From Local Spin Nematicity to Altermagnets: Footprints of Band Topology

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Altermagnets are crystallographic rotational symmetry breaking spin-ordered states, possessing a net zero magnetization despite manifesting Kramers non-degenerate bands. Here, we show that momentum-independent local spin nematic orders in monolayer, Bernal bilayer and rhombohedral trilayer graphene give rise to p-wave, d-wave and f-wave altermagnets, respectively, thereby inheriting topology of linear, quadratic and cubic free fermion band dispersions that are also described in terms of angular momentum $\ell = 1,\ 2$ and 3 harmonics in the reciprocal space. The same conclusions also hold inside a spin-triplet nematic superconductor, featuring Majorana altermagnets. Altogether, these findings highlight the importance of electronic band structure in identifying such exotic magnetic orders in quantum materials. We depict the effects of in-plane magnetic fields on altermagnets, and propose novel spin-disordered alter-valleymagnets in these systems.

Introduction. Magnetic materials commonly appear inside modern-day electronic devices. When doped, often they also source unconventional and high-temperature superconductors. Therefore, identifying new magnetic phases and materials are of both fundamental and technological importance, possibly paving a path toward the long sought room temperature superconductors.

Typically, magnetic materials are grouped into two families, ferromagnet and anti-ferromagnet. The former breaks only the time-reversal symmetry, thereby lifting the Kramers degeneracy of electronic bands. It possesses a finite magnetic moment, resulting from a population imbalance between electrons with opposite spins. By contrast, the Kramers degeneracy of electronic states is protected in an anti-ferromagnet, stemming from the simultaneous lifting of the time-reversal and inversion symmetries, yielding a net zero magnetization.

Recently, a new type of magnetic order has been proposed theoretically [1–20], and unearthed in quantum materials [21–32]: Altermagnet. Despite lifting the Kramers degeneracy, they manifest no net magnetization, a peculiarity accomplished at the cost of discrete crystallographic rotational symmetry with opposite signs for complementary spin projections. They are represented in terms of spherical harmonics (Y_ℓ^m), taking a generic form $\boldsymbol{\sigma} Y_\ell^m(\theta,\phi)|\boldsymbol{k}|^\ell$. Vector Pauli matrix $\boldsymbol{\sigma}$ operates on the spin space, $m = -\ell, \cdots, \ell$, θ (ϕ) is the polar (azimuthal) angle in the reciprocal space, and $\boldsymbol{k}$ is the momentum. This classification allows p-wave ($\ell = 1$), d-wave ($\ell = 2$), and f-wave ($\ell = 3$) altermagnets, to name a few.

Although strongly correlated materials can in principle harbor such exotic magnetic orders, their non-locality or momentum-dependence can be energetically expensive, forcing us to the raise the following question. *Can altermagnets emerge from momentum-independent local magnetic orders?* We show that its affirmative answer establishes a topology-based guiding principle to identify quantum materials, capable of fostering altermagnets.

This question arises from a seemingly unrelated topic, topological superconductors (TSCs), worth mentioning despite a short detour. Consider their prime member, the B-phase of ^{3}He, a fully gapped p-wave paired state [33]. It can emerge from *local* or *on-site* odd-parity Cooper pairing in 3D Dirac materials [34, 35], also modeled in terms of odd-parity p-wave harmonics. Therefore, neutral Bogoliubov de Gennes (BdG) quasiparticles inherit topology from normal state charged Dirac quasiparticles. Moreover, when such a local odd-parity pairing is projected on the Fermi surface, realized by intercalating or doping topological insulators, it takes the form of the B-phase of ^{3}He [36, 37]. This one-to-one correspondence between the normal state band topology and paired state emergent topology guides us to identify candidate materials, fostering charged TSCs, with $Cu_xBi_2Se_3$ and $In_xSn_{1-x}Te$ standing as promising candidates [38–40]. A similar avenue has also been built to identify candidate materials for higher-order TSCs [41–43]. In light of these observations, the question from the last paragraph can be rephrased in the following way. *How does electronic band topology get imprinted on altermagnets?*

