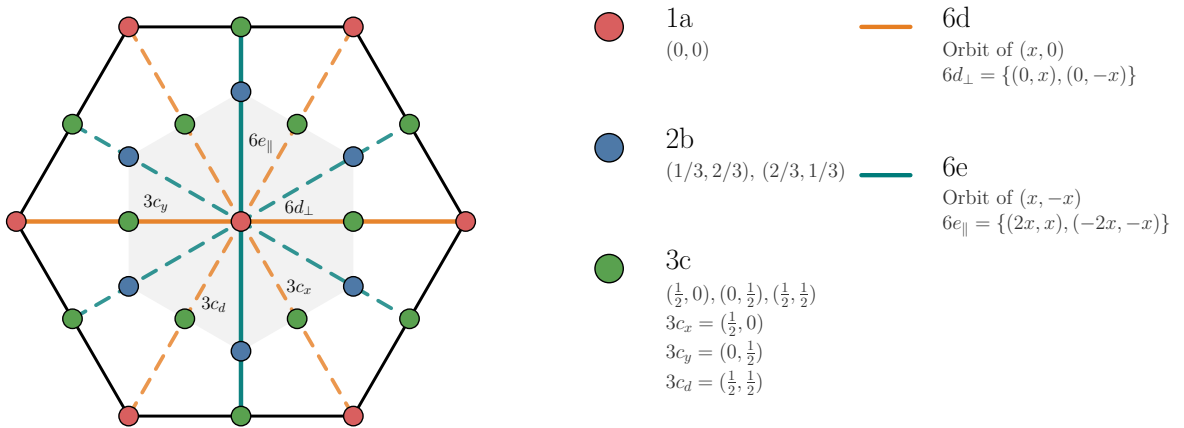


FIG. S15. **Unit cell and Wyckoff positions for $p6m$.** In the Cartesian reciprocal convention $\mathbf{b}_1 = (0, 2\pi)$ and $\mathbf{b}_2 = (\sqrt{3}\pi, \pi)$, the selected edge-centre momentum is $M_1 = \frac{1}{2}\mathbf{b}_1 = (0, \pi)$. Marker labels distinguish $3c_x$, $3c_y$, and $3c_d$ for M_1 ; the $2b$ family remains unsplit. The solid horizontal orange mirror is $6d_\perp$ and the solid vertical teal mirror is $6e_\parallel$. Dashed orange and teal lines are the remaining C_6 -related members of the $6d$ and $6e$ orbits.

S2. GAUGE INVARIANCE OF THE DARK SET

The band representation of a wave function depends on the definition of the symmetries: for instance, whether threefold rotation is defined relative to the origin or relative to another threefold symmetric point in the unit cell. Consequently, one is naturally led to ask the question: are the symmetry-enforced zeros of the wave function gauge invariant? This is particularly important for comparing with scanning tunnelling microscopy which images the charge density — a gauge-invariant observable.

In this section we show that upon a redefinition of the symmetries, while the irrep of the wave function changes, the physical position of these zeros does not. That is to say, the locations of the symmetry-enforced zeros in a new coordinate system are related to the locations of the zeros in the old coordinate system by the associated coordinate transformation.

A. Proof of gauge invariance

Using the same notation as in the main text, we let $h = \{R \mid \mathbf{t}_h\}$ be a space-group operation, acting on real-space coordinates as $\mathbf{r} \mapsto R\mathbf{r} + \mathbf{t}_h$. Let $\mathbf{k}_*$ be a high-symmetry momentum and let $\mathbf{r}_*$ be a high-symmetry point in the unit cell. The common stabiliser is $H_{\mathbf{k}_*, \mathbf{r}_*} = \{h \in G : R\mathbf{k}_* = \mathbf{k}_* + \mathbf{G}_h, R\mathbf{r}_* + \mathbf{t}_h = \mathbf{r}_*\}$. The symmetry action on the Bloch wavefunctions is

$$U_h \Psi_{\mathbf{k}_*, a} = e^{-i\mathbf{k}_* \cdot \mathbf{t}_h} \sum_b [D_{\rho, \mathbf{k}_*}(h)]_{ba} \Psi_{\mathbf{k}_*, b}. \quad (\text{S2})$$

Since $h \in G_{\mathbf{k}_*}$ implies $R\mathbf{k}_* = \mathbf{k}_* + \mathbf{G}_h$, the factors $e^{-i\mathbf{k}_* \cdot \mathbf{t}_h}$ multiply consistently under the stabiliser group law, the residual reciprocal-lattice phases being equal to unity. More precisely, from the composition rule $\mathbf{t}_{hh'} = \mathbf{t}_h + R\mathbf{t}_{h'}$ the assigned phases obey $e^{-i\mathbf{k}_* \cdot \mathbf{t}_h} e^{-i\mathbf{k}_* \cdot \mathbf{t}_{h'}} = e^{-i(R_h^{-1} \mathbf{G}_h) \cdot \mathbf{t}_{h'}} e^{-i\mathbf{k}_* \cdot \mathbf{t}_{hh'}}$. The allowed local values are obtained by taking the trace of the projector

$$P_{\mathbf{k}_*, \mathbf{r}_*} = \frac{1}{|H_{\mathbf{k}_*, \mathbf{r}_*}|} \sum_{h \in H_{\mathbf{k}_*, \mathbf{r}_*}} e^{-i\mathbf{k}_* \cdot \mathbf{t}_h} D_{\rho, \mathbf{k}_*}(h). \quad (\text{S3})$$

That is, the selection rule is $m_{\mathbf{k}_*, \mathbf{r}_*} = \text{Tr } P_{\mathbf{k}_*, \mathbf{r}_*} \neq 0$.

Now shift the coordinate origin by δ , so that $\mathbf{r}' = \mathbf{r} - \delta$. The same physical operation h is written in the new coordinates as $h' = \{R \mid \mathbf{t}'_h\}$, with $\mathbf{t}'_h = \mathbf{t}_h + (R - 1)\delta$. Indeed,

$$\mathbf{r}' \mapsto R\mathbf{r}' + \mathbf{t}_h + (R - 1)\delta. \quad (\text{S4})$$

If h fixes $\mathbf{r}_*$ in the old coordinates, then h' fixes $\mathbf{r}'_* = \mathbf{r}_* - \delta$ in the new coordinates, since $R\mathbf{r}'_* + \mathbf{t}'_h = R\mathbf{r}_* + \mathbf{t}_h - \delta = \mathbf{r}_* - \delta = \mathbf{r}'_*$. Hence the stabilisers $H_{\mathbf{k}_*, \mathbf{r}_*}$ and $H'_{\mathbf{k}_*, \mathbf{r}'_*}$ are the same physical group, written in two coordinate systems. That is, for a site-symmetry element of a symmorphic group the Seitz translation $\mathbf{t}_{h'} = (1 - R_{h'})\mathbf{r}_*$ is a Bravais lattice vector, so the residual phase is unity and $h \mapsto e^{-i\mathbf{k}_* \cdot \mathbf{t}_h} D_{\rho, \mathbf{k}_*}(h)$ is a representation of $H_{\mathbf{k}_*, \mathbf{r}_*}$.

Now, the matrix representing the full unitary action of the symmetry changes under a Bloch-basis gauge transformation $\Psi'_{\mathbf{k}_*} = W_{\mathbf{k}_*}^{-1} \Psi_{\mathbf{k}_*}$ through

$$e^{-i\mathbf{k}_* \cdot \mathbf{t}'_h} D'_{\rho, \mathbf{k}_*}(h') = W_{\mathbf{k}_*}^{-1} e^{-i\mathbf{k}_* \cdot \mathbf{t}_h} D_{\rho, \mathbf{k}_*}(h) W_{\mathbf{k}_*}. \quad (\text{S5})$$

Equivalently,

$$D'_{\rho, \mathbf{k}_*}(h') = e^{i\mathbf{k}_* \cdot (\mathbf{t}'_h - \mathbf{t}_h)} W_{\mathbf{k}_*}^{-1} D_{\rho, \mathbf{k}_*}(h) W_{\mathbf{k}_*}. \quad (\text{S6})$$

The transformed local projector is therefore

$$P'_{\mathbf{k}_*, \mathbf{r}'_*} = W_{\mathbf{k}_*}^{-1} P_{\mathbf{k}_*, \mathbf{r}_*} W_{\mathbf{k}_*}. \quad (\text{S7})$$

Hence $m'_{\mathbf{k}_*, \mathbf{r}'_*} = \text{Tr } P'_{\mathbf{k}_*, \mathbf{r}'_*} = \text{Tr } P_{\mathbf{k}_*, \mathbf{r}_*} = m_{\mathbf{k}_*, \mathbf{r}_*}$. In particular,

$$m_{\mathbf{k}_*, \mathbf{r}_*} = 0 \iff m'_{\mathbf{k}_*, \mathbf{r}'_*} = 0. \quad (\text{S8})$$

Thus symmetry-enforced zeros are invariant under a passive change of origin. The same argument covers embedding-gauge changes in tight-binding descriptions, as such a change is a unitary transformation $W_{\mathbf{k}}$ of the Bloch basis; since the projector changes by conjugation, its rank and trace do not change. Similarly, global reorientation of the rotation axes acts on the operations $\{R \mid \mathbf{t}_h\}$ by conjugation with a fixed point-group element and on the Bloch basis by a $\mathbf{k}$ -independent unitary; the projector again transforms by conjugation, so its trace, and with it the dark set, is unchanged.

TABLE XVI. Rotation-centre data for the 1H-TMD triangular lattice in two coordinate systems. We define the positions $\mathbf{r}_*$ with the origin at the 1a position. The columns $\mathbf{t}_{C_3}$ and $\mathbf{t}_{C_3^2}$ are the Seitz translations of C_3 and C_3^2 when the rotation axis is at 1a. The columns $\mathbf{t}'_{C_3}$ and $\mathbf{t}'_{C_3^2}$ give the Seitz translations after shifting the rotation axis to the hollow site 1c.

Site	$\mathbf{r}_*$	$\mathbf{t}_{C_3}$	$\mathbf{t}_{C_3^2}$	$\mathbf{t}'_{C_3}$	$\mathbf{t}'_{C_3^2}$
1a	0	0	0	$-\mathbf{R}_1$	$-\mathbf{R}_1 - \mathbf{R}_2$
1b	$\frac{1}{3}\mathbf{R}_1 + \frac{2}{3}\mathbf{R}_2$	$\mathbf{R}_1 + \mathbf{R}_2$	$\mathbf{R}_2$	$\mathbf{R}_2$	$-\mathbf{R}_1$
1c	$\frac{2}{3}\mathbf{R}_1 + \frac{1}{3}\mathbf{R}_2$	$\mathbf{R}_1$	$\mathbf{R}_1 + \mathbf{R}_2$	0	0

B. Worked example: shifting the origin from 1a to 1c in 1H-TMDs

Here we consider the example of changing the origin in the 1H-TMD example from the 1a position to the 1c position, noting that both sites have the exact same triangular symmetry. The selection rules for the origin at 1a are discussed in the main text; now we shift the origin by $\boldsymbol{\delta} = \mathbf{r}_{1c}$. For the C_3 generator and its square, the old Seitz translations are $\mathbf{t}_{\mathbf{r}_*,n}$, while the new translations after shifting the origin to 1c are (Table XVI)

$$\mathbf{t}'_{\mathbf{r}_*,n} = \mathbf{t}_{\mathbf{r}_*,n} - \mathbf{t}_{1c,n}, \quad n = 1, 2. \quad (\text{S9})$$

Since the new C_3 generator is the old hollow-centred rotation, its character is

$$\chi'_{\mathbf{k}}(C_3^n) = e^{-i\mathbf{k} \cdot \mathbf{t}_{1c,n}} \chi_{\mathbf{k}}(C_3^n), \quad n = 1, 2. \quad (\text{S10})$$

For the valence band at the K point, we use $\chi_K(C_3) = \omega$, $\chi_K(C_3^2) = \omega^2$, $\omega = e^{2\pi i/3}$, and $K \cdot \mathbf{R}_1 = K \cdot \mathbf{R}_2 = \frac{2\pi}{3}$. Hence, the new characters are $\chi'_K(C_3) = e^{-iK \cdot \mathbf{R}_1} \omega = 1$ and $\chi'_K(C_3^2) = e^{-iK \cdot (\mathbf{R}_1 + \mathbf{R}_2)} \omega^2 = 1$. So, in the 1c-origin convention, the same valence band has a trivial C_3 character at K , consistent with the fact that the valence band can be represented by an s -like orbital on the hollow site. The new selection-rule index is

$$m'_{\mathbf{k},\mathbf{r}_*} = \frac{1}{3} \sum_{n=0}^2 e^{-i\mathbf{k} \cdot \mathbf{t}'_{\mathbf{r}_*,n}} \chi'_{\mathbf{k}}(C_3^n), \quad (\text{S11})$$

with $\mathbf{t}'_{\mathbf{r}_*,0} = 0$ and $\chi'_{\mathbf{k}}(C_3^0) = 1$. At K , because $\chi'_K(C_3) = \chi'_K(C_3^2) = 1$, the shifted-origin columns of Table XVI give $m'_{K,1a} = 0$, $m'_{K,1b} = 0$, and $m'_{K,1c} = 1$, exactly as in the main text. The physical dark and bright sites are unchanged; what changed is the representation of the C_3 generator, and that change is exactly cancelled by the change in the Seitz translations entering the selection rule.

S3. STM SIMULATIONS

In this section, we describe how the simulated STM data are computed and details of the model Hamiltonians used.

A. Calculating STM data from tight-binding models

The differential tunnelling current imaged in STM is proportional to $\text{LDOS}(\text{eV}, \mathbf{r})$, where eV is the bias voltage, and the local density of states (LDOS) is given by the expectation value of the density at fixed energy,

$$\text{LDOS}(E, \mathbf{r}) = -\frac{1}{\pi} \text{Im} \langle c_{\mathbf{r}} c_{\mathbf{r}}^{\dagger} \rangle_E = -\frac{1}{\pi} \text{Im} G(E, \mathbf{r}) \quad (\text{S12})$$

where $c_{\mathbf{r}}^{\dagger}$ is the electron creation operator and $G(E, \mathbf{r})$ is the electron Green's function. To relate the continuum electronic density of states to the wavefunctions of a lattice model, we expand the continuum electron operator in terms of lattice creation operators associated to an orbital σ and a lattice site $\mathbf{R}$, via $c_{\mathbf{r}}^{\dagger} = \sum_{\sigma \mathbf{R}} w_{\sigma \mathbf{R}}(\mathbf{r}) c_{\sigma \mathbf{R}}^{\dagger}$ where $w_{\sigma \mathbf{R}}(\mathbf{r})$ are a set of real space orbitals indexed by σ and centred at the lattice sites $\mathbf{R}$, e.g. [5–13]. One obtains

$$\begin{aligned} \text{LDOS}(E, \mathbf{r}) &= -\frac{1}{\pi} \text{Im} \sum_{\sigma \sigma', \mathbf{R} \mathbf{R}'} w_{\sigma \mathbf{R}}^*(\mathbf{r}) w_{\sigma' \mathbf{R}'}(\mathbf{r}) \langle c_{\sigma \mathbf{R}} c_{\sigma' \mathbf{R}'}^{\dagger} \rangle_E \\ &= -\frac{1}{\pi} \text{Im} \sum_{\sigma \sigma', \mathbf{R} \mathbf{R}'} w_{\sigma \mathbf{R}}^*(\mathbf{r}) w_{\sigma' \mathbf{R}'}(\mathbf{r}) G(E, \mathbf{R} - \mathbf{R}')_{\sigma \sigma'} \end{aligned} \quad (\text{S13})$$

where $G(E, \mathbf{R} - \mathbf{R}')_{\sigma \sigma'}$ is the Green's function of the lattice model,

$$G(E, \mathbf{R} - \mathbf{R}')_{\sigma \sigma'} = \int \frac{d^d \mathbf{k}}{(2\pi)^d} \left(\frac{1}{E - \mathcal{H}(\mathbf{k}) + i0} \right)_{\sigma \sigma'} e^{i\mathbf{k} \cdot (\mathbf{R} - \mathbf{R}')} \quad (\text{S14})$$

where $\mathcal{H}(\mathbf{k})_{\sigma \sigma'}$ is the tight-binding Hamiltonian, defined as a matrix acting in orbital basis.

B. Numerical implementation

For the simulated STM data, we evaluate a band-projected version of Eq. (S14). Let $\mathcal{B}$ denote the set of tight-binding bands included in the projected LDOS at the chosen probe energy E . For a finite momentum mesh $\mathcal{K}$, the lattice Green function used in the simulations is

$$G_{\alpha \beta}(E, \Delta \mathbf{R}) = \frac{1}{N_{\mathcal{K}}} \sum_{\mathbf{k} \in \mathcal{K}} \sum_{n \in \mathcal{B}} \frac{e^{i\mathbf{k} \cdot \Delta \mathbf{R}} u_{\alpha n}(\mathbf{k}) u_{\beta n}^*(\mathbf{k})}{E + i\eta - \varepsilon_n(\mathbf{k})}, \quad (\text{S15})$$

where α, β label the tight-binding orbitals, $\varepsilon_n(\mathbf{k})$ is the band energy, $u_{\alpha n}(\mathbf{k})$ is the corresponding normalised eigenvector, and η is the Lorentzian broadening. In figures where the targeted momentum is related to symmetry-equivalent points by point-group rotations, the numerical quadrature is symmetrised by averaging over the corresponding rotated momenta.

The continuum LDOS is then reconstructed from the lattice Green function by

$$\text{LDOS}(E, \mathbf{r}) = -\frac{1}{\pi} \text{Im} \sum_{\alpha \beta} \sum_{\mathbf{R}, \mathbf{R}'} w_{\alpha}^*(\mathbf{r} - \mathbf{R} - \boldsymbol{\tau}_{\alpha}) w_{\beta}(\mathbf{r} - \mathbf{R}' - \boldsymbol{\tau}_{\beta}) G_{\alpha \beta}(E, \mathbf{R} - \mathbf{R}'). \quad (\text{S16})$$

The vectors $\boldsymbol{\tau}_{\alpha}$ specify the intracell orbital positions. The real-space sums are evaluated on finite patches large enough that increasing the patch changes the plotted LDOS only below the visual resolution of the figures. All LDOS panels in Figs. 1, 2, 3, S17, and S18 are normalised independently according to

$$Z_{\text{plot}}(\mathbf{r}) = \frac{\text{LDOS}(E, \mathbf{r})}{\max_{\mathbf{r} \in \Omega} \text{LDOS}(E, \mathbf{r})}, \quad (\text{S17})$$

where Ω is the plotted real-space region.

