

Designing topological high-order Van Hove singularities: Twisted bilayer kagome

David T. S. Perkins , Anirudh Chandrasekaran , and Joseph J. Betouras 

Department of Physics, Loughborough University, Loughborough LE11 3TU, United Kingdom



(Received 22 April 2025; revised 6 August 2025; accepted 5 November 2025; published 10 December 2025)

The interplay of high-order Van Hove singularities and topology plays a central role in determining the nature of the electronic correlations governing the phase of a system with unique signatures characterizing their presence. Layered van der Waals heterostructures are ideal systems for band engineering through the use of twisting and proximity effects. Here, we use symmetry to demonstrate how twisted kagome bilayers can host topological high-order Van Hove singularities. We study a commensurate system with a large twist angle and demonstrate how the initial choice of high-symmetry stacking order can greatly influence the electronic structure and topology of the system. Furthermore, we study the possibility of sublattice interference in the system. Our results illustrate the rich energy landscape of twisted kagome bilayers and unveil large Chern numbers (of order 10), establishing twisted bilayer kagome as a natural playground for probing the mixing of strong correlations and topology.

DOI: [10.1103/8y2v-kx2w](https://doi.org/10.1103/8y2v-kx2w)

I. INTRODUCTION

Electronic instabilities are facilitated when the kinetic energy of electrons is dominated by the characteristic energy scale of their interactions, resulting in the emergence of different phases. Naturally, the study of vanishing Fermi velocities, the occurrence of flat bands, and their associated divergences in the density of states (DOS) play a central role in determining the electronic phases, transport, and thermodynamic properties of materials [1]. The simplest example of this is the Van Hove singularity (VHS), a saddle point within the band structure that yields a logarithmic divergence in the DOS [2]. More recently, higher-order VHSs (HOVHSs) and flat bands have attracted much attention due to their appearance in several systems exhibiting exotic phenomena: unusual thermodynamics, strange metallicity, and non-Fermi-liquid behavior have been observed in $\text{Sr}_3\text{Ru}_2\text{O}_7$ [3–6] and twisted WSe_2 bilayers [7], while unconventional superconductivity manifests in multilayer graphene both with and without twisting [8–12]. By tuning a system to a HOVHS, a system's phase diagram can be altered drastically, as has been shown for bernal bilayer graphene where the presence of a HOVHS enabled ferromagnetism, spin-singlet superconductivity, and charge, spin, and pair density waves [13,14]. Every perturbation is relevant because the Fermi velocity tends to zero. HOVHSs are central in the realization of a supermetal phase [15]. The telltale sign of a HOVHS is a more severe divergence of the DOS, scaling according to a power-law, $g(\varepsilon) \sim \varepsilon^{-\alpha}$ ($\alpha > 0$), rather than a logarithm [5,16], where ε is the distance in energy space from the singularity. A detailed classification scheme has recently been developed for the various types of HOVHS [16,17] in conjunction with methods to

engineer and analyze their nature [18,19] as well as a study of their resilience to disorder [20]. As a result, the exact connection between HOVHSs and the observed phenomena, as well as methods to engineer quantum materials with desired properties as a consequence of HOVHSs and flat bands, are areas of intense research and discussion.

An exemplary system for probing the physics of strong correlations is the kagome lattice, which possesses a perfectly flat band across the entire Brillouin zone (BZ), while hosting Dirac electrons around the BZ corners and VHSs at the BZ edge. The kagome lattice with nearest-neighbor hopping is the line graph of a honeycomb lattice. Graph theory guarantees that such lattices possess at least one flat band [21–23]. At the same time, the kagome lattice appears in both its monolayer and bilayer forms in several materials, including the vanadium-based antimonides (AV_3Sb_5 ; $A = \text{K, Rb, Cs}$) [24–27], CsTi_3Bi_5 [28,29], and kagome magnets [30–32]. In these cases, the collection of atoms forming the kagome lattice are embedded in a network of atoms that do not form part of the kagome lattice. These atomic cages prevent band engineering through methods that have proven extremely powerful in the field of van der Waals (vdW) heterostructures, where various two-dimensional (2D) materials may be stacked and offset by a relative twist angle to manifest HOVHSs and flat bands, enable strong correlations, induce topological phases, and tune proximity-induced couplings [8,10,33–41]. There is a recent comprehensive study that predicts many more stoichiometric materials with kagome lattice structures [42]. An alternative family of 2D materials exhibiting signatures of kagome physics are metalorganic frameworks (MOFs), which may be constructed to host a kagome pattern without an atomic cage [43–48].