Such broadly defined questions can be efficiently answered by considering minimal model Hamiltonian for crystalline graphene heterostructures. Here, we focus on monolayer graphene (MLG), Bernal bilayer graphene (BBLG) and rhombohedral trilayer graphene (RTLG) displaying linear, bi-quadratic and bi-cubic touching of valence and conduction bands at two inequivalent corners of the hexagonal Brillouin zone, described by p-wave, d-wave and f-wave harmonics in the momentum space, respectively [44]. In such systems, we show that local spin nematic orders, transforming under the irreducible E_g or E_u representation of the D_{3d} group, give birth to emergent p-wave, d-wave and f-wave altermagnets, respectively, inheriting topology from the normal state band dispersion. See Fig. 1. By the same token, a spin-triplet nematic superconductor, belonging to the E_u representation, fosters altermagnet for neutral Majorana fermions, hereafter coined Majorana altermagnet. We recognize that the valley or pseudo-spin degree of freedom permits a spin-disordered charge nematic order, leading to (unnested) displaced or distorted Fermi surfaces near two valleys, a phase hereafter named alter-valleymagnet.

Free fermions. The continuum models, resulting from a minimal tight-binding Hamiltonian involving nearest-neighbor intra-layer (t) and inter-layer dimer ($t_\perp$) hopping [44], in MLG, BBLG and RTLG graphene in a sixteen component Nambu-doubled spinor basis read as

$$\hat{h}_\ell(\boldsymbol{k}) = \alpha_\ell |\boldsymbol{k}|^\ell \left[\Gamma^1_\ell \cos(\ell\phi) - \Gamma^2_\ell \sin(\ell\phi)\right] - \Delta_{\rm Z}\Gamma_{0100}, \quad (1)$$

with $\ell = 1, 2$ and 3, respectively. Here, $\alpha_\ell = (ta)^\ell / t_\perp^{\ell-1}$, bearing the dimension of Fermi velocity (inverse mass) for $\ell = 1(2)$, for example, a is the lattice spacing, $\Gamma^1_{1/3} = \Gamma_{3031}$, $\Gamma^2_{1/3} = \Gamma_{3002}$, $\Gamma^1_2 = \Gamma_{3001}$ and $\Gamma^2_2 = \Gamma_{3032}$. Hermitian matrices are $\Gamma_{\kappa\nu\rho\lambda} = \eta_\kappa \sigma_\nu \tau_\rho \beta_\lambda$, where $\{\eta_\kappa\}$, $\{\sigma_\kappa\}$, $\{\tau_\kappa\}$, $\{\beta_\kappa\}$ are Pauli matrices for $\kappa = 0, \cdots, 3$, operating on the particle-hole, spin, valley and sublattice or layer indices, respectively. The Nambu spinor is $\Psi^\top_{\rm Nam}(\boldsymbol{k}) = [\Psi(\boldsymbol{k}), \sigma_2\tau_1\beta_0\Psi^\star(-\boldsymbol{k})]$, where the eight-component spinor $\Psi^\top(\boldsymbol{k}) = [\Psi_\uparrow(\boldsymbol{k}), \Psi_\downarrow(\boldsymbol{k})]$ with $\sigma = \uparrow, \downarrow$ as two projections of electrons spin in the z direction and $\Psi^\top_\sigma(\boldsymbol{k}) = [\Psi_{\sigma,+}(\boldsymbol{k}), \Psi_{\sigma,-}(\boldsymbol{k})]$. Here $\top$ denotes transposition. For each spin projection, the two-component spinor near two opposite valleys at $\tau\mathbf{K}$ is defined as $\Psi_{\sigma,\tau}(\boldsymbol{k}) = [A_\sigma(\tau\mathbf{K} + \boldsymbol{k}), B_\sigma(\tau\mathbf{K} + \boldsymbol{k})]$, where $\tau = \pm$. A and B are fermionic annihilation operator on the sites of two triangular sublattices of the honeycomb lattice. They, however, live on the top and bottom layers of BBLG and RTLG. Therefore, the sublattice and layer degrees of freedom are synonymous. Momentum $|\boldsymbol{k}|(\ll |\mathbf{K}|)$ is measured from the respective valley. We introduced the Nambu doubling to facilitate a forthcoming discussion on Majorana altermagnet. Until then, it is redundant. The Zeeman term ($\Delta_{\rm Z}$) is due to in-plane magnetic fields. In its absence, spherically symmetric energy spectra of $\hat{h}_\ell(\boldsymbol{k})$ are $\pm E_\ell(\boldsymbol{k})$, where $+$ ($-$) corresponds to the conduction (valence) band, and $E_\ell(\boldsymbol{k}) = \alpha_\ell |\boldsymbol{k}|^\ell$ [45–50].