C. Three-orbital model of TMDs

Our calculations of the LDOS for TMDs employ the minimal three-band model of Ref. [14], comprised of d_{z^2} , d_{xy} , and $d_{x^2-y^2}$ orbitals located on the triangular lattice formed by the tungsten atoms. The model is given by

$$H^{\text{NN}}(\mathbf{k}) = \begin{bmatrix} V_0 & V_1 & V_2 \\ V_1^* & V_{11} & V_{12} \\ V_2^* & V_{12}^* & V_{22} \end{bmatrix} \quad (\text{S18})$$

where

$$V_0 = \epsilon_1 - \epsilon_0 + 2t_0(2\cos\alpha\cos\beta + \cos 2\alpha) + 2r_0(2\cos 3\alpha\cos\beta + \cos 2\beta) + 2u_0(2\cos 2\alpha\cos 2\beta + \cos 4\alpha) \quad (\text{S19})$$

$$\text{Re}[V_1] = -2\sqrt{3}t_2\sin\alpha\sin\beta + 2(r_1 + r_2)\sin 3\alpha\sin\beta - 2\sqrt{3}u_2\sin 2\alpha\sin 2\beta, \quad (\text{S20})$$

$$\text{Im}[V_1] = 2t_1\sin\alpha(2\cos\alpha + \cos\beta) + 2(r_1 - r_2)\sin 3\alpha\cos\beta + 2u_1\sin 2\alpha(2\cos 2\alpha + \cos 2\beta), \quad (\text{S21})$$

$$\text{Re}[V_2] = 2t_2(\cos 2\alpha - \cos\alpha\cos\beta) - \frac{2}{\sqrt{3}}(r_1 + r_2)(\cos 3\alpha\cos\beta - \cos 2\beta) + 2u_2(\cos 4\alpha - \cos 2\alpha\cos 2\beta), \quad (\text{S22})$$

$$\text{Im}[V_2] = 2\sqrt{3}t_1\cos\alpha\sin\beta + \frac{2}{\sqrt{3}}(r_1 - r_2)\sin\beta(\cos 3\alpha + 2\cos\beta) + 2\sqrt{3}u_1\cos 2\alpha\sin 2\beta, \quad (\text{S23})$$

$$V_{11} = \epsilon_2 - \epsilon_0 + (t_{11} + 3t_{22})\cos\alpha\cos\beta + 2t_{11}\cos 2\alpha + 4r_{11}\cos 3\alpha\cos\beta + 2(r_{11} + \sqrt{3}r_{12})\cos 2\beta \quad (\text{S24})$$

$$+ (u_{11} + 3u_{22})\cos 2\alpha\cos 2\beta + 2u_{11}\cos 4\alpha, \quad (\text{S25})$$

$$\text{Re}[V_{12}] = \sqrt{3}(t_{22} - t_{11})\sin\alpha\sin\beta + 4r_{12}\sin 3\alpha\sin\beta + \sqrt{3}(u_{22} - u_{11})\sin 2\alpha\sin 2\beta, \quad (\text{S26})$$

$$\text{Im}[V_{12}] = 4t_{12}\sin\alpha(\cos\alpha - \cos\beta) + 4u_{12}\sin 2\alpha(\cos 2\alpha - \cos 2\beta), \quad (\text{S27})$$

$$V_{22} = \epsilon_2 - \epsilon_0 + (3t_{11} + t_{22})\cos\alpha\cos\beta + 2t_{22}\cos 2\alpha + 2r_{11}(2\cos 3\alpha\cos\beta + \cos 2\beta) \quad (\text{S28})$$

$$+ \frac{2}{\sqrt{3}}r_{12}(4\cos 3\alpha\cos\beta - \cos 2\beta) + (3u_{11} + u_{22})\cos 2\alpha\cos 2\beta + 2u_{22}\cos 4\alpha \quad (\text{S29})$$

$$(\alpha, \beta) = (k_x a/2, \sqrt{3}k_y a/2) \quad (\text{S30})$$

We perform numerical simulations using parameters for WSe₂; when only nearest-neighbour hoppings are retained, the optimal fit to DFT for WSe₂ is given by $t_0 = -0.146$, $t_1 = -0.124$, $t_2 = 0.507$, $t_{11} = 0.117$, $t_{12} = 0.127$, $t_{22} = 0.015$, $\epsilon_1 = 0.728$, $\epsilon_2 = 1.655$ (all units in eV). Our results incorporated next-nearest-neighbour hoppings r_i , u_i , (values from Ref. [14]), but the STM simulations are essentially unchanged if only nearest-neighbour terms are used.

For the STM simulations, the continuum orbital envelopes used are

$$w_{z^2}(\mathbf{r}) = \frac{1}{4}\sqrt{\frac{5}{\pi}}g(\mathbf{r}), \quad w_{xy}(\mathbf{r}) = \frac{1}{2}\sqrt{\frac{15}{2\pi}}\frac{2xy}{|\mathbf{r}|}g(\mathbf{r}), \quad w_{x^2-y^2}(\mathbf{r}) = \frac{1}{2}\sqrt{\frac{15}{2\pi}}\frac{x^2-y^2}{|\mathbf{r}|}g(\mathbf{r}), \quad (\text{S31})$$

$$g(\mathbf{r}) = \exp(-|\mathbf{r}|^2/0.2) \quad (\text{S32})$$

At $\mathbf{r} = 0$, the two in-plane components w_{xy} and $w_{x^2-y^2}$ are set to zero by continuity of the plotted envelope.

The real-space sum is evaluated over the hexagonal patch

$$\mathbf{R} = n\mathbf{R}_1 + m\mathbf{R}_2, \quad \max(|n|, |m|, |n+m|) \leq 4. \quad (\text{S33})$$

The plotted grid has 401×347 points over the hexagonal region

$$-1 \leq x \leq 1, \quad -\frac{\sqrt{3}}{2} \leq y \leq \frac{\sqrt{3}}{2}. \quad (\text{S34})$$

The colour scale is unit-normalised independently for each plot at a given high-symmetry momentum, e.g. Γ and K .

195

Let $\omega = e^{2\pi i/3}$. At the three C_3 centres $1a$, $1c$, and $1b$, the C_3 phases differ at K and K' . Note that we use the high-symmetry-position labels of the layer group $p\bar{6}m2$ rather than of the 3D space group $P\bar{6}m2$ (No. 187), as we work in two dimensions; in the space-group notation, $(\frac{1}{3}, \frac{2}{3}, 0)$ is the $1c$ rather than the $1b$ position. A d_{z^2} orbital transforms in the A' irreducible representation of D_{3h} ; such an orbital situated at the three C_3 centres induces the C_3 characters

$$A'@1a : \Gamma : 1, \quad K : 1, \quad K' : 1, \quad (\text{S35})$$

$$A'@1c : \Gamma : 1, \quad K : \omega, \quad K' : \omega^2, \quad (\text{S36})$$

$$A'@1b : \Gamma : 1, \quad K : \omega^2, \quad K' : \omega. \quad (\text{S37})$$

Likewise, an E' doublet (the $d_{xy}/d_{x^2-y^2}$ orbitals) centred at these same positions gives

$$E'@1a : \Gamma : \omega^\pm, \quad K : \omega \oplus \omega^2, \quad K' : \omega^2 \oplus \omega, \quad (\text{S38})$$

$$E'@1c : \Gamma : \omega^\pm, \quad K : 1 \oplus \omega^2, \quad K' : 1 \oplus \omega, \quad (\text{S39})$$

$$E'@1b : \Gamma : \omega^\pm, \quad K : 1 \oplus \omega, \quad K' : 1 \oplus \omega^2. \quad (\text{S40})$$

For the isolated valence band of the three-band model one finds the C_3 characters

$$\Gamma : 1, \quad K : \omega, \quad K' : \omega^2. \quad (\text{S41})$$

This matches $A'@1c$. Thus, the valence-band Wannier centre is at the hollow-site position $1c$; since the atomic positions of the metals are at $1a$ and the chalcogens are at $1b$, this implies the valence band is described by an obstructed atomic limit. For the connected upper two-band subspace one instead finds

$$\Gamma : \omega^\pm, \quad K : 1 \oplus \omega^2, \quad K' : 1 \oplus \omega. \quad (\text{S42})$$

Among the multiplicity-one C_3 -centred candidates, this matches $E'@1c$. Therefore, the connected conduction doublet is also centred at $1c$.

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Unobstructed counterfactual

To highlight how the local density of states would appear for WSe_2 in the case of a hypothetical unobstructed band, we also consider a deliberately simplified counterfactual model. In the physical three-band model of WSe_2 , the isolated valence band has representation data consistent with an A' orbital centred at the hollow $1c$ position, while the connected upper two-band subspace has the symmetry data of an E' doublet centred at $1c$. The counterfactual model instead realises an E' doublet of D_{3h} , built from the same $(d_{xy}, d_{x^2-y^2})$ orbital sector, while using the same real-space orbital envelopes and STM reconstruction as in the physical TMD calculation. The inter-orbital hybridisations in Eq. (S18) are removed, the d_{z^2} band is pushed away, and the doublet dispersion is chosen so that the K valley is spectrally clean. Thus the model is a simplified unobstructed atomic doublet rather than the obstructed valence-band representation of WSe_2 .

Let $V_0(\mathbf{k})$ denote the d_{z^2} diagonal entry of Eq. (S18). We define the counterfactual Hamiltonian in the same orbital basis $(d_{z^2}, d_{xy}, d_{x^2-y^2})$ by setting all inter-orbital matrix elements to zero and writing

$$H_{\text{cf}}(\mathbf{k}) = \begin{pmatrix} H_{z^2}^{\text{cf}}(\mathbf{k}) & 0 \\ 0 & H_E^{\text{cf}}(\mathbf{k}) \end{pmatrix}. \quad (\text{S43})$$

The d_{z^2} block is shifted down in energy,

$$H_{z^2}^{\text{cf}}(\mathbf{k}) = (\epsilon_1 - 1.0) + \frac{1}{2} (V_0(\mathbf{k}) - \epsilon_1), \quad (\text{S44})$$

where $\epsilon_1 = 0.728 \text{ eV}$ is the onsite energy of the d_{z^2} orbital in the three-band model. This places the d_{z^2} band below the $d_{xy}/d_{x^2-y^2}$ sector, so that the latter can be imaged without spectral overlap.

The in-plane doublet is replaced by a simple triangular-lattice doublet dispersion,

$$H_E^{\text{cf}}(\mathbf{k}) = (E_E + T_E f_1(\mathbf{k})) \mathbb{1}_2 + \lambda s_1(\mathbf{k}) \tau_y, \quad (\text{S45})$$

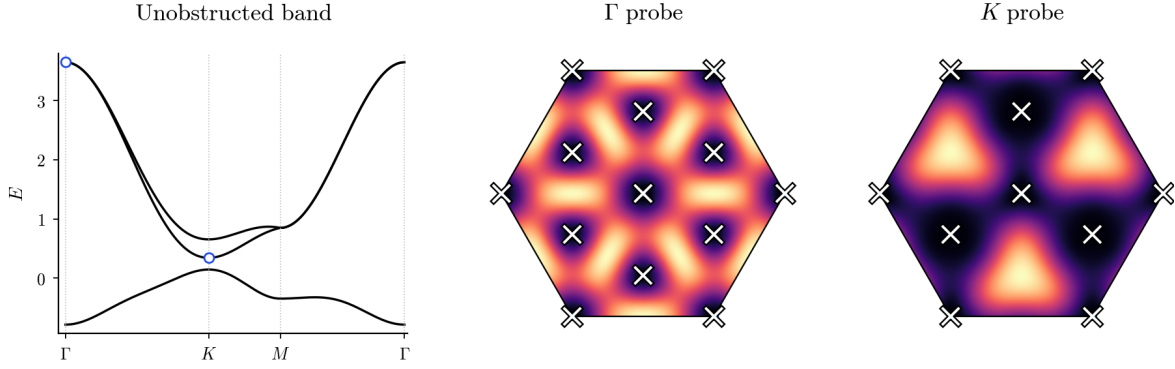


FIG. S16. **Unobstructed hypothetical TMD model.** Bandstructure (left), as well as the LDOS at Γ (middle) and K (right) for a hypothetical model of TMDs in which the hoppings were purely intra orbital type, so that the bands are atomic in nature. The LDOS at K resembles that of the actual TMD model, since the bright/dark spots are determined by the symmetry properties — which remain the same. The difference manifests near the Γ point, where the differing symmetry representation results in nodes at the 1a, 1b, and 1c positions, in contrast with the nodeless LDOS in Fig. 1.

where τ_y is a Pauli matrix acting in the real doublet basis $(d_{xy}, d_{x^2-y^2})$. We take $E_E = 1.55$ eV, $T_E = 1.55$ eV, and $\lambda = 0.18$ eV. The two scalar form factors are

$$f_1(\mathbf{k}) = 2 [\cos(\mathbf{k} \cdot \mathbf{R}_1) + \cos(\mathbf{k} \cdot \mathbf{R}_2) + \cos(\mathbf{k} \cdot (\mathbf{R}_1 + \mathbf{R}_2))], \quad (\text{S46})$$

$$s_1(\mathbf{k}) = \frac{1}{3} [\sin(\mathbf{k} \cdot \mathbf{R}_1) + \sin(\mathbf{k} \cdot \mathbf{R}_2) - \sin(\mathbf{k} \cdot (\mathbf{R}_1 + \mathbf{R}_2))]. \quad (\text{S47})$$

The first form factor gives a maximum at Γ and a minimum at K/K' , while the second is a C_3 -invariant odd function of momentum. Consequently $s_1(-\mathbf{k}) = -s_1(\mathbf{k})$, and since $\tau_y^* = -\tau_y$, the Hamiltonian obeys time-reversal symmetry,

$$H_E^{\text{cf}}(-\mathbf{k}) = H_E^{\text{cf}}(\mathbf{k})^* \quad (\text{S48})$$

This term therefore splits the doublet at K without breaking time reversal. By contrast, the E doublet at Γ remains degenerate because $s_1(\Gamma) = 0$ and the little group at Γ has a two-dimensional E irrep.

The Γ probe images the degenerate E doublet at $E = 3.650$ eV. The K probe images only the lower split state of the doublet, at $E = 0.344$ eV. The figure is generated from the same band-resolved Green-function LDOS procedure used in the other STM simulations. At Γ , the projected subspace contains both members of the degenerate E doublet. At K , the projected subspace contains only the lower split K state.

Using the dark set formalism, the crossed positions in the Γ -probe panel are the symmetry-enforced zeros of the imaged E doublet: within the plotted hexagonal cell they occur at the metal sites together with the centres of both the upward- and downward-pointing triangular plaquettes. For the lower split K state, the crossed positions are the metal sites together with the centres of the downward-pointing triangular plaquettes. These are the high-symmetry positions at which the corresponding Bloch wavefunctions vanish identically by symmetry.

D. Haldane model

For the Haldane simulations, we use the triangular Bravais lattice

$$\mathbf{R}_1 = (1, 0), \quad \mathbf{R}_2 = \left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right), \quad (\text{S49})$$

with reciprocal vectors defined by $\mathbf{G}_i \cdot \mathbf{R}_j = 2\pi\delta_{ij}$. The hexagon centre is the 1a position, while the two honeycomb sublattices are embedded at

$$\tau_A = \frac{1}{3}(\mathbf{R}_1 + 2\mathbf{R}_2) \quad (1b), \quad \tau_B = \frac{1}{3}(2\mathbf{R}_1 + \mathbf{R}_2) \quad (1c). \quad (\text{S50})$$

Here 1b and 1c refer to the $p3$ labelling appropriate to the generic model with both M and ϕ nonzero. When the symmetry is enhanced to $p6$, these two positions form the single Wyckoff orbit 2b.

We work in the sublattice basis $\Psi_{\mathbf{k}} = (c_{A\mathbf{k}}, c_{B\mathbf{k}})^T$, with the embedded Bloch convention

$$c_{\mu\mathbf{k}} = N^{-1/2} \sum_{\mathbf{R}} e^{-i\mathbf{k} \cdot (\mathbf{R} + \tau_{\mu})} c_{\mu\mathbf{R}}, \quad \mu = A, B. \quad (\text{S51})$$

245 The three nearest-neighbour vectors point from sublattice A to sublattice B ,

$$\{\boldsymbol{\alpha}_n\}_{n=1}^3 = \{\frac{1}{3}(\mathbf{R}_1 - \mathbf{R}_2), -\frac{1}{3}(2\mathbf{R}_1 + \mathbf{R}_2), \frac{1}{3}(\mathbf{R}_1 + 2\mathbf{R}_2)\}, \quad (\text{S52})$$

246 and the oriented next-nearest-neighbour vectors are

$$\{\boldsymbol{\beta}_n\}_{n=1}^3 = \{\mathbf{R}_1, \mathbf{R}_2, -\mathbf{R}_1 - \mathbf{R}_2\}. \quad (\text{S53})$$

247 The hoppings along $+\boldsymbol{\beta}_n$ carry phase $+\phi$ on sublattice A and phase $-\phi$ on sublattice B ; the reverse hoppings carry
248 the complex-conjugate phases. Defining

$$f_{\mathbf{k}} = \sum_{n=1}^3 e^{i\mathbf{k} \cdot \boldsymbol{\alpha}_n}, \quad g_{\mathbf{k}} = \sum_{n=1}^3 e^{i\mathbf{k} \cdot \boldsymbol{\beta}_n}, \quad (\text{S54})$$

249 the Hamiltonian is

$$H_{\text{H}}(\mathbf{k}) = \begin{pmatrix} d_0(\mathbf{k}) + d_z(\mathbf{k}) & -t_1 f_{\mathbf{k}} \\ -t_1 f_{\mathbf{k}}^* & d_0(\mathbf{k}) - d_z(\mathbf{k}) \end{pmatrix}, \quad (\text{S55})$$

250 where

$$d_0(\mathbf{k}) = 2t_2 \cos \phi \Re g_{\mathbf{k}}, \quad \mathbf{d}(\mathbf{k}) = (-t_1 \Re f_{\mathbf{k}}, t_1 \Im f_{\mathbf{k}}, d_z(\mathbf{k})), \quad d_z(\mathbf{k}) = M - 2t_2 \sin \phi \Im g_{\mathbf{k}}. \quad (\text{S56})$$

251 Noting that $\mathbf{K} = \frac{1}{3}(\mathbf{G}_1 + \mathbf{G}_2)$, $\mathbf{K}' = -\mathbf{K}$, then $f_{\mathbf{K}} = f_{\mathbf{K}'} = 0$, $g_{\mathbf{K}} = 3e^{2\pi i/3}$, and $g_{\mathbf{K}'} = 3e^{-2\pi i/3}$. The Dirac
252 masses $d_z(\pm\mathbf{K})$ are therefore

$$m_K = M - 3\sqrt{3}t_2 \sin \phi, \quad m_{K'} = M + 3\sqrt{3}t_2 \sin \phi. \quad (\text{S57})$$

253 The Chern number is nonzero when m_K and $m_{K'}$ have opposite signs. For the occupied lower band,

$$C = -\frac{1}{4\pi} \int_{\text{BZ}} d^2k \, \hat{\mathbf{d}} \cdot (\partial_{k_x} \hat{\mathbf{d}} \times \partial_{k_y} \hat{\mathbf{d}}). \quad (\text{S58})$$

254 For the parameter set for the topological regime quoted below this gives $C = -1$, in agreement with the inference from
255 the sign of the mass terms.