It is therefore natural to consider kagome-based vdW heterostructures when designing bespoke band structures hosting HOVHSs and near-flat bands which may be further tuned through straining [49] and twisting [50]. Moreover, topological kagome effects will become more accessible through the plethora of potential 2D partner materials and the tunability

granted by twisting, allowing for the realization of topological HOVHSs (i.e., HOVHSs situated in bands with nonzero Chern numbers); these are expected to play a key role in the formation of phases when incorporating interactions. For example, the superconducting phase and charge ordering in AV_3Sb_5 are understood to stem from the topological nature of the band structure [51], suggesting that twisting may enrich the phase space of kagome materials. Topological VHSs have been studied in a 3D context via Weyl metals [52], while topological HOVHSs have only very recently been considered in a kagome monolayer [53].

In this work, we demonstrate how topological HOVHSs with two- (C_{2z}), three- (C_{3z}), and sixfold (C_{6z}) rotational symmetry can be engineered in twisted kagome bilayers for all possible high-symmetry stackings of the kagome bilayer [54], and how the choice of stacking can greatly influence the nature and number of HOVHSs present in the band structure. We introduce the three high-symmetry stacking configurations and illustrate how the electronic structure is affected by tunneling asymmetry (dimerization) and complex next-nearest-neighbor (NNN) hopping. We then show how the structural symmetry of twisted bilayer kagome (TBK) is reduced upon twisting to a commensurate angle. Next, we model TBK using a tight-binding Hamiltonian that generalizes the Hamiltonian of Ref. [50] by including dimerization, complex NNN tunneling, and an interlayer potential (i.e., out-of-plane electric field) to enable band engineering for creating topological HOVHSs. To establish HOVHSs and illustrate the importance of stacking order, we focus on TBK with a 38.2° twist corresponding to the minimum moiré unit cell achievable.

We find that monkey saddles (third-order VHSs) appear around the moiré BZ (MBZ) corners for a large range of parameter values in several bands, while cuspid singularities (elongated VHSs) appear around the MBZ edges without any need for tuning, and we identify two classes of singularities that arise for both. Moreover, the stacking configurations with an effective C_{6z} symmetry in momentum space also host very sensitive sixth-order HOVHSs at the center of the MBZ. We use symmetry arguments to establish the exact number of singularities that may occur simultaneously within each band. Finally, when a HOVHS is created through the use of complex NNN tunneling, the breaking of time-reversal symmetry lifts the degeneracy between bands and allows us to calculate the Chern index for each one. We unveil bands with a Chern number of order 10 while simultaneously hosting a HOVHS, establishing a zoo of topological HOVHSs in TBK. The results we present here outline the electronic and topological signatures of twisted kagome systems and, given the growing family of kagome materials and the bespoke nature of vdW heterostructures, will help the design and investigation of topological kagome HOVHSs and nearly flat bands with exciting properties.

II. HIGH-SYMMETRY STACKING AND COMMENSURATE TWISTING

A. Stacking configurations

An untwisted bilayer formed out of two identical kagome lattices has three high-symmetry stacking orders [Fig. 1(a)]:

AA, in which the sublattices of both layers are perfectly aligned and retain the D_{6h} symmetry of the monolayer; *AB*, where one layer is shifted by a bond length relative to the other, resulting in only two directly overlapping sublattices and reducing the point group symmetry to D_2 ; and *interlocked*, reminiscent of Bernal stacked graphene, wherein the up triangles of one layer are aligned with the down triangles of the other layer to reduce the bilayer's symmetry to D_{3d} . The band crossing at the K point of the Brillouin zone is protected by inversion symmetry, C_i , and time-reversal symmetry, $\mathcal{T}$, meaning that only the *AB* bilayer will naturally have a gapped structure around the Dirac point of the original monolayer [Fig. 1(b)]. We note that the band structure around the K point for the *AA* and interlocked systems strongly resembles those of *AA* and Bernal stacked graphene, respectively. We interpret this as a triangle exchange symmetry, like that of the sublattice exchange symmetry in graphene [55], that can be either even (*AA*) or odd (interlocked). Details of each bilayer's Hamiltonian are provided in Ref. [56].