The effective Hamiltonian preserves the sublattice or layer (S) and valley (T) reflection symmetries, generated by Γ_{0001} and Γ_{0010}, respectively, and accompanied by momentum reflections $\boldsymbol{k} \to (k_x, -k_y)$ and $\boldsymbol{k} \to (-k_x, k_y)$. Its time reversal symmetry is generated by $\mathcal{T} = \Gamma_{0210}\mathcal{K}$, where $\mathcal{K}$ is the complex conjugation and $\mathcal{T}^2 = -1$. Thus electronic bands near two valleys are Kramers (spin) degenerate. In the hole part of $\Psi_{\rm Nam}$, we absorb the unitary part of the time-reversal operator. The generator of spatial rotation is Γ_{0033}, and the low-energy Hamiltonian possesses a rotational symmetry, generated by $R_{\pi/2} = \exp[i\pi\Gamma_{0033}/4]$, when the momentum axes are rotated by an angle $\pi/(2\ell)$. The U(1) translational symmetry is generated by Γ_{0030}. Light mass of carbon atoms allows us to neglect any spin-orbit coupling, and all the Hamiltonian are invariant under SU(2) spin rotation, generated by Γ_{0s00} with $s = 1, 2, 3$ [45, 49, 50].

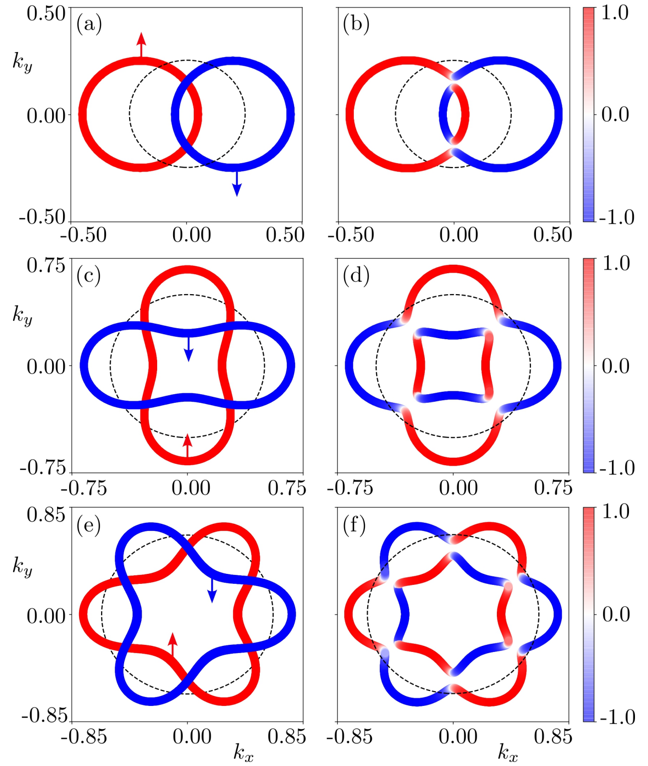

FIG. 1. Constant energy ($E = 0.25$) contours, yielding Fermi surfaces at chemical doping $\mu = E = 0.25$, near the $+\mathbf{K}$ valley for spin up ($\uparrow$) and spin down ($\downarrow$) electrons in the presence of local spin nematic orders (belonging to the E_g or E_u representation) without the Zeeman coupling in (a) MLG, (c) BBLG and (e) RTLG, displaying p-wave, d-wave and f-wave altermagnets, respectively. Here, we set $\Delta_j = 0.2$ and $\theta_j = 0$, where $j = E_g$ and E_u [Eq. (2)]. The numbers in the color bar represent the spin projection in the z-direction (in units of $\hbar/2$). It is zero where the contours for opposite spin projections cross. They get split by a Zeeman coupling (Δ_Z) of an in-plane magnetic field, as shown for (b) MLG ($\Delta_Z = 0.025$), (d) BBLG ($\Delta_Z = 0.05$) and (f) RTLG ($\Delta_Z = 0.05$). Near the $-\mathbf{K}$ valley, the spin projection on each contour gets reversed (stays the same) in MLG and RTLG (BBLG) for the E_g altermagnet. For the E_u altermagnet, this correspondence is exactly the opposite. Momentum $\boldsymbol{k}$ is measured about the valley momentum $\mathbf{K}$. We set $\alpha_\ell = 1$ [Eq. (1)]. Black dashed lines represent spin degenerate Fermi surface of free fermions.