256 The continuum orbital attached to each honeycomb site is an s -like Gaussian,

$$w_s(\mathbf{r}) = \frac{1}{\sqrt{2\pi}\sigma_H} \exp(-|\mathbf{r}|^2/(2\sigma_H^2)), \quad \sigma_H = 0.65. \quad (\text{S59})$$

257 The real-space patch used in the Haldane LDOS contraction contains all cells satisfying

$$\max(|n|, |m|, |n+m|) \leq 5, \quad \mathbf{R} = n\mathbf{R}_1 + m\mathbf{R}_2, \quad (\text{S60})$$

258 and the Green function is computed for displacements satisfying

$$\max(|n|, |m|, |n+m|) \leq 7. \quad (\text{S61})$$

259 The LDOS is evaluated using the upper band with Lorentzian broadening $\eta = 0.025$ and a 48×48 uniform
260 Brillouin-zone mesh. The plotted real-space grid is 81×81 over $-3 \leq x, y \leq 3$ before restricting to the displayed
261 hexagonal region. The K -probe panel is evaluated at the valley energy; since K and K' are degenerate for both
262 main-text parameter sets, the energy-resolved LDOS contains both valley contributions. In Fig. 2, we used the
263 parameters $t_1 = 1.0$ and $t_2 = 0.15$ for both scenarios, setting $\phi = 0$, $M = 0.575$, $m_K = 0.575$, and $m_{K'} = 0.575$ for the
264 trivial case ($C = 0$), and $\phi = \pi/3$, $M = 0$, $m_K = -0.675$, and $m_{K'} = 0.675$ for the Chern case ($C = -1$ for the lower
265 band and $C = 1$ for the upper band).

E. BHZ model

For the BHZ simulations, we use a square Bravais lattice $\mathbf{R}_1 = (1, 0)$, $\mathbf{R}_2 = (0, 1)$ with one site per unit cell. For clarity, we explicitly state the high-symmetry momenta

$$\Gamma = (0, 0), \quad X = (\pi, 0), \quad Y = (0, \pi), \quad M = (\pi, \pi). \quad (\text{S62})$$

The tight-binding basis is

$$(s_\uparrow, p_{+, \uparrow}, s_\downarrow, p_{-, \downarrow}). \quad (\text{S63})$$

where $p_\pm = p_x \pm ip_y$ and in which the spin-conserving BHZ Hamiltonian is

$$H_{\text{BHZ}}(\mathbf{k}) = \begin{pmatrix} h_\uparrow(\mathbf{k}) & 0 \\ 0 & h_\downarrow(\mathbf{k}) \end{pmatrix} + D(\cos k_x + \cos k_y) \mathbb{1}_4, \quad (\text{S64})$$

with

$$h_\uparrow(\mathbf{k}) = \begin{pmatrix} m_{\mathbf{k}} & A \sin k_x - iA \sin k_y \\ A \sin k_x + iA \sin k_y & -m_{\mathbf{k}} \end{pmatrix}, \quad (\text{S65})$$

where $m_{\mathbf{k}} = -(m + \cos k_x + \cos k_y)$ and for which $h_\downarrow(\mathbf{k}) = h_\uparrow^*(-\mathbf{k})$. The continuum orbitals are taken to be

$$w_s(\mathbf{r}) = \frac{1}{\sqrt{\pi}\sigma_B} \exp(-|\mathbf{r}|^2/(2\sigma_B^2)), \quad (\text{S66})$$

$$w_{p+}(\mathbf{r}) = \frac{\sqrt{2}}{\sqrt{\pi}\sigma_B^2} (x + iy) \exp(-|\mathbf{r}|^2/(2\sigma_B^2)), \quad (\text{S67})$$

$$w_{p-}(\mathbf{r}) = \frac{\sqrt{2}}{\sqrt{\pi}\sigma_B^2} (x - iy) \exp(-|\mathbf{r}|^2/(2\sigma_B^2)), \quad (\text{S68})$$

with $\sigma_B = 0.40$. The real-space patch used in the BHZ LDOS contraction contains the square-lattice cells

$$\mathbf{R} = n\mathbf{R}_1 + m\mathbf{R}_2, \quad -4 \leq n, m \leq 4. \quad (\text{S69})$$

The main-text BHZ figure uses the parameters $A = 1.0$ and $D = 0.2$ for both scenarios, setting $m = 2.5$ and $\nu = 0$ for the trivial case, and $m = 1.5$ and $\nu = 1$ for the QSH case. The probe energies are

$$E_\Gamma^{\text{triv}} = -4.1, \quad E_M^{\text{triv}} = -0.9, \quad E_\Gamma^{\text{QSH}} = -3.1, \quad E_M^{\text{QSH}} = -0.9. \quad (\text{S70})$$

The finite-energy LDOS uses $\eta = 0.025$, a 48×48 uniform Brillouin-zone mesh, C_4 -rotation averaging, and an 81×81 real-space grid over $-1 \leq x, y \leq 1$. Each panel is independently normalised to its maximum inside the plotted square.

S4. DARK SET IMAGING WITH FURTHER SYMMETRY BREAKING

In the generalised Haldane model in which both a chiral hopping and Semenoff mass are present, K and K' are no longer degenerate as they are in Fig. 2. In Fig. S17 we show imaging of the charge density at the high-symmetry points in the generalised Haldane model. In the trivial case, as one lowers the bias energy to first image K then K' , only one sublattice stays bright. By contrast, when the bias energy intersects K' in the topological case, the other sublattice suddenly turns bright — providing a sharp signature of the Chern number. In experiment, the valley-resolved LDOS can also be explored through strain-induced pseudomagnetic fields, which have been used to resolve the sublattice structure of pseudo-Landau levels in buckled graphene superlattices [15].

In this simulation, we used the parameters $t_1 = 1.0$ and probed the lowest band for both scenarios, setting $t_2 = 0.06$, $\phi = 0.675$, $M = 0.46$, $C = 0$, $m_K = 0.265$, and $m_{K'} = 0.655$ for the trivial case, and $t_2 = 0.09$, $\phi = 1.25$, $M = 0.18$, $C = -1$, $m_K = -0.264$, and $m_{K'} = 0.624$ for the Chern case.

Similarly, we consider a generalised BHZ model in which C_4 symmetry is broken to lift the degeneracy of X and Y present in Fig. 3. We add the C_4 -breaking scalar perturbation

$$H_{\text{gen}}(\mathbf{k}) = H_{\text{BHZ}}(\mathbf{k}) + \delta(\cos k_x - \cos k_y) \mathbb{1}_4. \quad (\text{S71})$$

This perturbation shifts the energies at X and Y without changing the high-symmetry eigenvectors, because it is proportional to the identity in orbital space. Fig. S18 uses the scalar perturbation $\delta = -0.15$; the remaining parameters are the same as in the ordinary BHZ simulation described in the previous section.

In these examples, several of the high-symmetry points being imaged are not energetically isolated, yet crucially the qualitative bright/dark structure is dominated by the selection rules near the relevant high-symmetry momenta.

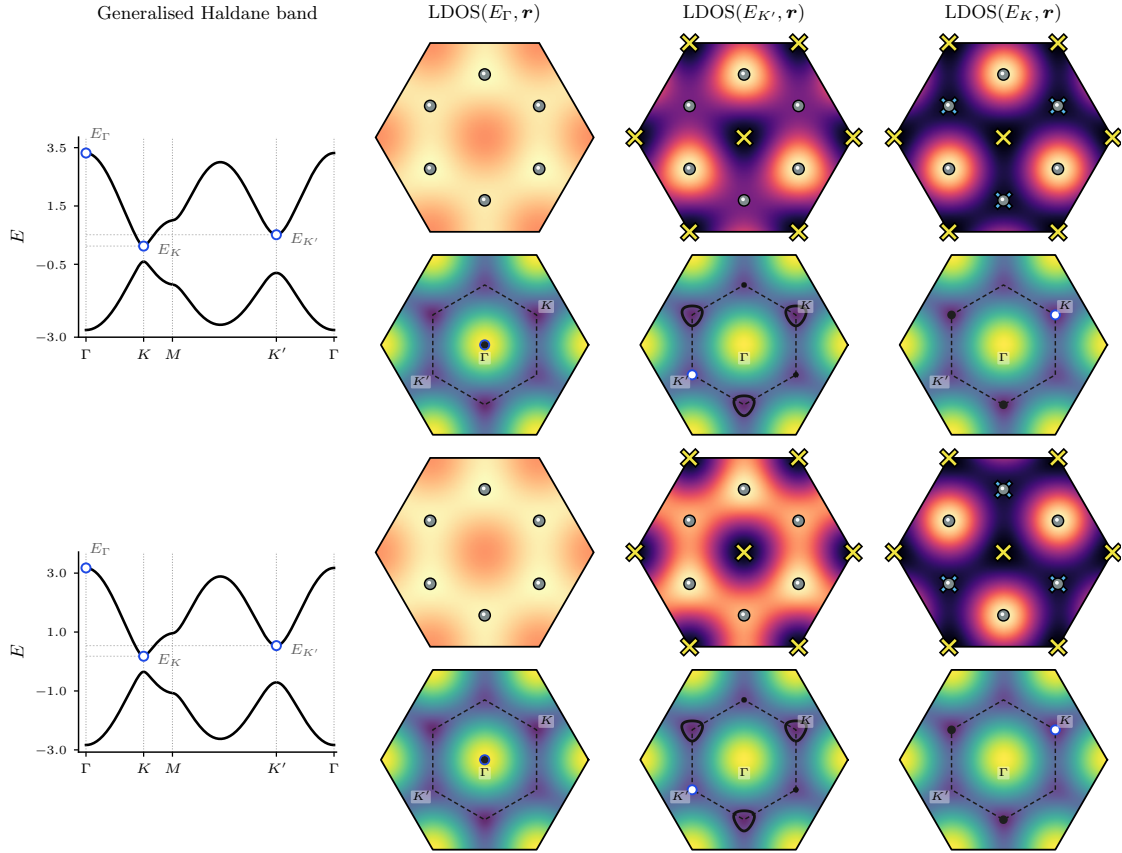


FIG. S17. **Generalised Haldane model.** Top: $C = 0$ case, Bottom: $|C| = 1$ case. Left: cut bandstructure in each case with high-symmetry points marked with blue circles. Subsequent columns left-right: LDOS computed at the energies associated to high-symmetry momenta, with the associated Fermi contour underneath. The boundary of the first Brillouin zone is denoted by a dashed black line. The LDOS involves integrating over all states with a fixed energy; the associated Fermi contour is represented by a solid grey line. At the K point, the contour is a set of small dots at the three equivalent K points. At K' , the contour comprises small dots at the K' corner and pockets encircling K . At the Γ point the contour is a small dot at the centre of the Brillouin zone.

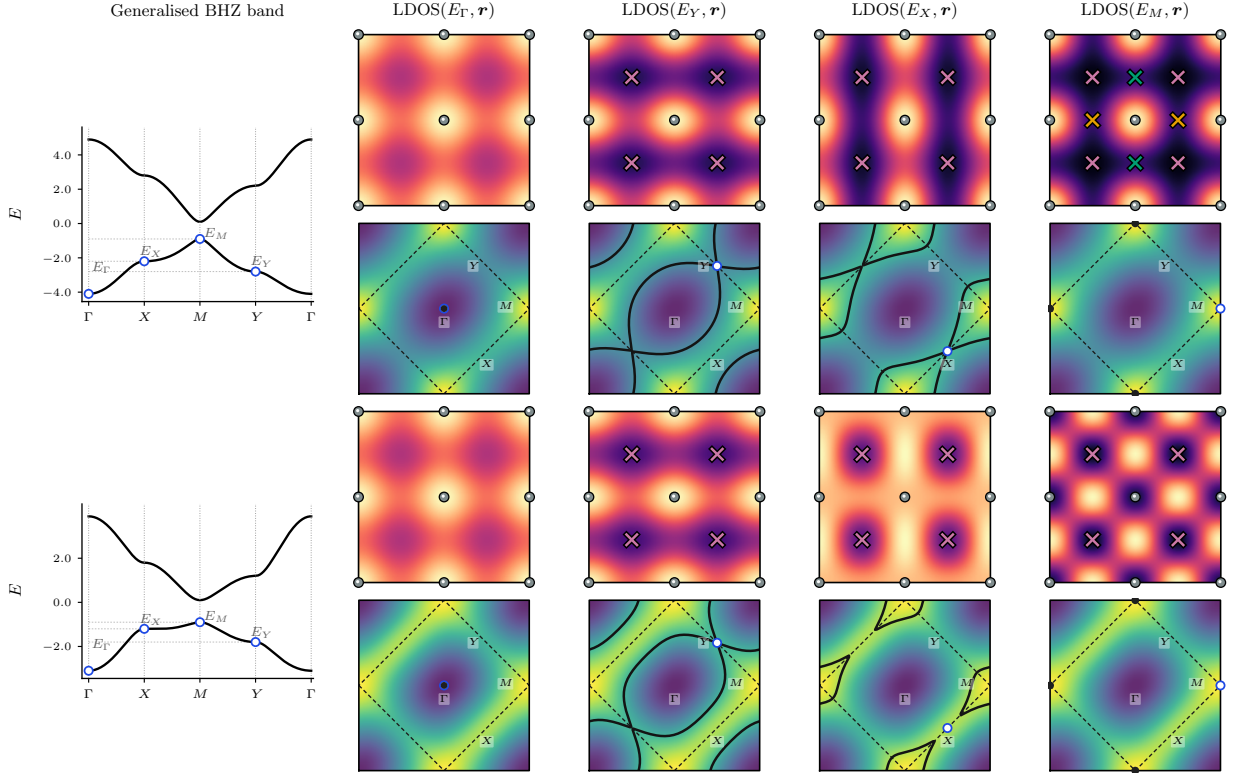


FIG. S18. **Generalised BHZ model.** Top: $\nu = 0$ case, Bottom: $\nu = 1$ case. Left: cut bandstructure in each case with high-symmetry points marked with blue circles. Plotting convention is the same as in Fig. S17. Subsequent columns from left-right: LDOS and associated energy contours. At the M point, the contour is a set of small dots at the four equivalent M points. At X/Y , the contours touch X/Y but also extend along an arc in the interior of the Brillouin zone. Since the Fermi contour is not solely composed of the high-symmetry momentum, the LDOS does not strictly vanish at the indicated nodes, but since the density of states is dominated by the X/Y points in each case, images are dominated by the bright/dark features at X/Y .

S5. MOMENTUM-RESOLVED WAVEFUNCTIONS

The STM simulations we have presented represent the LDOS, which involves averaging the wavefunction density across a constant energy contour in the Brillouin zone. In cases where this contour includes points away from a high-symmetry momentum, the dark set does not produce exact zeros of the LDOS. A more general and explicit visualisation of the dark set can be arrived at through a momentum-resolved plot of the charge density. In this section, we show $|\Psi_{\mathbf{k}_*}(\mathbf{r})|^2$ at all the high-symmetry momenta $\mathbf{k}_*$ for the models we have considered, allowing a momentum-resolved illustration of the dark sets. Specifically, at fixed high-symmetry crystal momentum $\mathbf{k}_*$, we plot the probability density $\rho_{n\mathbf{k}_*}(\mathbf{r})$ obtained by reconstructing the Bloch eigenstate from its local-orbital amplitudes. We have

$$\Psi_{n\mathbf{k}_*}(\mathbf{r}) = \sum_{\mathbf{R}, \alpha} e^{i\mathbf{k}_* \cdot \mathbf{R}} u_{n\alpha}(\mathbf{k}_*) w_{\alpha}(\mathbf{r} - \mathbf{R} - \boldsymbol{\tau}_{\alpha}), \quad \rho_{n\mathbf{k}_*}(\mathbf{r}) = |\Psi_{n\mathbf{k}_*}(\mathbf{r})|^2. \quad (\text{S72})$$

where $\mathbf{R}$ are the Bravais-lattice vectors, $\boldsymbol{\tau}_{\alpha}$ are the orbital positions, $u_{n\alpha}$ are the wavefunctions found by direct diagonalisation of the Bloch Hamiltonian. Crosses mark symmetry-enforced zeros.

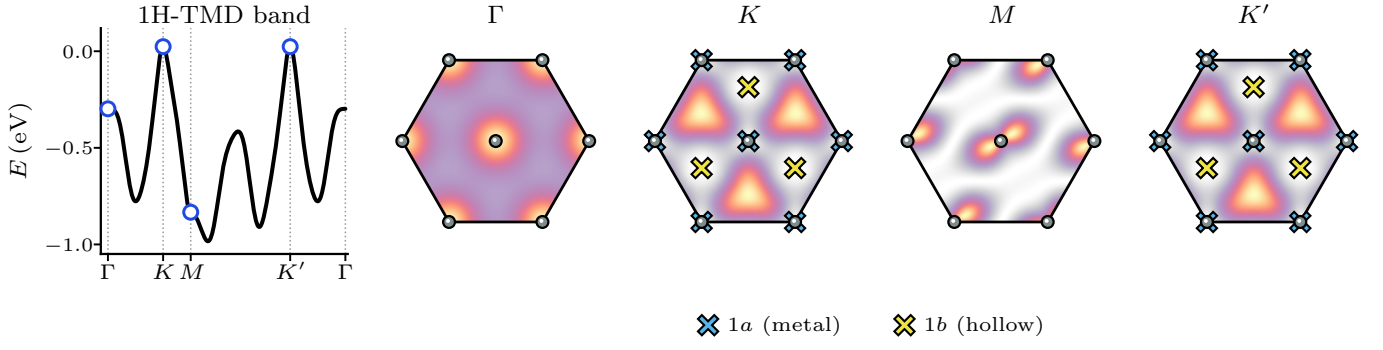


FIG. S19. **1H-TMD Bloch wavefunctions at high-symmetry momenta.** Amplitude $|\Psi_{\mathbf{k}_*}(\mathbf{r})|^2$ of the 1H-TMD wavefunctions at the high-symmetry momenta $\mathbf{k}_* = \Gamma, K, M, K'$, with the associated energies indicated on the bandstructure.