To achieve monkey saddle HOVHSs around the MBZ corners, it is necessary to eliminate the linear band crossings at the Dirac points in the twisted bilayer and gain control over the emergent gaps by breaking either C_i or $\mathcal{T}$; whether or not a Dirac cone can be flattened is ultimately determined by the symmetries of the system [57]. Inversion symmetry is broken in breathing kagome lattices whose up and down triangles are of different sizes, leading to an enhanced tunneling via up triangles and a reduced tunneling via down triangles [Fig. 1(c)] [58,59]. Niobium halides [60], their chalcogen substituted counterparts [61], and Fe_3Sn_2 [30] are all examples of systems possessing such a lattice. To break $\mathcal{T}$, we may either apply a magnetic field or introduce a complex Haldane-type NNN tunneling [53,62], whereby hopping anticlockwise (clockwise) carries a phase factor of $e^{i\phi}$ ($e^{-i\phi}$) [Fig. 1(d)]. While both approaches will gap the Dirac cone, they ultimately yield different symmetries for the system. Dimerization is a geometric effect and will reduce the point-group symmetry of the bilayer: $D_{6h} \rightarrow D_{3h}$, $D_{3d} \rightarrow C_{3v}$, and $D_2 \rightarrow D_1$. In contrast, Haldane-type hopping possesses a C_{6z} symmetry, thus not affecting the principal rotational symmetry. However, applying the in-plane dihedral rotation associated with the lattice will reverse the direction of the Haldane-type hopping ($e^{i\phi} \leftrightarrow e^{-i\phi}$). Therefore, the point-group symmetry will be reduced from $D_{6h} \rightarrow C_{6h}$, $D_{3d} \rightarrow C_{3v}$, and $D_2 \rightarrow C_2$.

B. Commensurate twist angles

When introducing a twist into kagome bilayers, only certain angles will produce commensurate structures with a finite moiré unit cell (MUC), with smaller twists possessing larger MUCs and many thousands of lattice sites. Whether the bilayer is commensurate or not is determined by its underlying triangular lattice. We can label each twist angle yielding a commensurate bilayer, $\theta_c \in [0, 60^\circ)$, by a unique pair of coprime integers, (m, n) , such that [63–65]

$$\cos \theta_c = \frac{3m^2 - n^2}{3m^2 + n^2}, \quad \sin \theta_c = \frac{2\sqrt{3}mn}{3m^2 + n^2}. \quad (1)$$

We apply the twist to the kagome bilayer by rotating one layer about a C_{6z} hexagon center to maintain 60° twist periodicity,