Spin nematicity. The underlying D_{3d} group allows two spin nematic orders transforming under the irreducible E_g and E_u representations. With respective amplitudes Δ_{E_g} and Δ_{E_u}, effective single-particle Hamiltonian are

$$\hat{h}^{\rm spin}_{E_g}(\Delta_{E_g}, \theta_{E_g}) = \Delta_{E_g}\left[\Gamma_{0301}\cos\theta_{E_g} - \Gamma_{0332}\sin\theta_{E_g}\right],$$
$$\hat{h}^{\rm spin}_{E_u}(\Delta_{E_u}, \theta_{E_u}) = \Delta_{E_u}\left[\Gamma_{3331}\cos\theta_{E_u} - \Gamma_{3302}\sin\theta_{E_u}\right]. \quad (2)$$

The internal angles θ_{E_g} and θ_{E_u} are chosen spontaneously in the ordered states [51], in which without any loss of generality, the spin projection is picked in the z direction. Two matrices of $\hat{h}^{\rm spin}_{E_g/E_u}$ constitute a vector under spatial rotation, generated by Γ_{0033}. So, the ordered state (with a fixed θ_{E_g} or θ_{E_u}) breaks the spatial rotational symmetry, yielding nematicity. The E_g (E_u) spin nematicity breaks (preserved) the $\mathcal{T}$ symmetry. Nucleation of either order lifts the Kramers (spin) degeneracy of the bands near each valley, which we discuss next.

The reconstructed band structure with the onset of the spin nematic orders can be computed by diagonalizing

$$\hat{h}^{\rm alt}_j(\Delta_j, \theta_j) = \hat{h}_\ell(\boldsymbol{k}) + \hat{h}^{\rm spin}_j(\Delta_j, \theta_j), \tag{3}$$

with $j = E_g$ and E_u. Near the $+\mathbf{K}$ valley, Kramers non-degenerate bands touch each other at Weyl points, located at $|\boldsymbol{k}| = \left([\Delta_j^2 + \Delta_Z^2]^{1/2}/\alpha_\ell\right)^{1/\ell}$ and $\phi = (\theta_j + m\pi)/\ell$. For spin-up ($\uparrow$) fermions, odd integer $m = 1, \cdots, 2\ell - 1$, while for spin-down ($\downarrow$) fermions even integer $m = 0, \cdots, 2\ell - 2$. Therefore, for each spin projection, the linear band touching point of MLG shifts to a new position in the reciprocal space, whereas the bi-quadratic (bi-cubic) band touching point of BBLG (RTLG) splits into two (three) Weyl points around which the energy-momentum dispersion is linear. In the E_g spin nematic phase, such a shift/splitting of the band touching points for spin-up (spin-down) fermions near $-\mathbf{K}$ valley is same as that of the spin-down (spin-up) fermions near $+\mathbf{K}$ valley in MLG and RTLG, but is identical for each spin projection near opposite valleys in BBLG. In the E_u spin nematic state, this shift/splitting near the opposite valleys is identical in MLG and RTLG for each spin projection, whereas in BBLG such a shift/splitting near $-\mathbf{K}$ valley for spin-down (spin-up) fermions is same as that of the spin-up (spin-down) fermions near $+\mathbf{K}$ valley. The resulting reconstruction of electronic bands and its Kramers degeneracy lifting lead to altermagnetism in these spin nematic states, which we promote now.

Altermagnets. Emergent altermagnetism in the spin nematic phases can be recognized from the constant energy contours for opposite spin projections either in the valence or conduction band of the corresponding effective single-particle Hamiltonian [Eq. (2)]. The results are shown in Fig. 1 (left column). Such contours for spin up and spin down electrons do not overlap, but always enclose equal area in the reciprocal space (Fermi area). Thus these phases do not possess any net magnetic moment, despite lifting the Kramers degeneracy from electronic bands. Hence, they represent altermagnets. Spin polarized constant energy contours cross each other at two, four and six points in MLG, BBLG and RTLG, respectively. From the topology of such contours, it is evident that the same spin nematic order gives birth to p-wave, d-wave and f-wave altermagnets in MLG, BBLG and RTLG, respectively. Shortly, we will justify this claim quantitatively and attribute this emergent phenomena to the normal state band topology.