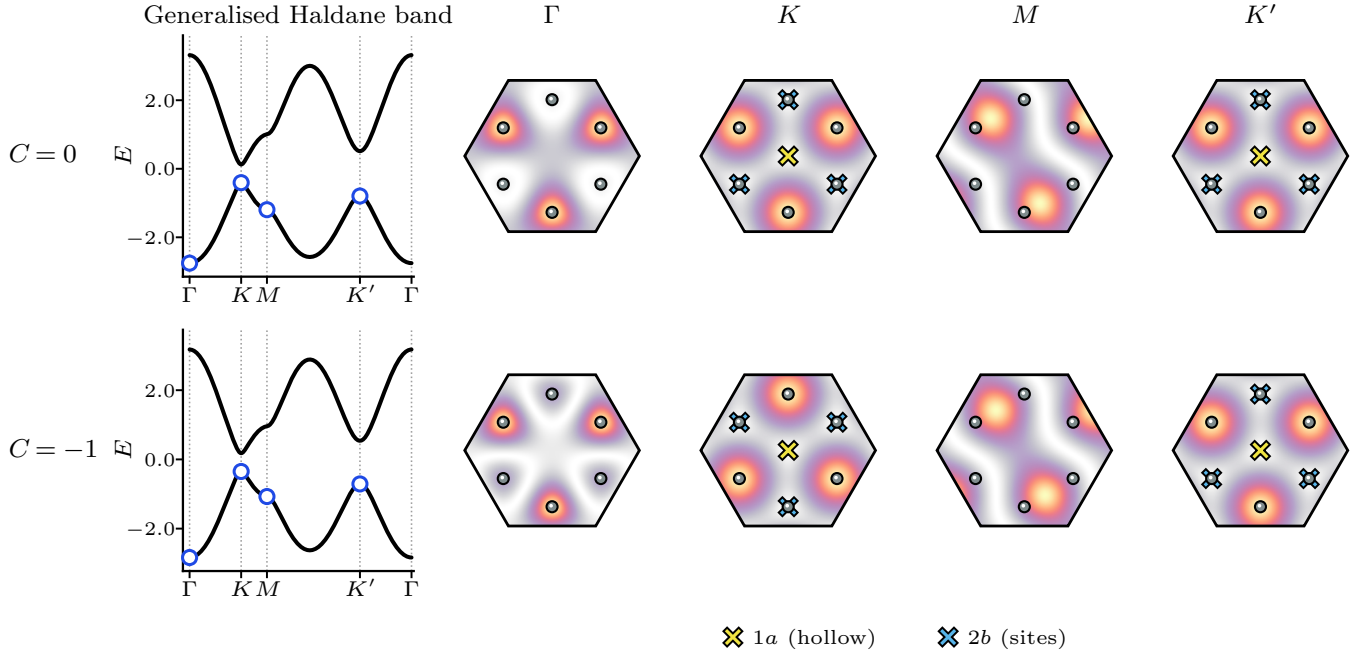


FIG. S20. **Generalised Haldane Bloch wavefunctions at high-symmetry momenta.** Amplitude $|\Psi_{\mathbf{k}_*}(\mathbf{r})|^2$ of the generalised Haldane wavefunctions at the high-symmetry momenta $\mathbf{k}_* = \Gamma, K, M, K'$, with the associated energies indicated on the bandstructure.

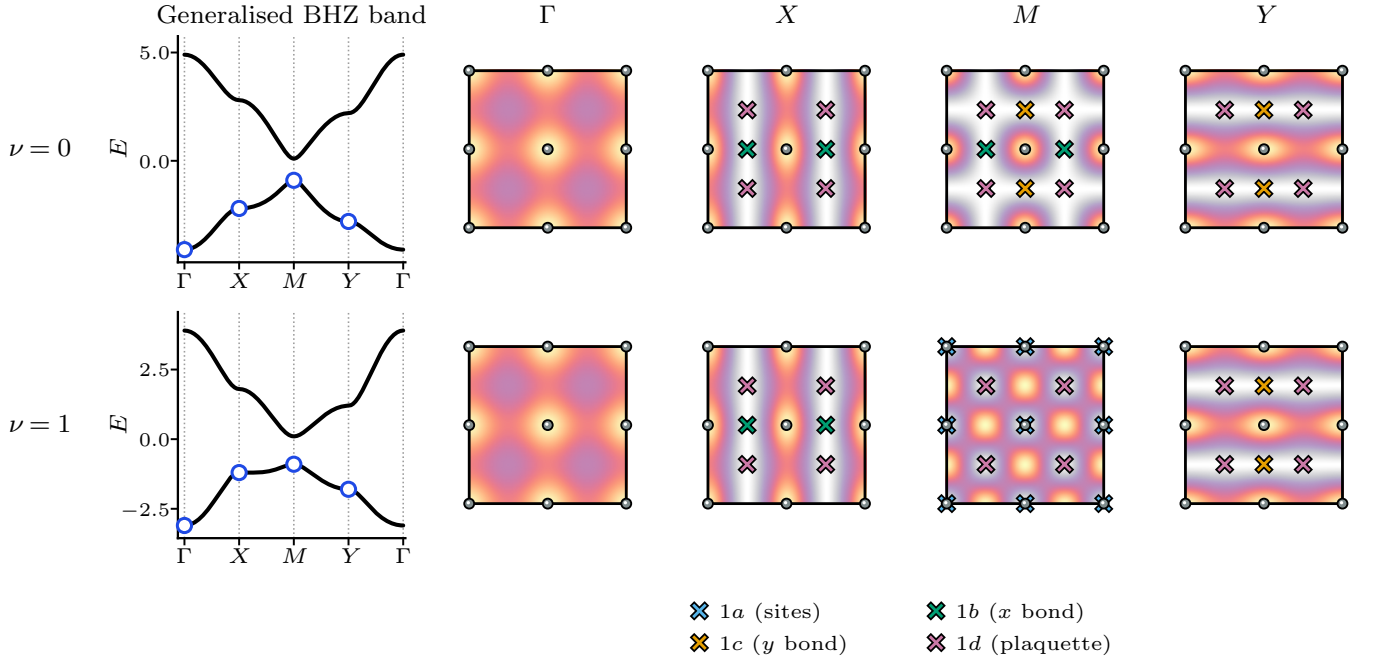


FIG. S21. **Generalised BHZ Bloch wavefunctions at high-symmetry momenta.** Amplitude $|\Psi_{\mathbf{k}_*}(\mathbf{r})|^2$ of the generalised BHZ wavefunctions at the high-symmetry momenta $\mathbf{k}_* = \Gamma, X, M, Y$, with the associated energies indicated on the bandstructure.

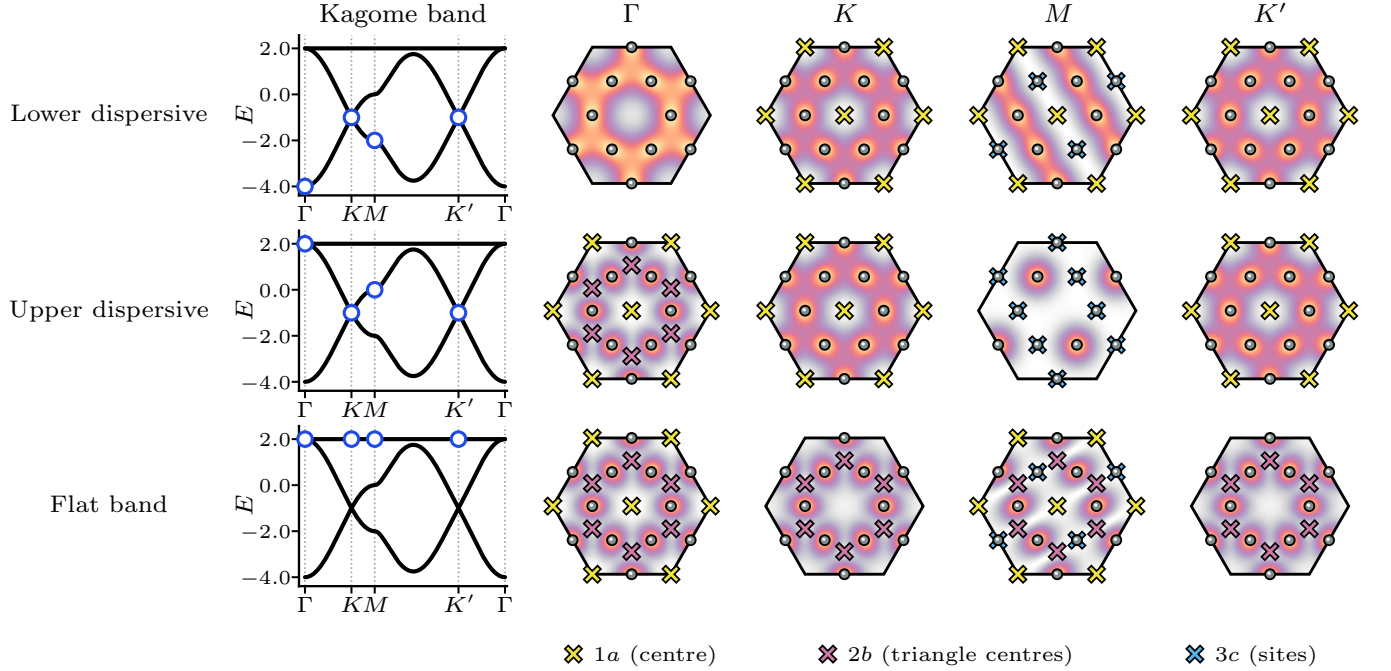


FIG. S22. **Kagome Bloch wavefunctions at high-symmetry momenta.** Amplitude $|\Psi_{\mathbf{k}_*}(\mathbf{r})|^2$ of the kagome wavefunctions at the high-symmetry momenta $\mathbf{k}_* = \Gamma, K, M, K'$, with the associated energies indicated on the bandstructure.

S6. DERIVATION OF THE KANE-MELE INVARIANT AS A ZERO COUNT

In this section, we derive that the Kane-Mele invariant can be rewritten as a count of the number of dark set zeros at an inversion centre, for systems with inversion symmetry. The proof assumes the Fu-Kane indicator, which relates the Kane-Mele invariant to the inversion eigenvalues; in forthcoming work we present a proof which does not assume, but rather derives the Fu-Kane indicator using zero counting. Fix one inversion centre $\mathbf{r}$. For an occupied Kramers pair a at a TRIM $\mathbf{\Lambda}$, let $\zeta_{I,a}(\mathbf{\Lambda}) = \pm 1$ be the inversion eigenvalue. We define

$$d_a(\mathbf{\Lambda}; \mathbf{r}) = \frac{1}{2} (1 - e^{-2i\mathbf{\Lambda} \cdot \mathbf{r}} \zeta_{I,a}(\mathbf{\Lambda})). \quad (\text{S73})$$

The variable $d_a(\mathbf{\Lambda}; \mathbf{r})$ equals one precisely when inversion about $\mathbf{r}$ forces the Kramers pair to vanish at $\mathbf{r}$, and equals zero otherwise. Summing over occupied Kramers pairs and TRIM,

$$\mathcal{N}(\mathbf{r}) = \sum_{\mathbf{\Lambda} \in \text{TRIM}} \sum_{a=1}^N d_a(\mathbf{\Lambda}; \mathbf{r}) \pmod{2}. \quad (\text{S74})$$

The function $\mathcal{N}(\mathbf{r})$ counts, at the fixed inversion centre $\mathbf{r}$, the number of inversion-forced dark occupied Kramers pairs accumulated over the four TRIM.

Since

$$(-1)^{d_a(\mathbf{\Lambda}; \mathbf{r})} = e^{-2i\mathbf{\Lambda} \cdot \mathbf{r}} \zeta_{I,a}(\mathbf{\Lambda}), \quad (\text{S75})$$

we obtain

$$(-1)^{\mathcal{N}(\mathbf{r})} = \left[\prod_{\mathbf{\Lambda} \in \text{TRIM}} e^{-2i\mathbf{\Lambda} \cdot \mathbf{r}} \right]^N \prod_{\mathbf{\Lambda}, a} \zeta_{I,a}(\mathbf{\Lambda}). \quad (\text{S76})$$

The four two-dimensional TRIM obey

$$\sum_{\mathbf{\Lambda} \in \text{TRIM}} \mathbf{\Lambda} = \mathbf{b}_1 + \mathbf{b}_2, \quad (\text{S77})$$

where $\mathbf{b}_1, \mathbf{b}_2$ are the reciprocal lattice vectors. Since $\mathbf{r}$ is an inversion centre, $2\mathbf{r}$ is a Bravais-lattice vector. Therefore

$$\prod_{\mathbf{\Lambda} \in \text{TRIM}} e^{-2i\mathbf{\Lambda} \cdot \mathbf{r}} = e^{-2i(\mathbf{b}_1 + \mathbf{b}_2) \cdot \mathbf{r}} = 1. \quad (\text{S78})$$

Using the Fu-Kane inversion product,

$$(-1)^\nu = \prod_{\mathbf{\Lambda}, a} \zeta_{I,a}(\mathbf{\Lambda}), \quad (\text{S79})$$

we conclude that

$$\boxed{\mathcal{N}(\mathbf{r}) = \nu \pmod{2}}. \quad (\text{S80})$$

At any fixed inversion centre, the parity of the number of inversion-forced dark occupied Kramers pairs over all four TRIM is the Kane-Mele invariant.

A position with a larger site stabiliser may have additional zeros enforced by rotations or mirrors. Those additional zeros are not included in $\mathcal{N}(\mathbf{r})$ unless they are already forced by the inversion subgroup; for this reason, the diagnostic is sharpest when probing an inversion centre with no other symmetry.

A. Reduction in the presence of C_4 symmetry

In the standard C_4 -symmetric BHZ geometry, the site and plaquette centres are also C_4 centres at Γ and M . A zero at one of these positions can therefore be forced by the inclusion of C_4 characters in the projector sum. That is, a location can be bright when accounting solely for the constraints implied by inversion symmetry, but forced-dark when

C_4 is accounted for; such zeros are removed if C_4 symmetry is broken. The upshot is that the origin and plaquette centres are ambiguous as a probe of the inversion characters, as their darkness is also determined by C_4 .

The bond centres B_x and B_y avoid this ambiguity: at Γ and M they probe the inversion condition without an additional C_4 constraint. On the other hand, exact C_4 symmetry relates X and Y , so an energy-resolved STM image does not isolate one from the other while preserving the symmetry. Yet, since the occupied inversion-eigenvalue multisets at X and Y are then identical, their contribution to the fixed-bond zero parity is a known constant — this suggests that it should be possible to rewrite the invariant in a way that makes it sufficient to image only Γ and M . The reduction below demonstrates this, rewriting the inversion zero count using only bond-centre data at Γ and M .

Now assume that inversion is accompanied by C_4 symmetry on a square lattice. Choose primitive reciprocal vectors $\mathbf{b}_1, \mathbf{b}_2$, and write

$$\Gamma = \mathbf{0}, \quad X = \frac{1}{2}\mathbf{b}_1, \quad Y = \frac{1}{2}\mathbf{b}_2, \quad M = \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_2). \quad (\text{S81})$$

Let the two bond-centred inversion centres be

$$B_x = \frac{1}{2}\mathbf{a}_1, \quad B_y = \frac{1}{2}\mathbf{a}_2. \quad (\text{S82})$$

At B_x , the inversion phases at (Γ, X, Y, M) are $(+1, -1, +1, -1)$. Therefore

$$d_a(\Gamma; B_x) = \frac{1}{2}(1 - \zeta_{I,a}(\Gamma)), \quad (\text{S83})$$

$$d_a(X; B_x) = \frac{1}{2}(1 + \zeta_{I,a}(X)), \quad (\text{S84})$$

$$d_a(Y; B_x) = \frac{1}{2}(1 - \zeta_{I,a}(Y)), \quad (\text{S85})$$

$$d_a(M; B_x) = \frac{1}{2}(1 + \zeta_{I,a}(M)). \quad (\text{S86})$$

At B_y , the roles of X and Y are exchanged.

Since C_4 maps X to Y , the occupied inversion eigenvalue multisets at X and Y are identical. Hence, at either fixed bond centre,

$$\sum_{a=1}^N d_a(X; B_{x,y}) + \sum_{a=1}^N d_a(Y; B_{x,y}) = N. \quad (\text{S87})$$

The X and Y contribution to the fixed-bond zero parity is therefore a known constant.

Define

$$z_{\Gamma}^{\text{bond}} = \sum_{a=1}^N d_a(\Gamma; B_x) = \sum_{a=1}^N d_a(\Gamma; B_y), \quad (\text{S88})$$

$$z_M^{\text{bond}} = \sum_{a=1}^N d_a(M; B_x) = \sum_{a=1}^N d_a(M; B_y). \quad (\text{S89})$$

Then the fixed-centre formula reduces to

$$\nu \equiv N + z_{\Gamma}^{\text{bond}} + z_M^{\text{bond}} \pmod{2}. \quad (\text{S90})$$

Thus, in a C_4 -symmetric system, the X, Y data can be eliminated from the bond-centred zero count. The remaining information is the bond-centre contrast at Γ and M , together with the known constant N .

Equivalently, let N_{Γ}^{bond} and N_M^{bond} denote the total number of dark occupied Kramers pairs over the two C_4 -related bond centres at Γ and M . Since the two bonds are symmetry-related at both Γ and M ,

$$N_{\Gamma}^{\text{bond}} = 2z_{\Gamma}^{\text{bond}}, \quad N_M^{\text{bond}} = 2z_M^{\text{bond}}. \quad (\text{S91})$$

The same formula may be written as

$$\nu \equiv N + \frac{1}{2}(N_{\Gamma}^{\text{bond}} + N_M^{\text{bond}}) \pmod{2}. \quad (\text{S92})$$

For a single occupied Kramers pair, $N = 1$. If $z_{\Gamma}, z_M \in \{0, 1\}$ denote whether the bond pair is dark at Γ and at M , then

$$\boxed{\nu \equiv 1 + z_{\Gamma} + z_M \pmod{2}.} \quad (\text{S93})$$

Thus the topological phase has the same bond-centre contrast at Γ and M , while the trivial phase has opposite bond-centre contrast.