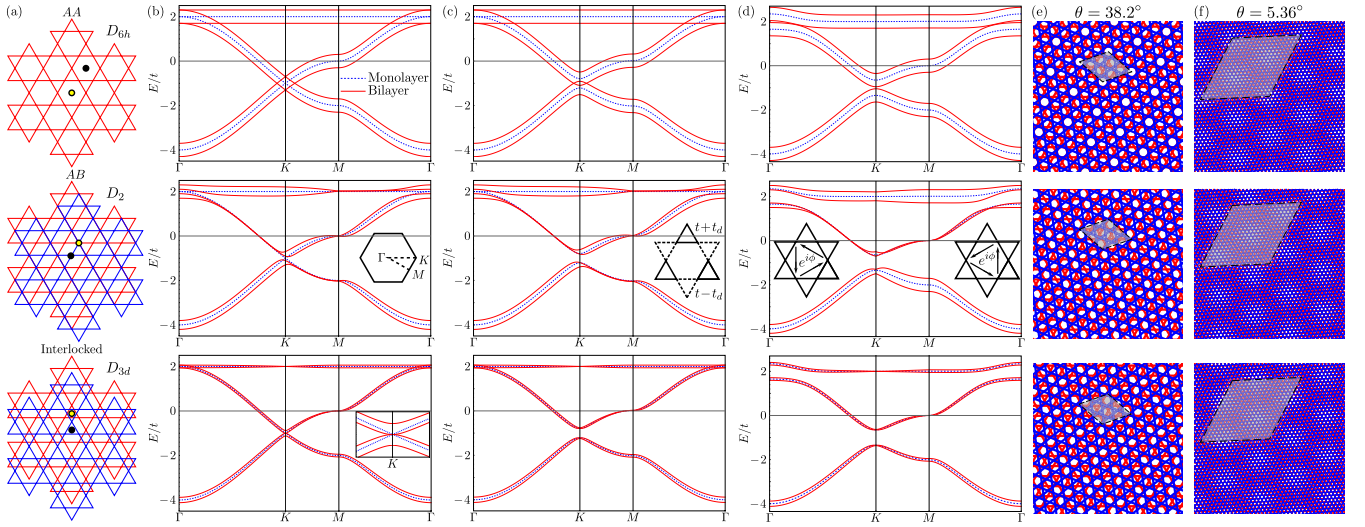


FIG. 1. Unique high-symmetry stacking orders of a kagome bilayer and their effect upon the band structure and moiré pattern. (a) High-symmetry stacking orders with their real-space high-symmetry point (i.e., that which exhibits the full point group symmetry) highlighted by the yellow dot and twist centers used to create twisted bilayers denoted by the black dots. (b) Band structures associated with each stacking choice compared against the monolayer kagome bands in units of the intralayer tunneling amplitude, t . We use $t_{\perp} = 0.3t$ for the interlayer tunneling energy in the AA and AB stackings, while taking $\tilde{t}_{\perp} = 0.2t_{\perp}$ for the reduced interlayer hopping in the interlocked scenario due to no sites overlapping directly. The inset for the interlocked case shows how the Dirac cone is flattened. (c) Band structure under dimerization ($t_d = 0.07t$) for the three stackings compared to the dimerized monolayer, with the bands being gapped out around the original MDP due to breaking of inversion symmetry. The schematic in the AB plot illustrates the enhancement/reduction (solid/dashed triangles) of tunneling energy due to dimerization. (d) Band structure due to complex NNN tunneling with $t_H = 0.1t$ and $\phi = \pi/2$ for the Haldane hopping strength and phase, respectively, where degeneracies are lifted by the breaking of $\mathcal{T}$. The schematics in the AB panel shows the hopping processes yielding phase factors of $e^{i\phi}$. Reversal of hopping direction instead yields $e^{-i\phi}$. (e), (f) Moiré patterns for TBK with $(m, n) = (5, 3)$ (e) and $(m, n) = (37, 3)$ (f).

see Fig. 1(a), and we note that this labeling of commensurate angles yields two families [54,65]: (i) where n is divisible by 3, and (ii) where n is not divisible by 3. These two sets can be simply related via $\theta'_c = \pi/3 - \theta_c$ such that if θ_c is defined by a choice of n that is divisible by 3, then θ'_c will be associated with a value of n that is not divisible by 3 [65]. For example, $(m, n) = (5, 3)$ yields $\theta_c = 38.2^\circ$, which in turn has the partner angle $\theta'_c = 21.8^\circ$, which can be obtained with $(m, n) = (3, 1)$. It was shown in Ref. [54] that the point group symmetries for both families of commensurate angles were identical when the twist is applied about a hexagon center. However, differences between the two can be seen both at the superlattice level and in the Hamiltonian.

Working in the twist-symmetric frame (i.e., layer 1 is rotated by $-\theta_c/2$ and layer 2 is rotated by $\theta_c/2$), the cases where n is divisible by 3 will always possess a moiré lattice vector parallel to the x -axis, while those with n not divisible by 3 will always possess a moiré lattice vector parallel to the y -axis. Using graphene nomenclature, we refer to these orientations of the unit cell as zigzag and armchair, respectively, based upon the Wigner-Seitz cell constructed with the twist origin at its center. To see this, let us denote the lattice sites of a triangular lattice by $\mathbf{r}_i(k, l) = k\mathbf{a}_1 + l\mathbf{a}_2$, where i is the layer index and $k, l \in \mathbb{Z}$, and their rotated forms by $\mathbf{r}_i^\theta = R_\theta \mathbf{r}_i$. In the twist-symmetric frame, the triangular lattice is guaranteed to have dihedral symmetry along the x -axis, which manifests as a $y \rightarrow -y$ reflection symmetry between the layers. Consequently, a moiré lattice vector must lie parallel to either the x -axis or the y -axis.