Application of a weak external in-plane magnetic field (no Landau quantization) splits the crossing points between contours belonging to opposite spin projections, where the z-component of electronic spin is zero, as seen in Fig. 1 (right column). The Zeeman coupling then takes place between the magnetic field and in-plane components (such as x) of electronic spin. The orbital effect of sufficiently weak in-plane magnetic fields is negligible in BBLG and RTLG in comparison to its Zeeman cousin, and is thus omitted here [52]. In-plane magnetic fields project the spin of altermagnets in the orthogonal easy-plane, and gap out the contour crossing points.

Classification of altermagnets, resulting from local spin nematic orders, in terms of the spherical harmonics is accomplished by casting their effective single-particle Hamiltonian [Eq. (2)] in the band electron basis. Then the kinetic energy term $\hat{h}^{\rm band}_\ell(\boldsymbol{k}) = \alpha_\ell |\boldsymbol{k}|^\ell \bar{\Gamma}_{3003} - \Delta_{\rm Z} \bar{\Gamma}_{0100}$ becomes diagonal, achieved after a unitary rotation by U, constructed by columnwise arranging the eigenvectors of $\hat{h}_\ell(\boldsymbol{k})$ with $\Delta_{\rm Z} = 0$. Here, $\bar{\Gamma}_{\kappa\nu\rho\lambda} = \eta_\kappa \sigma_\nu \tau_\rho \zeta_\lambda$ and the newly introduced Pauli matrices $\{\zeta_\kappa\}$ operate on the band index (conduction and valence). In this basis, the local spin nematic orders from Eq. (2) take the form

$$\begin{aligned}\hat{h}^{\rm alt}_{j,{\rm band}} \;=\; \Delta_j \Big\{ & [\cos\theta_j \cos(\ell\phi) + \sin\theta_j \sin(\ell\phi)]\, \bar{\Gamma}^{j,\ell}_{\rm intra} \\ & + \; [\cos\theta_j \sin(\ell\phi) - \sin\theta_j \cos(\ell\phi)]\, \bar{\Gamma}^{j,\ell}_{\rm inter} \Big\}. \end{aligned} \tag{4}$$

The first (second) term captures the intraband (interband) component of the $j = E_g$ and E_u nematic orders, ensured by the accompanying matrices taking the following form with $\kappa = 3$ (0) for $j = E_g$ (E_u)

$$\begin{aligned}&\bar{\Gamma}^{E_g,1/3}_{\rm intra} = \bar{\Gamma}^{E_u,2}_{\rm intra} = \bar{\Gamma}_{\kappa 333}, \quad \bar{\Gamma}^{E_g,2}_{\rm intra} = \bar{\Gamma}^{E_u,1/3}_{\rm intra} = \bar{\Gamma}_{\kappa 303} \\ &\bar{\Gamma}^{E_g,1/3}_{\rm inter} = \bar{\Gamma}^{E_u,2}_{\rm inter} = \bar{\Gamma}_{\kappa 302}, \text{ and } \bar{\Gamma}^{E_g,2}_{\rm inter} = \bar{\Gamma}^{E_u,1/3}_{\rm inter} = \bar{\Gamma}_{\kappa 332}.\end{aligned}$$

The intraband component is responsible for the topology of the constant energy contours (Fermi surface). From the definitions of cubic harmonics in two dimensions

$$\left\{ \begin{array}{c} \cos(\ell\phi) \\ \sin(\ell\phi) \end{array} \right\} \propto Y^{-\ell}_\ell \left(\frac{\pi}{2}, \phi\right) \left\{ \begin{array}{c} + \\ - \end{array} \right\} (-1)^\ell Y^\ell_\ell \left(\frac{\pi}{2}, \phi\right), \tag{5}$$

we identify that the altermagnets are p-wave, d-wave and f-wave in nature in MLG ($\ell = 1$), BBLG ($\ell = 2$) and RTLG ($\ell = 3$), respectively, resulting from their normal state band topology, described by the same harmonics.