S7. SUBLATTICE INTERFERENCE EFFECT ON THE S-ORBITAL KAGOME LATTICE

A. Geometry and tight-binding model

We take the triangular Bravais lattice, with real space lattice vectors $\mathbf{a}_1 = (1, 0)$ and $\mathbf{a}_2 = (\frac{1}{2}, \frac{\sqrt{3}}{2})$, and with reciprocal lattice vectors $\mathbf{b}_1 = (2\pi, -\frac{2\pi}{\sqrt{3}})$ and $\mathbf{b}_2 = (0, \frac{4\pi}{\sqrt{3}})$. The three kagome sites in one unit cell are located at the 3c positions,

$$\mathbf{r}_A = \frac{1}{2}\mathbf{a}_1 = (\frac{1}{2}, 0), \quad \mathbf{r}_B = \frac{1}{2}\mathbf{a}_2 = (\frac{1}{4}, \frac{\sqrt{3}}{4}), \quad \mathbf{r}_C = \frac{1}{2}(\mathbf{a}_1 + \mathbf{a}_2) = (\frac{3}{4}, \frac{\sqrt{3}}{4}). \quad (\text{S94})$$

For the nearest-neighbour kagome tight-binding model, it is convenient to define

$$\mathbf{d}_{AB} = \frac{1}{2}(\mathbf{a}_1 - \mathbf{a}_2) = (\frac{1}{4}, -\frac{\sqrt{3}}{4}), \quad (\text{S95})$$

$$\mathbf{d}_{BC} = \frac{1}{2}\mathbf{a}_1 = (\frac{1}{2}, 0), \quad (\text{S96})$$

$$\mathbf{d}_{CA} = \frac{1}{2}\mathbf{a}_2 = (\frac{1}{4}, \frac{\sqrt{3}}{4}). \quad (\text{S97})$$

In the (A, B, C) basis the Bloch Hamiltonian is

$$H_0(\mathbf{k}) = -2t \begin{pmatrix} 0 & \cos(\mathbf{k} \cdot \mathbf{d}_{AB}) & \cos(\mathbf{k} \cdot \mathbf{d}_{CA}) \\ \cos(\mathbf{k} \cdot \mathbf{d}_{AB}) & 0 & \cos(\mathbf{k} \cdot \mathbf{d}_{BC}) \\ \cos(\mathbf{k} \cdot \mathbf{d}_{CA}) & \cos(\mathbf{k} \cdot \mathbf{d}_{BC}) & 0 \end{pmatrix}. \quad (\text{S98})$$

The three inequivalent M points are

$$\mathbf{M}_1 = \frac{1}{2}\mathbf{b}_2 = (0, \frac{2\pi}{\sqrt{3}}), \quad (\text{S99})$$

$$\mathbf{M}_2 = \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_2) = (\pi, \frac{\pi}{\sqrt{3}}), \quad (\text{S100})$$

$$\mathbf{M}_3 = \frac{1}{2}\mathbf{b}_1 = (\pi, -\frac{\pi}{\sqrt{3}}). \quad (\text{S101})$$

We choose the labelling so that $\mathbf{M}_1$ singles out sublattice A , while $\mathbf{M}_2$ and $\mathbf{M}_3$ are obtained by C_3 rotation.

B. Induced representations at M_1

We now consider the properties of the wavefunction at $\mathbf{k} = \mathbf{M}_1 = (0, \frac{2\pi}{\sqrt{3}})$. The Bloch functions are (see Eq. (E1))

$$|\alpha\rangle \equiv |\alpha, \mathbf{M}_1\rangle = \sum_{\mathbf{R}} e^{i\mathbf{M}_1 \cdot (\mathbf{R} + \mathbf{r}_\alpha)} |\mathbf{R}, \alpha\rangle, \quad \alpha = A, B, C, \quad (\text{S102})$$

where α indexes the three sublattices and $|\mathbf{R}, \alpha\rangle$ correspond to localised s -like orbitals at the 3c positions. The little co-group of the M -point is $C_{2v} = \{E, C_2, \sigma_1, \sigma_2\}$. We now follow the standard site-symmetry-induction construction of a band representation from a localised orbital on the 3c Wyckoff orbit [16–18]; we choose σ_1 to be the mirror that fixes the A site and swaps $B \leftrightarrow C$, and $\sigma_2 = C_2\sigma_1$. Under C_2 ,

$$A \mapsto A - \mathbf{a}_1, \quad B \mapsto B - \mathbf{a}_2, \quad C \mapsto C - \mathbf{a}_1 - \mathbf{a}_2. \quad (\text{S103})$$

At $\mathbf{M}_1$ the corresponding Bloch phases are

$$e^{-i\mathbf{M}_1 \cdot \mathbf{a}_1} = 1, \quad (\text{S104})$$

$$e^{-i\mathbf{M}_1 \cdot \mathbf{a}_2} = -1, \quad (\text{S105})$$

$$e^{-i\mathbf{M}_1 \cdot (\mathbf{a}_1 + \mathbf{a}_2)} = -1, \quad (\text{S106})$$

and so the representation of C_2 symmetry in the sublattice basis is

$$D(C_2) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \quad (\text{S107})$$

For σ_1 , we have

$$A \mapsto A, \quad B \mapsto C - \mathbf{a}_2, \quad C \mapsto B + \mathbf{a}_1 - \mathbf{a}_2. \quad (\text{S108})$$

Accounting for the Bloch phases appropriately, one finds

$$D(\sigma_1) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}. \quad (\text{S109})$$

For σ_2 , we have

$$A \mapsto A - \mathbf{a}_1, \quad B \mapsto C - \mathbf{a}_1, \quad C \mapsto B - \mathbf{a}_1, \quad (\text{S110})$$

and the Bloch phase is now +1, giving

$$D(\sigma_2) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \quad (\text{S111})$$

The characters of the three-dimensional band representation induced from an s orbital on the $3c$ orbit are given by the traces of these matrices,

$$\chi_{\mathbf{M}_1}^{(s@3c)}(E, C_2, \sigma_1, \sigma_2) = (3, -1, 1, 1). \quad (\text{S112})$$

Using the C_{2v} character table

$$\chi_{A_1} = (1, 1, 1, 1), \quad \chi_{A_2} = (1, 1, -1, -1), \quad (\text{S113})$$

$$\chi_{B_1} = (1, -1, 1, -1), \quad \chi_{B_2} = (1, -1, -1, 1), \quad (\text{S114})$$

we can use the orthogonality of characters [19] to decompose these characters into irreps; one immediately finds

$$\chi_{\mathbf{M}_1}^{(s@3c)} = A_1 \oplus B_1 \oplus B_2. \quad (\text{S115})$$

Thus the $s@3c$ elementary band representation contributes exactly three one-dimensional irreducible representations at each M point

$$(s@3c) \uparrow G \Big|_{\mathbf{M}_1} = A_1 \oplus B_1 \oplus B_2. \quad (\text{S116})$$

These are the symmetry representations which appear in the kagome s orbital tight-binding model near the M -point.

C. Dark set on the three kagome sublattices

We now compute the dark set index

$$m_\rho(\mathbf{M}_1, \mathbf{r}) = \frac{1}{|H_{\mathbf{M}_1, \mathbf{r}}|} \sum_{h \in H_{\mathbf{M}_1, \mathbf{r}}} e^{-i\mathbf{M}_1 \cdot (1-R_h)\mathbf{r}} \chi_\rho(h). \quad (\text{S117})$$

We first consider sublattice A ; for $\mathbf{r} = \mathbf{r}_A$, all four little-group elements fix A modulo lattice translation, so

$$H_{\mathbf{M}_1, A} = C_{2v}. \quad (\text{S118})$$

The translation phase is trivial for all four elements, and so

$$m_\rho(\mathbf{M}_1, A) = \frac{1}{4} [\chi_\rho(E) + \chi_\rho(C_2) + \chi_\rho(\sigma_1) + \chi_\rho(\sigma_2)]. \quad (\text{S119})$$

Consulting the character table for C_{2v} allows us to evaluate this for different ρ ; this gives the value of the index as

$$m_{A_1}(\mathbf{M}_1, \mathbf{r}_A) = 1, \quad (\text{S120})$$

$$m_{A_2}(\mathbf{M}_1, \mathbf{r}_A) = 0, \quad (\text{S121})$$

$$m_{B_1}(\mathbf{M}_1, \mathbf{r}_A) = 0, \quad (\text{S122})$$

$$m_{B_2}(\mathbf{M}_1, \mathbf{r}_A) = 0. \quad (\text{S123})$$

Hence of the four irreps of C_{2v} , at $\mathbf{M}_1$ all are dark on sublattice A except the A_1 irrep.

At the B sublattice $\mathbf{r} = \mathbf{r}_B$, only E and C_2 fix the point modulo a lattice vector, so

$$H_{\mathbf{M}_1, B} = \{E, C_2\} \cong C_2. \quad (\text{S124})$$

The C_2 action sends $B \mapsto B - \mathbf{a}_2$, i.e. $(1 - C_2)\mathbf{r}_B = \mathbf{a}_2$, yielding the Bloch phase

$$e^{-i\mathbf{M}_1 \cdot \mathbf{a}_2} = -1. \quad (\text{S125})$$

Hence

$$m_\rho(\mathbf{M}_1, B) = \frac{1}{2} [\chi_\rho(E) - \chi_\rho(C_2)]. \quad (\text{S126})$$

Therefore, using the character table for C_{2v} again

$$m_{A_1}(\mathbf{M}_1, B) = 0, \quad (\text{S127})$$

$$m_{A_2}(\mathbf{M}_1, B) = 0, \quad (\text{S128})$$

$$m_{B_1}(\mathbf{M}_1, B) = 1, \quad (\text{S129})$$

$$m_{B_2}(\mathbf{M}_1, B) = 1. \quad (\text{S130})$$

So the A_1 state is dark on B , while both B_1 and B_2 are allowed there. Exactly the same logic holds for $\mathbf{r} = \mathbf{r}_C$, because C_2 sends $C \mapsto C - \mathbf{a}_1 - \mathbf{a}_2$ and

$$e^{-i\mathbf{M}_1 \cdot (\mathbf{a}_1 + \mathbf{a}_2)} = -1. \quad (\text{S131})$$

Thus

$$m_\rho(\mathbf{M}_1, C) = \frac{1}{2} [\chi_\rho(E) - \chi_\rho(C_2)], \quad (\text{S132})$$

and therefore

$$m_{A_1}(\mathbf{M}_1, C) = 0, \quad (\text{S133})$$

$$m_{A_2}(\mathbf{M}_1, C) = 0, \quad (\text{S134})$$

$$m_{B_1}(\mathbf{M}_1, C) = 1, \quad (\text{S135})$$

$$m_{B_2}(\mathbf{M}_1, C) = 1. \quad (\text{S136})$$

D. Site-resolved dark sets at the M points

Collecting the three site tests at $\mathbf{M}_1$, we obtain

$$D_{A_1}(\mathbf{M}_1) = \{B, C\}, \quad (\text{S137})$$

$$D_{B_1}(\mathbf{M}_1) = \{A\}, \quad (\text{S138})$$

$$D_{B_2}(\mathbf{M}_1) = \{A\}. \quad (\text{S139})$$

Thus the A_1 state is supported only on the singled-out sublattice A , whereas the B_1 and B_2 states avoid A and live on the complementary pair (B, C) .

By C_3 symmetry, the other two M points give the cyclic permutations

$$D_{A_1}(\mathbf{M}_2) = \{C, A\}, \quad D_{B_1}(\mathbf{M}_2) = D_{B_2}(\mathbf{M}_2) = \{B\}, \quad (\text{S140})$$

$$D_{A_1}(\mathbf{M}_3) = \{A, B\}, \quad D_{B_1}(\mathbf{M}_3) = D_{B_2}(\mathbf{M}_3) = \{C\}. \quad (\text{S141})$$

Hence, for each M patch, one irreducible representation is bright on exactly one kagome sublattice, while the other two are bright on exactly two sublattices.

E. Identification with the nearest-neighbour kagome bands

At $\mathbf{M}_1$ one has

$$\mathbf{M}_1 \cdot \mathbf{d}_{AB} = -\frac{\pi}{2}, \quad (\text{S142})$$

$$\mathbf{M}_1 \cdot \mathbf{d}_{CA} = \frac{\pi}{2}, \quad (\text{S143})$$

$$\mathbf{M}_1 \cdot \mathbf{d}_{BC} = 0, \quad (\text{S144})$$

so the nearest-neighbour Hamiltonian becomes

$$H_0(\mathbf{M}_1) = -2t \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \quad (\text{S145})$$

Its three eigenstates are

$$|p_1\rangle = |A\rangle, \quad E_{p_1} = 0, \quad (\text{S146})$$

$$|m_1\rangle = \frac{1}{\sqrt{2}}(|B\rangle + |C\rangle), \quad E_{m_1} = -2t, \quad (\text{S147})$$

$$|f_1\rangle = \frac{1}{\sqrt{2}}(|B\rangle - |C\rangle), \quad E_{f_1} = +2t. \quad (\text{S148})$$

Up to the overall hopping-sign convention, these are the middle (p -type VHS), lower (m -type VHS), and upper (flat-band) states. Comparing with the symmetry matrices above, one finds the symmetry eigenvalues:

$$|p_1\rangle : (1, 1, 1, 1) = A_1, \quad (\text{S149})$$

$$|m_1\rangle : (1, -1, -1, 1) = B_2, \quad (\text{S150})$$

$$|f_1\rangle : (1, -1, 1, -1) = B_1. \quad (\text{S151})$$

Thus, at $\mathbf{M}_1$,

$$D_{p_1} = \{B, C\}, \quad (\text{S152})$$

$$D_{m_1} = \{A\}, \quad (\text{S153})$$

$$D_{f_1} = \{A\}. \quad (\text{S154})$$

In other words, the p -type Van Hove state is supported on a single kagome sublattice, while the m -type Van Hove state avoids that sublattice and lives on the complementary pair.

One interesting aspect of this result is its robustness — unlike the flat band of the kagome lattice, which becomes dispersive upon the addition of hoppings other than the simplest nearest-neighbour term, the sublattice interference effect is purely a statement about the band representations at the M -point, and is therefore an *exact* statement in the presence of symmetries. Adding complicated additional hoppings or interaction-induced band renormalisation can change the energetic ordering of the irreps from those in the nearest-neighbour model, but their dark sets remain the same.

On the other hand, when C_2 or mirror $\sigma_{1,2}$ are broken, the sublattice texture can change — for instance, it has been previously noted that a breathing distortion of the kagome lattice, which breaks C_2 and retains mirror, can mix the m - and p -type VHS while leaving the sublattice structure of the flat band intact [11, 20].

F. Distinguishing the m -type band from the flat band

On the three kagome sites alone, the B_1 and B_2 irreps look identical: both are dark on A at $\mathbf{M}_1$. To distinguish them one may use an additional high-symmetry probe, namely the midpoint of the BC bond,

$$\mathbf{P}_A = \frac{1}{2}(\mathbf{r}_B + \mathbf{r}_C) = \left(\frac{1}{2}, \frac{\sqrt{3}}{4}\right). \quad (\text{S155})$$

For this point,

$$H_{\mathbf{M}_1, \mathbf{P}_A} = \{E, \sigma_2\}, \quad (\text{S156})$$

⁴³⁰ and the twist is trivial, so

$$m_\rho(\mathbf{M}_1, \mathbf{P}_A) = \frac{1}{2} \left[1 + \chi_\rho(\sigma_2) \right]. \quad (\text{S157})$$

⁴³¹ Hence

$$m_{A_1}(\mathbf{M}_1, \mathbf{P}_A) = 1, \quad (\text{S158})$$

$$m_{A_2}(\mathbf{M}_1, \mathbf{P}_A) = 0, \quad (\text{S159})$$

$$m_{B_1}(\mathbf{M}_1, \mathbf{P}_A) = 0, \quad (\text{S160})$$

$$m_{B_2}(\mathbf{M}_1, \mathbf{P}_A) = 1. \quad (\text{S161})$$

⁴³² So the lower m -type state $|m_1\rangle$ is symmetry-allowed on the BC bond midpoint, while the flat-band state $|f_1\rangle$ is
⁴³³ symmetry-forced-dark there.

S8. HARTREE RENORMALISATION OF THE FLAT BANDS IN MAGIC-ANGLE BILAYER GRAPHENE

This section describes the continuum Hamiltonian, the flat-band symmetry representations and dark sets, the one-shot Hartree calculation used, and the atomistic real-space embedding used for the wavefunction panels in Fig. 5.