Without loss of generality [54], we assume that n is divisible by 3 such that $n = 3\nu$ with $\nu \in \mathbb{Z}$, and we require the y -components of $\mathbf{r}_1^{\frac{\theta_c}{2}}(k, l)$ and $\mathbf{r}_2^{\frac{\theta_c}{2}}(p, q)$ to vanish ($\bar{\theta}_c = -\theta_c$). We find that $\mathbf{r}_1^{\frac{\theta_c}{2}}(k, l) = \mathbf{r}_2^{\frac{\theta_c}{2}}(p, q)$ is then satisfied by

$$\begin{aligned} k &= \alpha_{mv}(m - \nu), & l &= 2\alpha_{mv}\nu, \\ p &= \alpha_{mv}(m + \nu), & q &= -2\alpha_{mv}\nu, \end{aligned} \quad (2)$$

where

$$\alpha_{mv} = \begin{cases} 1, & m + \nu \text{ is odd,} \\ \frac{1}{2}, & m + \nu \text{ is even.} \end{cases} \quad (3)$$

The resulting moiré lattice constant is then $a_M = \alpha_{mv}\sqrt{m^2 + 3\nu^2}a$, where a is the monolayer lattice constant. If we instead demand that the x -component vanishes, we find a larger magnitude for the moiré lattice constant, $\tilde{a}_M = \alpha_{mv}\sqrt{3}\sqrt{m^2 + 3\nu^2}a$, clearly indicating that the commensurate superlattices defined by an n divisible by 3 will always be of zigzag orientation. Alternatively, we may assume that $n = 3\nu \pm 1$ and demand that the x -components of $\mathbf{r}_1^{\frac{\theta_c}{2}}(k, l)$ and $\mathbf{r}_2^{\frac{\theta_c}{2}}(p, q)$ vanish, where we find that $\mathbf{r}_1^{\frac{\theta_c}{2}}(k, l) = \mathbf{r}_2^{\frac{\theta_c}{2}}(p, q)$ is satisfied when

$$\begin{aligned} k &= \alpha_{mn}(m + n), & l &= -2\alpha_{mn}m, \\ p &= \alpha_{mn}(m - n), & q &= -2\alpha_{mn}m, \end{aligned} \quad (4)$$

yielding a moiré lattice constant of $a_M = \alpha_{mn}\sqrt{3m^2 + n^2}a$. Similar to the $n = 3\nu$ case, we find a larger moiré lattice

constant, $\tilde{a}_M = \alpha_{mn} \sqrt{3} \sqrt{3m^2 + n^2} a$, by seeking a moiré lattice vector parallel to the x -axis when n is not divisible by 3. Therefore, the orientation of the superlattice unit cell when n is not divisible by 3 will always be armchair. Lastly, we note that these two classes of superlattices are related by reflection in the $y = x$ line; see Appendix A for details.

Moving onto the Hamiltonians of these systems, in the absence of complex NNN hopping and dimerization, we see that the Hamiltonian with θ_c , $\mathcal{H}$, is related to the Hamiltonian with θ'_c by $\mathcal{H}(k_x, k_y) = \mathcal{H}'(k_y, k_x)$ when constructed in the twist-symmetric frame. Application of an out-of-plane electric field, which induces an interlayer potential, does not affect this observation. Including Haldane-type hopping, we must also flip the sign of the phase to obtain one Hamiltonian from the other, $\mathcal{H}(k_x, k_y, \phi) = \mathcal{H}'(k_y, k_x, -\phi)$. Finally, dimerization results in the largest difference between the two systems, with the asymmetric tunneling along up and down triangles appearing reversed in one layer and unchanged in the other after reflection in $y = x$. Specifically, the layer rotated anticlockwise by $\theta_c/2$ will appear to have its dimerization unchanged, while the layer rotated clockwise by $\theta_c/2$ will have its dimerization reversed; details are discussed in Appendix A. Therefore, the two families of twist angles may provide significant differences when dimerization is present.

Finally, while the choice of stacking order might initially seem irrelevant for small twist angles, it becomes apparent at large twist angles that the superlattice structure is completely dependent on the stacking order [Figs. 1(e) and 1(f)]. The point group symmetry of the resulting superlattice will always be dihedral and retain the rotational symmetry of the original untwisted kagome bilayer: D_6 for AA, D_3 for interlocked, and D_2 for AB [54]. This is further reflected in the electronic structure, where parabolic band touching at the K point is seen for interlocked TBK while a double well with a linear crossing is seen for AA TBK.