Majorana altermagnet. As a penultimate topic, we showcase the possibility of realizing altermagnets of neutral Majorana fermions in local spin-triplet nematic superconductors. The D_{3d} group allows only one such paired state, following the E_u representation [48, 49], with the effective single-particle BdG Hamiltonian

$$\hat{h}^{\rm pair}_{E_u}\left(\Delta^p_{E_u}, \theta^p_{E_u}\right) = \Delta^p_{E_u} \left[\Gamma_{\alpha j 31} \cos\theta^p_{E_u} - \Gamma_{\alpha j 02} \sin\theta^p_{E_u}\right]. \tag{6}$$

Here $\Delta^p_{E_u}$ is the pairing amplitude, $\theta^p_{E_u}$ determines the spatial orientation of Cooper pairs, and $\alpha = 1, 2$ reflects the U(1) gauge redundancy in defining the superconducting phase. For simplicity, we choose $\alpha = 1$ and the Cooper pair spin in the z-direction ($j = 3$). All the discussions for the E_u spin nematic order directly apply here with the caveat that the Weyl nodes feature gapless Majorana excitations. We now enjoy the liberty to completely neglect the inter-band component of the pairing Hamiltonian (Eq. (4) with $3 \to 1$ in the Nambu sector), as the effective attractive interaction exists only around the Fermi surface, realized within the valence or conduction band upon doping these systems. Thus, the paired state also hosts altermagnets, but for neutral Majorana fermions [Fig. 1]. We name them Majorana altermagnets. By the same analogy they are p-wave, d-wave and f-wave in nature in MLG, BBLG and RTLG, respectively.

Alter-valleymagnet. Symmetry protected valley degree of freedom in graphene heterostructures enters their low-energy models as spin degrees of freedom [Eq. (1)], thus named pseudo-spin. We envision to construct altermagnetic states in terms of valley or pseudo-spin. Spin up and down components in this case translate into two valleys at $\pm\mathbf{K}$, and exchange of spin projections $\uparrow\leftrightarrow\downarrow$, leading to a change in spin angular momentum $S_z = \pm 2$ (in units of $\hbar/2$), maps onto $\mathbf{K} \leftrightarrow -\mathbf{K}$, causing a $2\mathbf{K}$ momentum transfer. The proposed alter-valleymagnet is spin-disordered, and stems from the charge nematic orders, for which the effective single-particle Hamiltonian takes the form shown in Eq. (2), with $3 \leftrightarrow 0$ in the Nambu sector and $3 \to 0$ in the spin sector of the corresponding Γ matrices [49]. A charge nematic phase then represents an alter-valleymagnet if the displaced (in MLG) or distorted (in BBLG and RTLG) spin-degenerate Fermi surfaces near two inequivalent valleys do not map onto each other under a $2\mathbf{K}$ translation (pseudo-spin flip). With this definition in hand, we recognize E_g (in MLG and RTLG) and E_u (in BBLG) charge nematic orders as alter-valleymagnet, with the corresponding spin degenerate Fermi surfaces from the opposite valleys shown in a single frame in Fig. 1 (left column), where $\uparrow / \downarrow \equiv +/-\mathbf{K}$.

Summary & discussions. We show that the band topology of non-interacting electrons plays a decisive role in determining the geometry of emergent altermagnets from the local spin nematic orders. As examples, we consider graphene-based crystalline heterostructures, namely MLG, BBLG and RTLG, displaying linear, quadratic and cubic band dispersion, captured by $\ell = 1, 2$ and 3 harmonics, respectively. As a result, the local spin nematic orders foster p-wave, d-wave and f-wave altermagnets, respectively, inheriting their geometry from the free fermion band topology. The same conclusions hold in a spin-triplet nematic local superconductor, harboring Majorana altermagnets. In addition, the valley or pseudo-spin degree of freedom allows us to unfold the possibility of spin-disordered alter-valleymagnetic phases. Present discussion opens up various fascinating future directions, among which generalizing these concepts to strong spin-orbit coupled and three-dimensional materials, emergent superconductors in doped altermagnets [53–58] are the prominent ones.

Topological quantum chemistry nowadays is routinely employed to mine quantum materials with unusual electronic band dispersion [59–64]. Our proposed symmetry-based sufficiently general one-to-one correspondence between band topology and altermagnet geometry should therefore open an unexplored and fascinating avenue to harness these exotic quantum magnets in a predictive way. Within the landscape of graphene heterostructures recent experiments have unveiled several ordered phases (including superconductors) in doped BBLG and RTLG, when the layer-inversion symmetry is broken by an external displacement electric field [65–69]. New phases in their global phase diagram are still being discovered. They constitute a promising material platform, where our predicted altermagnets, including their Majorana and valley cousins, can in principle be observed, where the trigonal warping does not affect our predictions [51].

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