A. Continuum model

We use the single-valley continuum Dirac description of a twisted graphene bilayer [21–24]. We write the Hamiltonian for valley $\tau = +1$ throughout; the opposite valley is generated by time reversal, which also complex-conjugates all crystalline eigenvalues. The reciprocal primitive vectors of an untwisted graphene layer are denoted $\mathbf{G}_1, \mathbf{G}_2$, and the moiré reciprocal lattice vectors are

$$\mathbf{g}_i = (R_{\theta/2} - R_{-\theta/2})\mathbf{G}_i, \quad i = 1, 2, \quad (\text{S162})$$

with $\mathbf{a}_i \cdot \mathbf{g}_j = 2\pi\delta_{ij}$. We define,

$$\mathbf{q}_1 = -\frac{1}{3}(\mathbf{g}_1 + \mathbf{g}_2), \quad \mathbf{q}_2 = \mathbf{q}_1 + \mathbf{g}_1, \quad \mathbf{q}_3 = \mathbf{q}_1 + \mathbf{g}_2, \quad (\text{S163})$$

and the high symmetry momenta

$$K_M : \mathbf{k} = 0, \quad \Gamma_M : \mathbf{k} = \mathbf{q}_1, \quad M_M : \mathbf{k} = \mathbf{q}_1 + \frac{1}{2}\mathbf{g}_1, \quad K'_M : \mathbf{k} = -\mathbf{q}_1. \quad (\text{S164})$$

The plane-wave basis is $|\mathbf{g}, \ell, s\rangle$, where $\mathbf{g} = m\mathbf{g}_1 + n\mathbf{g}_2$, $\ell = 1, 2$ labels the layer, and $s = A, B$ labels the microscopic graphene sublattice. Using $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$, we define the intralayer Hamiltonian blocks

$$H_{11}(\mathbf{k} + \mathbf{g}) = -\hbar v_F \boldsymbol{\sigma} \cdot R_{-\theta/2}(\mathbf{k} + \mathbf{g}), \quad H_{22}(\mathbf{k} + \mathbf{g}) = -\hbar v_F \boldsymbol{\sigma} \cdot R_{\theta/2}(\mathbf{k} + \mathbf{g} + \mathbf{q}_1), \quad (\text{S165})$$

where subscripts 1, 2 index the layers, and

$$H_{12}(\mathbf{g}, \mathbf{g}') = T_1 \delta_{\mathbf{g}', \mathbf{g}} + T_2 \delta_{\mathbf{g}', \mathbf{g} + \mathbf{g}_1} + T_3 \delta_{\mathbf{g}', \mathbf{g} + \mathbf{g}_2}, \quad H_{21} = H_{12}^\dagger. \quad (\text{S166})$$

The tunnelling matrices are then

$$T_1 = \begin{pmatrix} w_{AA} & w_{AB} \\ w_{AB} & w_{AA} \end{pmatrix}, \quad T_2 = \begin{pmatrix} w_{AA} & w_{AB}\omega^{-1} \\ w_{AB}\omega & w_{AA} \end{pmatrix}, \quad T_3 = \begin{pmatrix} w_{AA} & w_{AB}\omega \\ w_{AB}\omega^{-1} & w_{AA} \end{pmatrix}. \quad (\text{S167})$$

The numerical parameters used for the magic-angle bandstructure are

$$\theta = 1.05^\circ, \quad w_{AA} = 80 \text{ meV}, \quad w_{AB} = 110 \text{ meV}, \quad v_F = 8.8 \times 10^5 \text{ m s}^{-1}, \quad a_0 = 0.246 \text{ nm}. \quad (\text{S168})$$

For the Hartree calculation, reciprocal vectors are retained within the radial cutoff $R_{\text{fac}} = 3.75$ about the physical Dirac momentum of each layer. This gives 55 layer-1 and 48 layer-2 reciprocal vectors, hence a one-valley Hamiltonian dimension of 206; the residual C_3 covariance error at K_M is 2.5×10^{-13} . The atomistic density panels use the separate high-symmetry-point-centred basis described in Sec. S8 E.

B. One-shot Hartree bands

Electrostatics is known to strongly reshape the active bands away from charge neutrality [25–29]. A complete mean-field calculation requires a choice of reference density matrix and, in general, a self-consistency loop. We use a charge-neutrality reference density in the sense reviewed in Ref. [30], but retain only the Hartree term and diagonalise once rather than perform a fully self-consistent calculation. Thus we compute

$$H^{1\text{shot}}(\nu) = H^0 + H_H[\delta P_\nu], \quad \delta P_\nu = P_\nu - P_{\nu=0}, \quad (\text{S169})$$

with no exchange term and no update of δP_ν after diagonalisation. This construction isolates the electrostatic form-factor mechanism responsible for the momentum-dependent reshaping, rather than attempting a self-consistent Hartree or Hartree–Fock prediction.

The interacting panel in Fig. 5 is evaluated at electron filling $\nu = 2$ with a spin-valley-symmetric occupation. Each of the four spin-valley flavours contributes one half electron per moiré unit cell to the central conduction band. On a uniform $N \times N$ mesh of the moiré Brillouin zone, the noninteracting central-conduction-band energies are sorted independently in the two valleys and the lowest half of the mesh points are occupied. Equivalently,

$$f_{\tau\mathbf{k}} = \Theta(\mu_\tau - \epsilon_{\tau c\mathbf{k}}^0), \quad \frac{1}{N^2} \sum_{\mathbf{k}} f_{\tau\mathbf{k}} = \frac{1}{2}, \quad (\text{S170})$$

where c labels the central conduction band. Let $\eta = \pm$ label the two time-reversed valleys generated from the $\tau = +1$ Hamiltonian of Sec. S8 A. The source density matrix is

$$\delta P_{\nu=2} = \frac{2}{N^2} \sum_{\eta=\pm} \sum_{\mathbf{k}} f_{\eta\mathbf{k}} |u_{\eta c\mathbf{k}}^0\rangle \langle u_{\eta c\mathbf{k}}^0|, \quad (\text{S171})$$

where $|u_{\eta c\mathbf{k}}^0\rangle$ is the normalised noninteracting eigenvector and the prefactor 2 is the spin degeneracy. This contains exactly two added electrons per moiré unit cell. At charge neutrality $P_\nu = P_{\nu=0}$, so the Hartree correction vanishes by construction.

For a moiré reciprocal vector $\delta\mathbf{g}$, the plane-wave density form factor and excess-density harmonic are

$$F_{\eta n\mathbf{k}}(\delta\mathbf{g}) = \sum_{\ell,s} \sum_{\mathbf{g}} u_{\eta n\mathbf{k}}^*(\mathbf{g}, \ell, s) u_{\eta n\mathbf{k}}(\mathbf{g} + \delta\mathbf{g}, \ell, s), \quad (\text{S172})$$

$$\delta n(\delta\mathbf{g}) = \frac{2}{N^2} \sum_{\eta=\pm} \sum_{\mathbf{k}} f_{\eta\mathbf{k}} F_{\eta c\mathbf{k}}(\delta\mathbf{g}), \quad (\text{S173})$$

where terms outside the finite plane-wave basis are omitted. We use $N = 72$ in the results presented in the main text, and no finite-temperature smearing. The uniform component $\delta\mathbf{g} = 0$ is removed because it is cancelled by the neutralising background or absorbed into the chemical potential.

The dual-gate screened Coulomb kernel is

$$V(g) = \frac{2\pi e^2}{\epsilon_r g} \tanh(g d_{\text{sc}}), \quad g = |\delta\mathbf{g}|, \quad (\text{S174})$$

where e^2 denotes $e^2/(4\pi\epsilon_0)$ in units of meV nm. We use $\epsilon_r = 10$ and $d_{\text{sc}} = 30$ nm. The resulting Hartree matrix is diagonal in layer and microscopic sublattice and is taken to be the same in both graphene layers,

$$[H_H]_{\mathbf{g}\ell s, \mathbf{g}'\ell' s'} = \delta_{\ell\ell'} \delta_{ss'} \frac{1}{\mathcal{A}_M} \sum_{\delta\mathbf{g} \neq 0} V(|\delta\mathbf{g}|) \delta n(\delta\mathbf{g}) \delta_{\mathbf{g}', \mathbf{g} + \delta\mathbf{g}}, \quad (\text{S175})$$

where $\mathcal{A}_M$ is the moiré unit-cell area. The microscopic interlayer separation is neglected in the interaction kernel, which is appropriate on the moiré length scale. After constructing Eq. (S175), we impose Hermiticity and average the matrix over the three C_3 rotations to remove residual quadrature and cutoff asymmetries.

The main text calculation retains the first two stars $\mathcal{S}_1 \cup \mathcal{S}_2$ of the triangular moiré reciprocal lattice, with $g_s/|\mathbf{g}_1| = 1$ and $\sqrt{3}$ and six vectors in each star. The first two stars give 96.80% of the three-star value of the relative $K_M - \Gamma_M$ shift; adding the third star, $g_3/|\mathbf{g}_1| = 2$, changes either central band by at most 0.85 meV along the complete $K_M \rightarrow \Gamma_M \rightarrow M_M \rightarrow K_M$ path. Replacing the 72×72 source mesh by a 60×60 mesh changes the quoted high-symmetry shifts by less than 2×10^{-4} meV. The qualitative reshaping is also robust to the screening parameters — at fixed $d_{\text{sc}} = 30$ nm, varying ϵ_r from 8 to 12 changes $\Delta_{K\Gamma}$ from 29.10 to 19.64 meV and $\Delta_{M\Gamma}$ from 29.37 to 19.80 meV, close to the expected $1/\epsilon_r$ scaling. At fixed $\epsilon_r = 10$, varying d_{sc} from 5 to 30 nm changes $\Delta_{K\Gamma}$ only from 23.280 to 23.466 meV; the finite-wavevector interaction is already nearly saturated at the shortest screening length considered. These variations alter the overall Hartree scale but not the pronounced minimum of the shift near Γ_M .

For the Brillouin-zone maps, $\boldsymbol{\kappa}$ denotes Cartesian momentum measured from Γ_M . We diagonalise the full one-shot Hamiltonian throughout the hexagonal moiré Brillouin zone and define

$$\Delta E_{\pm}(\boldsymbol{\kappa}) = E_{\pm}^{\text{1shot}}(\boldsymbol{\kappa}) - E_{\pm}^0(\boldsymbol{\kappa}), \quad \Delta \bar{E}(\boldsymbol{\kappa}) = \frac{1}{2} \{ \Delta E_+(\boldsymbol{\kappa}) + \Delta E_-(\boldsymbol{\kappa}) \}. \quad (\text{S176})$$

The raw central-pair mean shifts are 2.516 meV at Γ_M , 25.982 meV at K_M , and 26.189 meV at M_M . Thus $\Delta_{K\Gamma} \equiv \Delta \bar{E}(K_M) - \Delta \bar{E}(\Gamma_M) = 23.466$ meV and $\Delta_{M\Gamma} \equiv \Delta \bar{E}(M_M) - \Delta \bar{E}(\Gamma_M) = 23.673$ meV. The separate lower- and upper-band shifts need not be maximal at K_M : the symmetry-preserving Hartree potential produces a common shift of the Dirac doublet there, whereas away from the corner the branches can mix and redistribute the shift, giving the threefold structure in Fig. S23.

For the band path used in the main text, the noninteracting zero is the mean energy of the central pair at K_M . The Hartree spectrum is shifted by a constant so that the central-pair mean at Γ_M aligns with the noninteracting value; this removes no momentum-dependent information.

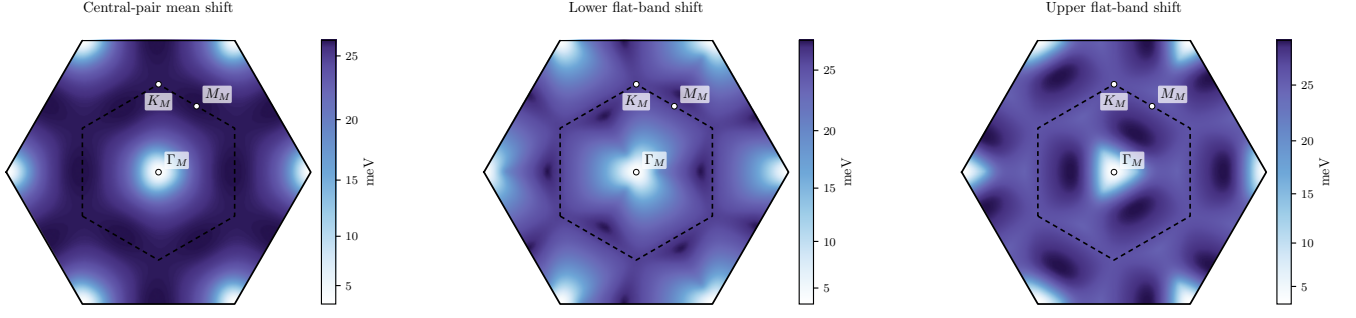


FIG. S23. One-shot band shifts throughout the hexagonal moiré Brillouin zone. Left: mean shift $\Delta\bar{E}$ of the central pair. Middle and right: shifts of the lower and upper central bands after diagonalising $H^0 + H_H$. The central-pair mean has a pronounced minimum at Γ_M , while the separate branches display the threefold redistribution of the common outer-Brillouin-zone shift.

C. Flat-band symmetry representations

The one-valley and two-valley symmetry groups must be distinguished. A single valley has magnetic space group $P6'2'2$, generated by C_{3z} , C_{2x} , $C_{2z}\mathcal{T}$, and moiré translations. Restoring the time-reversed valley gives the ordinary space group $P622$, whose point group is D_6 . The flat-band representations were identified in the early symmetry analyses of Refs. [31–35]; the same representation content is central to the heavy-fermion descriptions of Refs. [36–38]. For one valley, the central pair transforms as

$$\Gamma_M : \Gamma_1 \oplus \Gamma_2, \quad K_M : K_2K_3, \quad M_M : M_1 \oplus M_2. \quad (\text{S177})$$

The time-reversed corner K'_M carries the conjugate co-representation and is left implicit below. The two Γ_M states have C_{3z} eigenvalue 1 and opposite C_{2x} parities; the K_2K_3 co-representation has C_{3z} eigenvalues ω and ω^2 ; and the two M_M states have opposite C_{2x} parities. After the opposite valley is added, the four flat bands transform as

$$\Gamma_M : \Gamma_1 \oplus \Gamma_2 \oplus \Gamma_3 \oplus \Gamma_4, \quad K_M : 2K_3, \quad M_M : M_1 \oplus M_2 \oplus M_3 \oplus M_4. \quad (\text{S178})$$

At a selected K_M corner, the little co-group is the six-element proper-rotation group D_3 , generated in our convention by C_{3z} and C_{2y} . Although D_3 is abstractly isomorphic to C_{3v} , its order-two elements here are three-dimensional rotations, as we emphasise below. The crystallographic irrep K_3 is also denoted E , with $\chi_E(C_{3z}) = -1$ and $\chi_E(C_{2y}) = 0$. The operations C_{2x} and C_{2z} exchange K_M and K'_M . Table XVII gives the remaining generator characters at Γ_M and M_M . Using the conventional crystallographic C_{3z} generator, the central flat-band subspace in valley + has the C_{3z} -eigenvalue multisets

$$\Lambda_{\Gamma_M} = \{1, 1\}, \quad \Lambda_{K_M} = \Lambda_{K'_M} = \{\omega, \omega^2\}. \quad (\text{S179})$$

Time reversal complex-conjugates the eigenvalues and exchanges the laboratory-frame K_M and K'_M points. Since the corner eigenvalues form the conjugation-invariant set $\{\omega, \omega^2\}$, the unordered eigenvalue set is the same at the two corners.

Three-dimensional meaning of the order-two characters

The order-two characters are physically important, but their nodal consequences live partly outside the two-dimensional, layer-projected density plotted in Fig. 5. The distinction follows from the three-dimensional action of the point group. The abstract groups D_6 and C_{6v} are isomorphic, and restricting the coordinates to the plane $z = 0$ makes an in-plane twofold rotation look like a mirror. Their fixed sets in the physical bilayer are nevertheless different. In D_6 ,

$$C_{2x} : (x, y, z) \mapsto (x, -y, -z), \quad \mathcal{L}_x = \{(x, 0, 0) : x \in \mathbb{R}\}, \quad (\text{S180})$$

so the fixed positions lie on an axis in the midplane between the layers. An actual C_{6v} mirror would instead act as $(x, y, z) \mapsto (x, -y, z)$ and fix the whole vertical plane $y = 0$, including its intersections with both graphene sheets.

Let $g = \{C_2|\mathbf{t}_g\}$ leave $\mathbf{k}_*$ invariant and let $p_g = \pm 1$ be the physical eigenvalue of a one-dimensional small representation. At a point of the affine fixed set of g , the usual local selection rule reads

$$\Phi_{\mathbf{k}_*}(\mathbf{r}_*) = e^{-i\mathbf{k}_* \cdot \mathbf{t}_g} p_g \Phi_{\mathbf{k}_*}(\mathbf{r}_*). \quad (\text{S181})$$

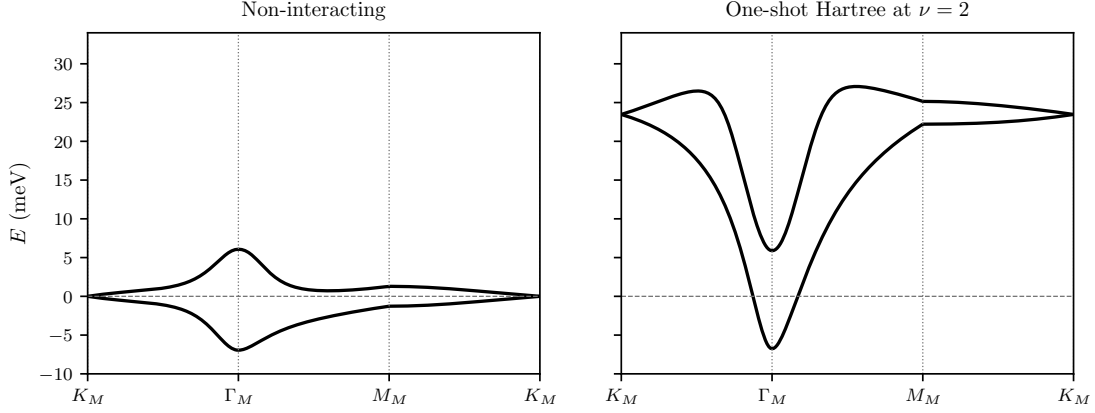


FIG. S24. Noninteracting bands and the charge-neutrality-subtracted one-shot Hartree bands at $\nu = 2$. The source density is evaluated on a 72×72 mesh and the first two moiré reciprocal stars are retained. The Hartree panel is aligned at Γ_M , highlighting a relative displacement of 23.47 meV at K_M and 23.67 meV at M_M .

Thus the full three-dimensional amplitude vanishes whenever the local parity

$$\pi_g(\mathbf{k}_*, \mathbf{r}_*) = e^{-i\mathbf{k}_* \cdot \mathbf{t}_g} p_g \quad (\text{S182})$$

is -1 . For the origin-centred C_{2x} axis at Γ_M , this reduces to

$$p_x = -1 \implies \Phi_{\mathbf{k}_*}(x, 0, 0) = 0. \quad (\text{S183})$$

The same statement holds on translated in-plane twofold axes, with the Bloch factor in Eq. (S182) deciding which parity is locally dark.

Another way to see this is to let φ_t be an orbital in the top layer and φ_b its C_{2x} partner in the bottom layer, with

$$\hat{C}_{2x}\varphi_t = s_x\varphi_b, \quad s_x = \pm 1. \quad (\text{S184})$$

The sign s_x includes both the microscopic transformation of the carbon p_z orbital and any basis convention. The parity eigenstates are

$$\Phi_{p_x} = \frac{1}{\sqrt{2}}(\varphi_t + p_x s_x \varphi_b). \quad (\text{S185})$$

On $\mathcal{L}_x$, invariance of the coordinate implies $\varphi_t = s_x\varphi_b$, and therefore

$$\Phi_{p_x}(\mathbf{r} \in \mathcal{L}_x) = \frac{1+p_x}{\sqrt{2}}\varphi_t(\mathbf{r}). \quad (\text{S186})$$

The odd state is forced to vanish exactly at the midpoint between the two C_{2x} -related orbitals, and more generally along the full fixed axis. This result is independent of the orbital sign s_x .