III. MODEL

A. Tight-binding Hamiltonian

We model the TBK system using a tight-binding model with one atomic orbital per lattice site, assuming an exponential decay of the tunneling energy with separation distance, r , of the form $f(r) = \exp[-\gamma(r - r_i)/r_i]$, where r_i is the NN separation ($\bar{a} = a/2$) for intralayer tunneling and the interlayer separation ($d_\perp$) for interlayer tunneling, while γ characterizes the hopping range [50]. By retaining tunneling between all lattice sites up to NNN MUCs, the resulting momentum space Hamiltonian becomes

$$H = - \sum_{\mathbf{k}} \sum_l \sum_{\alpha, \beta} \left[t^{\alpha\beta} \Gamma_l^{\alpha\beta}(\mathbf{k}) - s_l \frac{\Delta}{2} \delta_{\alpha\beta} \right] c_{\mathbf{k}l\alpha}^\dagger c_{\mathbf{k}l\beta} - \sum_{\mathbf{k}} \sum_{\alpha, \beta} t_\perp^{\alpha\beta} [\Gamma_\perp^{\alpha\beta}(\mathbf{k}) c_{\mathbf{k}1\alpha}^\dagger c_{\mathbf{k}2\beta} + \text{H.c.}], \quad (5)$$

where $c_{\mathbf{k}l\alpha}^\dagger$ ($c_{\mathbf{k}l\alpha}$) is the creation (annihilation) operator for an electron with momentum $\mathbf{k}$ in layer l for moiré sublattice site α , $t^{\alpha\beta} = t$ is the intralayer tunneling amplitude between sites α and β , $t_\perp^{\alpha\beta} = t_\perp$ is the interlayer tunneling amplitude between sites α and β of different layers, Δ is an interlayer

potential, $s_l = \pm 1$ for layer $l/2$, $\delta_{\alpha\beta}$ is the Kronecker delta, and $\Gamma_{l(\perp)}^{\alpha\beta}(\mathbf{k})$ are the structure factors containing the information about the decay of tunneling energy with distance (their explicit form is given in Appendix B). To include dimerization, we restrict intralayer hopping to only NN and let $t^{\alpha\beta} = t \pm t_d$ with the sign determined by whether the tunneling is via an up or down triangle. For the models we consider here with $\gamma = 20$, NN intralayer tunneling is sufficient to accurately model the system, since NNN intralayer hopping introduces negligible corrections $\sim 10^{-7}t$. Additionally, we may introduce an intralayer Haldane-type hopping via

$$H_H = -t_H \sum_{\mathbf{k}} \sum_l \sum_{\alpha, \beta} \Gamma_H^{\alpha\beta}(\mathbf{k}) e^{iS_{\alpha\beta}\phi} c_{\mathbf{k}l\alpha}^\dagger c_{\mathbf{k}l\beta}, \quad (6)$$

where $S_{\alpha\beta} = \pm 1$ and the details of the Haldane structure factor, $\Gamma_H^{\alpha\beta}(\mathbf{k})$, are given in Appendix B. Finally, we note that the Haldane hopping will not be subject to dimerization due to being a NNN tunneling process. The total Hamiltonian is thus given by $\mathcal{H}(t_d, t_H, \phi, \Delta; \theta) = H + H_H$. A detailed derivation of the total Hamiltonian is given in Appendix B.

B. Electronic structure and stacking

We illustrate the effects of stacking order, dimerization, and Haldane-type hopping in Fig. 2 for a TBK system based on Fe_3Sn_2 [30,50]. For a physical interpretation of dimerization in TBK systems, we note that dimerizations as large as $t_d \sim 0.5t$ are achievable with small changes to the interatomic distances on the order of 2–3 % [Fig. 2(a)]. Therefore, the dimerization term approximates well a TBK system comprised of breathing kagome lattices at large twist angles. The effective separation error compared to the modeled interlayer tunneling decay is presented in Fig. 2(b). Small changes to the tunneling energies will only renormalize the values of the parameters needed to tune a HOVHS.

Starting from $t_d = t_H = 0$, we see that the stacking order is particularly relevant around the M_M point with clear differences in both energy and structure [Fig. 2(c)]. We further observe the appearance of a characteristic densely packed near-flat-band region about the original monolayer flat band energy with a resolution of $\sim 0.3t$, where the stacking order greatly influences the fine details of each band, although no choice of stacking order prevents the loss of an exact flat band [Fig. 2(d)]. The nature of the electronic structure of the aligned bilayer at the K_M point is also preserved upon twisting to a commensurate angle [Fig. 2(e)]. Specifically, the gap and linear band crossing of the AA system persists while the interlocked stacking retains its parabolic band touching at the K_M point, with both sets of features occurring close to the original monolayer Dirac point (MDP) energy. These features prevent us from observing critical points that also possess a vanishing curvature in the absence of dimerization or Haldane-type hopping.