The layer-projected density used in Fig. 5 does not sample this fixed axis. It evaluates the amplitudes on the two sheets with $z = \pm d/2$ at two-dimensional coordinates $\boldsymbol{\rho}$, and adds their densities incoherently,

$$\rho_{\text{lay}}(\boldsymbol{\rho}) = |\Phi(\boldsymbol{\rho}, d/2)|^2 + |\Phi(\boldsymbol{\rho}, -d/2)|^2. \quad (\text{S187})$$

On the layer planes, C_{2x} relates the two terms and fixes their relative phase; it does not fix either point individually. The sign p_x is lost when the layer densities are added, while the destructive interference in Eq. (S186) occurs only in the interlayer region where the two orbital tails overlap coherently. Hence different C_{2x} eigenvalues cannot be distinguished from the layer-projected density. In the convention of Table XVII, the C_{2x} -odd one-dimensional irreps are Γ_2 (A_2), Γ_3 (B_2), M_2 (B_1), and M_3 (B_2) — each has an interlayer nodal axis whenever the local Bloch phase is trivial. The K_3 (E) doublet contains one even and one odd eigenvector of C_{2y} , so its two-dimensional projected density remains bright on the corresponding axis even though its odd member is individually dark there.

There is an analogous, but valley-sensitive, statement for C_{2z} ,

$$C_{2z} : (x, y, z) \mapsto (-x, -y, z), \quad \mathcal{L}_z = \{(0, 0, z) : z \in \mathbb{R}\}. \quad (\text{S188})$$

Momentum	Irrep	$\chi(C_{3z})$	$\chi(C_{2z})$	$\chi(C_{2x})$
Γ_M	$\Gamma_1 (A_1)$	1	+1	+1
Γ_M	$\Gamma_2 (A_2)$	1	+1	-1
Γ_M	$\Gamma_3 (B_2)$	1	-1	-1
Γ_M	$\Gamma_4 (B_1)$	1	-1	+1
K_M	$K_3 (E)$	-1	-	-
M_M	$M_1 (A)$	-	+1	+1
M_M	$M_2 (B_1)$	-	+1	-1
M_M	$M_3 (B_2)$	-	-1	-1
M_M	$M_4 (B_3)$	-	-1	+1

TABLE XVII. **Two-valley flat-band representation data for magic-angle graphene.** The first label in the Irrep column is the crystallographic small-representation label; the label in parentheses is the Mulliken notation for the associated little co-group. The little co-groups are D_6 at Γ_M , $D_3 \ni C_{3z}, C_{2y}$ at K_M , and $D_2 \ni C_{2y}$ at M_M . In the axis convention of the $P622$ character table, C_{2x} belongs to the C'_2 class and C_{2y} to the C''_2 class. The dashes in the K_M row indicate that C_{2z} and C_{2x} exchange the two corners. The flat band manifold contains one copy of each listed Γ_M and M_M irrep and two copies of K_3 .

At Γ_M and M_M , a full two-valley state with local C_{2z} parity -1 vanishes on the vertical rotation axis, including its intersections with the two graphene sheets. In the continuum theory, however, C_{2z} exchanges valleys and sublattices. If Φ_+ is a valley + amplitude and $\hat{C}_{2z}\Phi_+ = s_z\Phi_-$, then the coherent parity eigenstates are

$$\Phi_{p_z} = \frac{1}{\sqrt{2}}(\Phi_+ + p_z s_z \Phi_-), \quad (\text{S189})$$

and on $\mathcal{L}_z$ one obtains

$$\Phi_{p_z}(\mathbf{r} \in \mathcal{L}_z) = \frac{1+p_z}{\sqrt{2}}\Phi_+(\mathbf{r}). \quad (\text{S190})$$

Thus a C_{2z} -odd valley-coherent state has a vertical nodal line. A single-valley wavefunction is not a C_{2z} eigenstate, while the valley-incoherent density

$$\rho_{\text{val}}(\mathbf{r}) = |\Phi_+(\mathbf{r})|^2 + |\Phi_-(\mathbf{r})|^2 \quad (\text{S191})$$

contains no interference term and is blind to p_z . At K_M , C_{2z} exchanges K_M and K'_M , so a C_{2z} parity can only be assigned to a coherent superposition over the two-corner star, not to a state at one corner. The C_{2z} -odd one-dimensional irreps at the time-reversal-invariant momenta are $\Gamma_3 (B_2)$, $\Gamma_4 (B_1)$, $M_3 (B_2)$, and $M_4 (B_3)$.

The order-two characters therefore produce *three-dimensional dark sets* — the C_{2x} characters control interlayer-parity nodes on midplane axes, while the C_{2z} characters control vertical nodes of valley-coherent states. Neither effect is represented in the plots used here, which retain one valley and project the density onto the two graphene layers before adding the layers incoherently. The C_3 analysis below instead concerns zeros already present in the layer-resolved amplitudes at the maximal stacking centres, and is directly visible in those plots.

D. Calculation of the flat-band dark sets

We apply the main-text stabiliser projector to one embedded layer-sublattice component at a time. In valley +,

$$\psi_{1s}(\mathbf{r}) = \sum_{\mathbf{g}} u_{\mathbf{g},1s}(\mathbf{k}) e^{i(\mathbf{k}+\mathbf{g})\cdot\mathbf{r}}, \quad \psi_{2s}(\mathbf{r}) = \sum_{\mathbf{g}} u_{\mathbf{g},2s}(\mathbf{k}) e^{i(\mathbf{k}+\mathbf{g}+\mathbf{q}_1)\cdot\mathbf{r}}. \quad (\text{S192})$$

Let $\xi_A = 1$, $\xi_B = \omega$, and $\mathbf{t}_3(\mathbf{r}_*) = (1 - C_3)\mathbf{r}_*$. In the conventional C_3 gauge of Eq. (S179), the local phase is

$$\zeta_{\ell s}(\mathbf{k}_*, \mathbf{r}_*) = \omega \xi_s \exp\{i(\mathbf{k}_* + \delta_{\ell,2}\mathbf{q}_1) \cdot \mathbf{t}_3(\mathbf{r}_*)\}. \quad (\text{S193})$$

For a flat-band subspace $\mathcal{S}$, write $\Lambda_{\mathcal{S}} = \{\lambda_a\}_{a=1}^{\dim \mathcal{S}}$ for its set of C_{3z} eigenvalues, counted with multiplicity; thus λ_a is the rotation eigenvalue of the a th symmetry-resolved state in $\mathcal{S}$. The index gives

$$m_{\mathcal{S},\ell s}(\mathbf{k}_*, \mathbf{r}_*) = \sum_{\lambda_a \in \Lambda_{\mathcal{S}}} \frac{1}{3} \{1 + \lambda_a \zeta_{\ell s}^{-1} + (\lambda_a \zeta_{\ell s}^{-1})^2\}. \quad (\text{S194})$$

Channel	Γ_M, AA	Γ_M, AB	Γ_M, BA	K_M, AA	K_M, AB	K_M, BA	K'_M, AA	K'_M, AB	K'_M, BA
1A	ω	ω^2	1	ω	ω	ω	ω	1	ω^2
1B	ω^2	1	ω	ω^2	ω^2	ω^2	ω^2	ω	1
2A	ω	1	ω^2	ω	ω^2	1	ω	ω	ω
2B	ω^2	ω	1	ω^2	1	ω	ω^2	ω^2	ω^2

TABLE XVIII. Local C_3 phases of the four embedded layer-sublattice components in valley $+$. A component is bright when its entry matches one of the flat-band eigenvalues in Eq. (S179).

The component is bright precisely when one $\lambda_a = \zeta_{\ell s}$. The motivation for this slight reformulation of the equation in the main text is that this form is basis-independent at the Dirac points.

The maximal high-symmetry positions of the moiré cell are

$$\mathbf{r}_{AA} = 0, \quad \mathbf{r}_{AB} = \frac{1}{3}(\mathbf{a}_1 + 2\mathbf{a}_2), \quad \mathbf{r}_{BA} = \frac{1}{3}(2\mathbf{a}_1 + \mathbf{a}_2), \quad (\text{S195})$$

and the three saddle positions $\mathbf{s}_1 = \mathbf{a}_1/2$, $\mathbf{s}_2 = \mathbf{a}_2/2$, $\mathbf{s}_3 = (\mathbf{a}_1 + \mathbf{a}_2)/2$. The conventional local C_3 phases are listed in Table XVIII.

Combining this table with Eq. (S179) gives the channel-resolved result in Table XIX. This table samples amplitudes on the graphene layers and therefore records the C_3 -enforced layer-sublattice zeros relevant to Fig. 5. The order-two characters add the three-dimensional nodal axes derived in Sec. S8 C: a C_{2x} -odd state is dark on the appropriate interlayer fixed axis, and a C_{2z} -odd coherent two-valley state is dark on the corresponding vertical axis. Those nodes are absent from the present layer-projected, single-valley visualisation. At K_M , the K_3 (E) subspace contains both C_{2y} parities, so its subspace density has no order-two-enforced zero. The AB and BA centres are exchanged by the relevant order-two operations, which relate their amplitudes rather than imposing an additional one-point zero on a fixed layer.

The layer-projected density is the sum over all four layer-sublattice components. It vanishes at the positions D_{lay} when every component is dark, and therefore

$$D_{\text{lay}}(\Gamma_M) = \{AA\}, \quad D_{\text{lay}}(K_M) = D_{\text{lay}}(K'_M) = D_{\text{lay}}(M_M) = \emptyset. \quad (\text{S196})$$

While the wavefunction has components with exact zeros at AB and BA, other components remain bright, and so Eq. (S196) is the complete symmetry-enforced dark set for the layer-projected, valley-diagonal density at the maximal in-plane positions used in Fig. 5.

E. Wavefunction maps

The exact C_3 dark-set statement concerns the pointwise embedded continuum amplitude in a fixed valley; the time-reversed valley has the conjugate amplitude and therefore the same density. The real-space panels in Fig. 5 show the atomistically embedded density of the selected flat-band state at one high-symmetry momentum and energy.

We follow the microscopic reconstruction used in Refs. [39, 40]; the continuum eigenvector is first converted into a complex amplitude on every microscopic carbon site by restoring the rapidly varying valley momentum and the plane-wave phases. These complex site amplitudes are then used as coefficients of overlapping carbon-centred orbitals, and the orbitals are summed before the modulus square is taken. This reconstructs the wavefunction itself within each layer and retains interference between neighbouring carbon sites and between the two sublattices. For the plots used here, the z coordinate is suppressed and the two layer densities are added incoherently, so the interlayer C_{2x} cancellation and the valley-coherent C_{2z} cancellation of Sec. S8 C are not retained.

Let $\mathbf{A}_1, \mathbf{A}_2$ be graphene direct vectors dual to $\mathbf{G}_1, \mathbf{G}_2$, and define the sublattice displacement

$$\delta_{AB} = \frac{1}{3}\mathbf{A}_1 - \frac{1}{3}\mathbf{A}_2. \quad (\text{S197})$$

The microscopic carbon positions in layer ℓ are

$$\mathbf{R}_{mn}^{\ell A} = R_{\alpha_\ell}(m\mathbf{A}_1 + n\mathbf{A}_2), \quad (\text{S198})$$

$$\mathbf{R}_{mn}^{\ell B} = R_{\alpha_\ell}(m\mathbf{A}_1 + n\mathbf{A}_2 + \delta_{AB}), \quad (\text{S199})$$

where $m, n \in \mathbb{Z}$, $\alpha_1 = \theta/2$, and $\alpha_2 = -\theta/2$. The layer-dependent valley momenta are

$$\mathbf{K}_1 = R_{\theta/2}\mathbf{K}_0, \quad \mathbf{K}_2 = R_{-\theta/2}\mathbf{K}_0, \quad \mathbf{K}_0 = -\frac{1}{3}(\mathbf{G}_1 + \mathbf{G}_2). \quad (\text{S200})$$

Position	Γ_M	K_M	K'_M	M_M
AA	$1A, 1B, 2A, 2B$	None	None	None
AB	$1A, 2B$	$2B$	$1A$	None
BA	$1B, 2A$	$2A$	$1B$	None
$\mathbf{s}_1, \mathbf{s}_2, \mathbf{s}_3$	None	None	None	None

TABLE XIX. Component-resolved dark sets of the central two flat bands in one valley. The entries list the dark layer-sublattice components.

For a continuum eigenvector $u_{n\mathbf{k}}(\mathbf{g}, \ell, s)$, with band index n , moiré momentum $\mathbf{k}$, layer ℓ , and sublattice s , define the microscopic momentum carried by the corresponding plane-wave component as

$$\mathbf{p}_{\mathbf{k}\mathbf{g}}^\ell = \mathbf{K}_\ell + \mathbf{k} + \mathbf{g} + \delta_{\ell,2}\mathbf{q}_1. \quad (\text{S201})$$

The complex coefficient assigned to a carbon site $\mathbf{R}$ is then

$$\mathcal{A}_{n\mathbf{k}}^{\ell s}(\mathbf{R}) = \sum_{\mathbf{g}} u_{n\mathbf{k}}(\mathbf{g}, \ell, s) e^{i\mathbf{p}_{\mathbf{k}\mathbf{g}}^\ell \cdot \mathbf{R}}. \quad (\text{S202})$$

This is the continuum envelope evaluated on the microscopic lattice with the valley-scale Bloch phase restored.

We represent each carbon-centred orbital by the two-dimensional Gaussian

$$\phi_\sigma(\mathbf{r}) = \exp[-|\mathbf{r}|^2/(2\sigma^2)], \quad (\text{S203})$$

with the choice of $\sigma = 0.060$ nm. The reconstructed complex wavefunction in layer ℓ is

$$\Phi_{n\mathbf{k}}^\ell(\mathbf{r}) = \sum_{p,q \in \mathbb{Z}} \sum_{s=A,B} \mathcal{A}_{n\mathbf{k}}^{\ell s}(\mathbf{R}_{pq}^{\ell s}) \phi_\sigma(\mathbf{r} - \mathbf{R}_{pq}^{\ell s}), \quad (\text{S204})$$

where p, q label graphene unit cells. The sum is coherent over all carbon sites and both sublattices in a given layer.

For a selected state or degenerate subspace $\mathcal{S}$, the plotted density is

$$\rho_{\mathcal{S}}^{\text{atom}}(\mathbf{r}) = \sum_{n \in \mathcal{S}} \sum_{\ell=1}^2 |\Phi_{n\mathbf{k}}^\ell(\mathbf{r})|^2. \quad (\text{S205})$$

Eq. (S205) adds different bands and the two layers incoherently, while retaining all carbon-site interference within each layer through Eq. (S204).

The wavefunction panels in Fig. 5 are evaluated at the selected high-symmetry momentum and band energy. Their eigenvectors are calculated in a high-symmetry-point-centred radial basis with $R_{\text{fac}} = 2.5$, for which the dimensions are 80 at K_M and 84 at Γ_M . The basis is closed under C_3 at the relevant momentum to residuals below 2×10^{-13} . The atomistic density is evaluated on a 330×330 grid over the moiré Wigner-Seitz cell, averaged over the three C_3 rotations, and normalised independently in each panel,

$$Z_{\text{plot}}(\mathbf{r}) = \frac{\rho_{\mathcal{S}}^{\text{atom}}(\mathbf{r})}{\max_{\mathbf{r} \in \Omega_M} \rho_{\mathcal{S}}^{\text{atom}}(\mathbf{r})}, \quad (\text{S206})$$

where Ω_M is the plotted moiré Wigner-Seitz cell. The exact continuum envelope for the Γ_M wavefunction vanishes to numerical precision at the AA position.

S9. A MORE GENERAL PROOF

In SM Sec. S1, we verified the central theorem in two dimensions by explicitly computing the dark set for every irrep at every high-symmetry momentum of the 17 wallpaper groups. Here we give a less constructive proof for symmorphic wallpaper groups. The idea is that each real-space probe defines a linear functional of the little-group character. We prove that, for every symmorphic wallpaper little co-group, a sufficiently rich finite set probe positions makes the resulting map injective on the character space. The labelled zero pattern of these indices distinguishes the corresponding physical irrep. For nonsymmorphic groups, fixed-point-free symmetries are absent from every one-point stabiliser; the final subsection explains this obstruction, observable in the tables of Sec. S1.

A. Linear-algebra formulation of the uniqueness problem

A class function on G is a complex-valued function on the group that is constant on conjugacy classes. Characters are the most important examples: if ρ is a representation of G , then its character

$$\chi_\rho(g) = \text{Tr } \rho(g) \quad (\text{S207})$$

depends only on the conjugacy class of g . Since a finite group has finitely many conjugacy classes, the space $\text{Class}(G)$ of class functions is finite-dimensional.

For a probe position $\mathbf{r}_i$, define its stabiliser H_i and local phase

$$\vartheta_i(h) = e^{-i\mathbf{k}_* \cdot (1-R_h)\mathbf{r}_i}, \quad h \in H_i. \quad (\text{S208})$$

For an irrep ρ of G , the local index is

$$m_i(\rho) = \frac{1}{|H_i|} \sum_{h \in H_i} \vartheta_i(h) \chi_\rho(h). \quad (\text{S209})$$

This expression is linear in χ_ρ , so the uniqueness problem is naturally a problem in linear algebra on $\text{Class}(G)$.

B. Restriction, induction, and Frobenius reciprocity

If ρ is a representation of G , then

$$\text{Res}_{H_i}^G \rho \quad (\text{S210})$$

denotes the same representation viewed only on H_i . If σ is a representation of H_i , then

$$\text{Ind}_{H_i}^G \sigma \quad (\text{S211})$$

is the representation of G induced from σ .

With the standard inner product on class functions,

$$\langle f, g \rangle_G = \frac{1}{|G|} \sum_{h \in G} f(h)^* g(h), \quad (\text{S212})$$

the index of Eq. (4) can be written as the inner product

$$m_i(\rho) = \langle \vartheta_i^*, \text{Res}_{H_i}^G \chi_\rho \rangle_{H_i}. \quad (\text{S213})$$

As shown in Sec. S2, ϑ_i is a one-dimensional representation of the stabiliser. Frobenius reciprocity therefore gives

$$\langle \sigma, \text{Res}_H^G \chi \rangle_H = \langle \text{Ind}_H^G \sigma, \chi \rangle_G, \quad (\text{S214})$$

and hence

$$m_i(\rho) = \langle \text{Ind}_{H_i}^G \vartheta_i^*, \chi_\rho \rangle_G. \quad (\text{S215})$$

Define the probe-induced class function

$$\Psi_i \equiv \chi_{\text{Ind}_{H_i}^G \vartheta_i^*}. \quad (\text{S216})$$

Then

$$m_i(\rho) = \langle \Psi_i, \chi_\rho \rangle_G. \quad (\text{S217})$$

Thus each physical probe position defines one linear functional on the character table of the little group.

C. The visible class-function space

Let

$$\mathcal{V}_{\text{vis}}(\mathbf{k}_*) = \text{span}\{\Psi_{\mathbf{r}} : \text{all physical probe positions } \mathbf{r}\} \subseteq \text{Class}(G) \quad (\text{S218})$$

be the visible class-function space. Two characters have identical local indices at every probe position precisely when their difference is orthogonal to this space:

$$\chi_{\rho} - \chi_{\rho'} \in \mathcal{V}_{\text{vis}}(\mathbf{k}_*)^{\perp}. \quad (\text{S219})$$

Equivalently, the complete family of one-point probes determines exactly the projection of χ_{ρ} onto $\mathcal{V}_{\text{vis}}(\mathbf{k}_*)$.

D. Reduction of the probe family

For fixed $\mathbf{k}_*$, every probe position $\mathbf{r}$ determines a subgroup-character pair $(H_{\mathbf{r}}, \vartheta_{\mathbf{r}})$, and $\Psi_{\mathbf{r}}$ depends only on this pair. Since G is finite, it has finitely many subgroups, and each subgroup has finitely many one-dimensional characters. Hence only finitely many distinct probe-induced functions $\Psi_{\mathbf{r}}$ can occur.

Choose a maximal linearly independent subfamily

$$\Psi_1, \dots, \Psi_N. \quad (\text{S220})$$

It is a basis of $\mathcal{V}_{\text{vis}}(\mathbf{k}_*)$: if some $\Psi_{\mathbf{r}}$ lay outside its span, adjoining it would contradict maximality. Therefore a finite set of physical probe positions captures all information accessible to one-point probes. The substantive task below is to show that, for symmorphic wallpaper groups, physically realised rotation-centre and mirror-line probes span this space.

E. Matrix form and the uniqueness criterion

Choose probe positions $\mathbf{r}_1, \dots, \mathbf{r}_N$ such that $\Psi_1, \dots, \Psi_N$ form a basis of $\mathcal{V}_{\text{vis}}(\mathbf{k}_*)$. Write the visible part of an irrep character as

$$\chi_{\rho}^{\text{vis}} = \sum_{j=1}^N c_{\rho,j} \Psi_j. \quad (\text{S221})$$

Then

$$m_i(\rho) = \langle \Psi_i, \chi_{\rho}^{\text{vis}} \rangle_G = \sum_{j=1}^N P_{ij} c_{\rho,j}, \quad P_{ij} \equiv \langle \Psi_i, \Psi_j \rangle_G. \quad (\text{S222})$$

Equivalently,

$$\mathbf{m}_{\rho} = P \mathbf{c}_{\rho}, \quad (\text{S223})$$

where

$$\mathbf{m}_{\rho} = (m_1(\rho), \dots, m_N(\rho))^T. \quad (\text{S224})$$

For a basis $\{\Psi_i\}$, the Gram matrix P has full rank, so the local indices determine χ_{ρ}^{vis} . Consequently, to reconstruct the physical character it is enough to prove

$$\mathcal{V}_{\text{vis}}(\mathbf{k}_*) = \text{Class}_{\text{phys}}(G). \quad (\text{S225})$$

The following sections establish this equality by constructing the required physical probes.

F. Physical character space at a time-reversal invariant momentum

At a time-reversal invariant momentum, the local phases of a symmorphic stabiliser are real:

$$\vartheta_i(h) = \pm 1. \quad (\text{S226})$$

Consequently,

$$m_i(\bar{\rho}) = m_i(\rho). \quad (\text{S227})$$

A density measurement therefore cannot distinguish an ordinary complex irrep ρ from its conjugate $\bar{\rho}$.

Define the corresponding physical character by

$$\chi_{[\rho]} = \begin{cases} \chi_\rho, & \rho \simeq \bar{\rho}, \\ \chi_\rho + \chi_{\bar{\rho}}, & \rho \not\simeq \bar{\rho}. \end{cases} \quad (\text{S228})$$

The span of these characters is denoted

$$\text{Class}_{\text{phys}}(G). \quad (\text{S229})$$

In a time-reversal-symmetric system, a distinct pair $\rho, \bar{\rho}$ forms one irreducible corepresentation of the magnetic little group. Away from a time-reversal invariant momentum, no such pairing is imposed and we take

$$\text{Class}_{\text{phys}}(G) = \text{Class}(G). \quad (\text{S230})$$

G. Rotation centres and their local phases

Let $\mathcal{R}$ be an n -fold lattice rotation. A point $\mathbf{r}$ is a centre of an affine rotation with linear part $\mathcal{R}$ precisely when

$$(1 - \mathcal{R})\mathbf{r} = \mathbf{t} \in \Lambda, \quad (\text{S231})$$

where Λ is the Bravais lattice. Translating the centre by $\boldsymbol{\lambda} \in \Lambda$ changes its label by

$$\mathbf{t} \mapsto \mathbf{t} + (1 - \mathcal{R})\boldsymbol{\lambda}. \quad (\text{S232})$$

The translation-inequivalent centres are therefore classified by

$$Q_{\mathcal{R}} \equiv \Lambda / (1 - \mathcal{R})\Lambda. \quad (\text{S233})$$

For a two-dimensional rotation,

$$|Q_{\mathcal{R}}| = |\det(1 - \mathcal{R})| = 2 - 2 \cos\left(\frac{2\pi}{n}\right). \quad (\text{S234})$$

For the crystallographic orders,

$$n = 2, 3, 4, 6 \quad \implies \quad |Q_{\mathcal{R}}| = 4, 3, 2, 1. \quad (\text{S235})$$

These are the four twofold, three threefold, two fourfold, and one sixfold centre classes.

At a momentum satisfying

$$\mathcal{R}\mathbf{k}_* = \mathbf{k}_* + \mathbf{G}, \quad (\text{S236})$$

the local phase associated with the centre labelled by $\mathbf{t}$ is

$$\vartheta_{\mathbf{t}}(\mathcal{R}) = e^{-i\mathbf{k}_* \cdot \mathbf{t}}. \quad (\text{S237})$$

This phase is well defined on $Q_{\mathcal{R}}$, since

$$e^{-i\mathbf{k}_* \cdot (1 - \mathcal{R})\boldsymbol{\lambda}} = e^{-i(\mathbf{k}_* - \mathcal{R}^{-1}\mathbf{k}_*) \cdot \boldsymbol{\lambda}} = 1. \quad (\text{S238})$$

Thus the quotient determines both the available rotation centres and the local characters realised by them.

H. Physical realisation of the separating probes

a. Lemma. For every symmorphic wallpaper little co-group, the cyclic subgroups, local phases, and reflection classes used in the reconstruction below are realised by physical probe positions.

b. Proof. First consider a point group with maximal rotation order n . Applying the preceding quotient count to the powers of the maximal rotation, and removing centres already fixed by a higher-order rotation, gives

n	Rotational stabilisers	
2	$4 C_2$	
3	$3 C_3$	
4	$2 C_4$ and $2 C_2$	
6	$1 C_6$, $2 C_3$, and $3 C_2$.	(S239)

For $n = 4$, the two C_4 centres are among the four centres of the order-two power, leaving two exact C_2 centres. For $n = 6$, the unique C_6 centre is among both the three C_3 centres and the four C_2 centres. A point fixed by both a threefold and a twofold generator is fixed by the C_6 group they generate, so there is no further overlap. Hence every divisor subgroup required below is represented by an actual rotation centre. In a mirror-containing group, its full stabiliser may be D_d rather than C_d ; this case is treated explicitly below.

The pairing

$$([\mathbf{k}], [\mathbf{t}]) \mapsto e^{-i\mathbf{k} \cdot \mathbf{t}} \quad (\text{S240})$$

between $\mathcal{R}$ -invariant momentum classes and $Q_{\mathcal{R}}$ is perfect, meaning that it identifies the group of $\mathcal{R}$ -invariant momentum classes with the character group $\widehat{Q_{\mathcal{R}}}$. Triviality on every $[\mathbf{t}]$ forces $\mathbf{k}$ to be reciprocal-lattice equivalent to zero, and the two finite groups have the same order $|\det(1 - \mathcal{R})|$. Therefore the nonzero invariant momentum classes realise the nontrivial characters of $Q_{\mathcal{R}}$. In the crystallographic cases this gives

Case	Phases realised by the centre classes	
Nonzero C_2 -invariant momentum	$+1, -1$	
C_4 -invariant M	$+1, -1$	
C_3 -invariant corner	$1, \omega, \omega^2$.	(S241)

Finally, choose the symmorphic origin to be fixed by the point group. Every point-group reflection σ then has a representative $\{\sigma|0\}$ with a fixed mirror line. A generic point on that line, away from its intersections with other symmetry loci, has stabiliser C_s . For even n , representatives of the two reflection conjugacy classes give the two required mirror families. The origin itself has the full D_n stabiliser. This proves the claim. $\square$

I. Cyclic little co-groups at Γ

Let

$$G = C_n = \langle c \rangle, \quad n \in \{1, 2, 3, 4, 6\}. \quad (\text{S242})$$

The ordinary complex irreps are

$$\rho_j(c) = e^{2\pi i j/n}, \quad j \in \mathbb{Z}_n. \quad (\text{S243})$$

At a time-reversal invariant momentum, j and $-j$ belong to the same physical conjugation class. Define

$$e(j) = \text{ord} \left(e^{2\pi i j/n} \right) = \frac{n}{\gcd(j, n)}. \quad (\text{S244})$$

For $n = 1, 2, 3, 4, 6$, the order $e(j)$ uniquely determines the physical conjugation class.

For every divisor d of n , let

$$C_d = \langle c^{n/d} \rangle. \quad (\text{S245})$$

At Γ , the local phase is trivial. Let ρ_e denote the physical irrep whose rotation eigenvalue has order e , and let d_e be its real dimension. The C_d projector gives

$$m_d(\rho_e) = d_e \mathbf{1}_{e|n/d}. \quad (\text{S246})$$

Writing

$$q = \frac{n}{d}, \quad (\text{S247})$$

the normalised probe matrix is

$$Z_{eq} = \mathbf{1}_{e|q}, \quad e, q \mid n. \quad (\text{S248})$$

This is the incidence matrix of the divisor lattice. Its inverse is given by number-theoretic Möbius inversion. If

$$F(q) = \sum_{e|q} a(e), \quad (\text{S249})$$

then

$$a(e) = \sum_{q|e} \mu(e/q) F(q), \quad (\text{S250})$$

where μ is the Möbius function. Hence the divisor probes reconstruct every coefficient in $\text{Class}_{\text{phys}}(C_n)$.

The divisor set includes $d = 1$. The corresponding generic probe gives the dimension d_e . For example, at Γ in C_6 , the probes with stabilisers C_1, C_2, C_3, C_6 give

	C_1	C_2	C_3	C_6
A	1	1	1	1
B	1	0	1	0
E_1	2	0	0	0
E_2	2	2	0	0

. (S251)

This matrix has full rank. Omitting the C_1 column removes the dimension functional but does not create a collision between the four zero patterns.

J. Cyclic little co-groups at nonzero momentum

Let a probe have stabiliser C_d and local character

$$\vartheta(c^{n/d}) = e^{-2\pi i q/d}. \quad (\text{S252})$$

For the complex irrep ρ_j ,

$$m_{d,q}(j) = \frac{1}{d} \sum_{\ell=0}^{d-1} e^{-2\pi i q \ell/d} e^{2\pi i j \ell/d} \quad (\text{S253})$$

$$= \begin{cases} 1, & j = q \pmod{d}, \\ 0, & j \neq q \pmod{d}. \end{cases} \quad (\text{S254})$$

Thus a shifted rotation centre is a finite Fourier projector for the angular-momentum label modulo d .

The physical-realisation lemma exhausts the crystallographic possibilities. A nonzero C_2 -invariant momentum has centre phases ± 1 , which separate the two C_2 irreps. At the square-lattice M point, the two C_4 centres carry phases $+1$ and -1 , whilst the twofold centres supply the remaining divisor test. At a hexagonal corner, the three C_3 centres carry the phases $1, \omega, \omega^2$, and hence

$$m_s(\rho_j) = \frac{1}{3} \sum_{\ell=0}^2 \omega^{(s+j)\ell} = \delta_{s+j, 0 \pmod{3}}. \quad (\text{S255})$$

Every C_3 irrep is therefore allowed at exactly one member-resolved centre. A sixfold little co-group occurs only at Γ , which was covered by the divisor argument.

It follows that all cyclic symmorphic wallpaper little co-groups are separated, with only the unavoidable conjugation pairing at a time-reversal invariant momentum.

K. Mirror-containing little co-groups

Let

$$G = C_{nv} \simeq D_n. \quad (\text{S256})$$

A character of D_n is determined by its restriction to the rotation subgroup C_n and by its values on the reflection classes. There is one reflection class for odd n and two reflection classes for even n .

A generic point on a mirror line has stabiliser

$$C_s = \{E, \sigma\}. \quad (\text{S257})$$

Allowing for the known local sign $\epsilon_\sigma = \vartheta(\sigma) = \pm 1$, its projector rank is

$$m_{\sigma, \epsilon_\sigma}(\rho) = \frac{1}{2} [d_\rho + \epsilon_\sigma \chi_\rho(\sigma)]. \quad (\text{S258})$$

This determines the reflection character:

$$\chi_\rho(\sigma) = \epsilon_\sigma [2m_{\sigma, \epsilon_\sigma}(\rho) - d_\rho]. \quad (\text{S259})$$

One mirror family therefore determines the reflection class for odd n , whilst two inequivalent mirror families determine the two reflection classes for even n .

A rotation centre in a mirror group may have stabiliser D_d rather than C_d . Splitting the projector into rotation and reflection parts gives

$$m_{D_d, \vartheta}(\rho) = \frac{1}{2} m_{C_d, \vartheta|_{C_d}}(\rho) + \frac{1}{2d} \sum_{\tau \in D_d \setminus C_d} \vartheta(\tau) \chi_\rho(\tau). \quad (\text{S260})$$

The reflection characters in the second term have already been determined by the mirror-line probes. Therefore

$$m_{C_d, \vartheta|_{C_d}}(\rho) = 2m_{D_d, \vartheta}(\rho) - \frac{1}{d} \sum_{\tau \in D_d \setminus C_d} \vartheta(\tau) \chi_\rho(\tau). \quad (\text{S261})$$

The cyclic divisor and Fourier arguments then determine the rotational part of the character. Hence rotation-centre and mirror-line probes together span $\text{Class}_{\text{phys}}(D_n)$.

L. Uniqueness of the dark set

The preceding subsections prove that the complete index vector determines the physical character. We now show that the labelled zero pattern is itself sufficient for the symmorphic wallpaper little groups.

For a cyclic group at Γ , the nonzero divisor probes are exactly those satisfying $e \mid \frac{n}{d}$. This set determines the order e of the rotation eigenvalue. At a shifted centre, the Fourier projector determines the angular-momentum label directly.

For a one-dimensional irrep λ of D_n , a pure mirror probe has

$$m_\sigma(\lambda) = \frac{1}{2} [1 + \lambda(\sigma)]. \quad (\text{S262})$$

For odd n , the parity on the single reflection class determines λ . For even n , choose representatives s and cs of the two reflection classes. Their parities also determine the rotational sign, since

$$\lambda(c) = \lambda(cs)\lambda(s). \quad (\text{S263})$$

Thus the mirror zero pattern determines every one-dimensional irrep.

For a two-dimensional irrep E_j , every reflection character vanishes, so

$$m_\sigma(E_j) = 1 \quad (\text{S264})$$

for every mirror line. Any one-dimensional irrep with a dark mirror is therefore separated immediately from every E_j . The only one-dimensional irrep bright on all the pure mirror families is the trivial irrep. At the origin-centred probe with full stabiliser D_n ,

$$m_{D_n}(\mathbf{1}) = 1, \quad m_{D_n}(E_j) = 0, \quad (\text{S265})$$

because an irreducible two-dimensional representation contains no trivial D_n subrepresentation. This separates the remaining one-dimensional case from the two-dimensional irreps.

It remains to distinguish the different E_j . At a centre with stabiliser D_d , the reflection characters of E_j vanish, so the preceding decomposition reduces to

$$m_{D_d, \vartheta}(E_j) = \frac{1}{2} m_{C_d, \vartheta|_{C_d}}(E_j). \quad (\text{S266})$$

Consequently,

$$m_{D_d, \vartheta}(E_j) = 0 \iff m_{C_d, \vartheta|_{C_d}}(E_j) = 0. \quad (\text{S267})$$

The physically realised D_d centre therefore carries exactly the same zero-pattern information as the corresponding cyclic test on E_j . The cyclic argument distinguishes the different E_j .

Combining the cyclic and dihedral cases, we have proved the following:

Theorem. Let G be the little co-group of a symmorphic wallpaper group, and let ρ be a single isolated irrep. Probing all member-resolved rotation centres and mirror-line families determines ρ exactly at a non-TRIM and determines the pair $\{\rho, \bar{\rho}\}$ at a TRIM.

If time-reversal symmetry is present, a distinct pair $\rho, \bar{\rho}$ forms one irreducible corepresentation of the magnetic little group. In that formulation, the physical corepresentation is determined exactly.

M. Nonsymmorphic groups

A fixed-point-free glide cannot belong to a one-point real-space stabiliser and therefore never appears in any local projector sum. One-point probes can consequently resolve only character data carried by symmetries with fixed points. The symmorphic construction above succeeds because the required character space is spanned by probes associated with physical rotation centres and mirror lines. No analogous complete one-point basis can recover character directions carried only by fixed-point-free nonsymmorphic operations — for every nonsymmorphic symmetry, one fewer independent class function is available.

The preceding argument therefore gives a complete uniform proof for symmorphic wallpaper groups and identifies the structural obstruction in the nonsymmorphic case. The collisions between nonsymmorphic irreps are explicitly observed in Sec. S1.

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