C. Emergent symmetries that enable HOVHSs

Through dimerization and Haldane-type hopping, we can tune the gaps between previously degenerate bands at the K_M point to engineer a monkey saddle singularity for both the AA and interlocked TBK systems [Figs. 2(f) and 2(g)]. This type

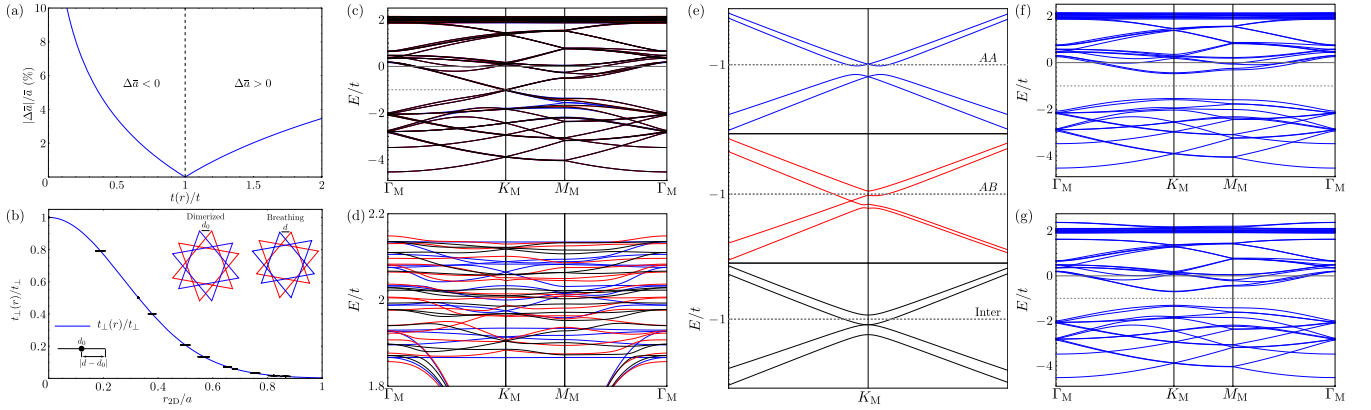


FIG. 2. Variation of the TBK band structure due to stacking, dimerization, and Haldane-type hopping. Here we consider a TBK system with $\theta_c = 38.2^\circ$, $a = 0.5338$ nm, $d_\perp = 0.6596$ nm, $t_\perp = 0.3t$, and $\gamma = 20$ [30,50]. (a) Change in NN separation distance required to achieve a given decay factor for intralayer tunneling. (b) Plot of the interlayer tunneling decay as a function of the in-plane separation of atoms, r_{2D} . The black dots correspond to the separations present within a twisted dimerized kagome bilayer with $\theta_c \simeq 38.2^\circ$, and the error bars indicate the magnitude of difference in 2D interlayer separations between the dimerized and breathing kagome bilayers such that they both yield a difference in tunneling along up and down triangles of $t_d = 0.5t$. (c)–(e) Band structure in the absence of dimerization and Haldane hopping for all high-symmetry stackings (blue: AA, red: AB, black: interlocked), with a focus on the near-flat band region (d) and on the MDP energy (e) marked by the gray dashed line. (f) The effect of dimerization on AA TBK with $t_d = 0.2t$, opening a gap between bands 14 and 15. Similar band structures for AB and interlocked TBK are obtained, with differences in stacking order becoming more apparent over a wider range of the high-symmetry path; see Ref. [56]. (g) AA TBK with $t_H = 0.1t$, which opens two gaps: one between bands 14 and 15, and a second between bands 28 and 29.

of HOVHS requires C_{3z} symmetry and therefore cannot be hosted by the AB configuration, and hence we shall only focus on the AA and interlocked systems from hereon. Moreover, we can explore the possibility of engineering a HOVHS with sixfold rotational symmetry at Γ_M in both the AA and interlocked TBK systems. Naturally, this will be achieved most easily using an AA stacking due to its inherent C_{6z} symmetry. When $t_d \neq 0$ and $t_H = 0$, the system possesses an effective C_{6z} symmetry in momentum space due to the system possessing C_{3z} and $\mathcal{T}$ (the same is true for interlocked TBK). For the opposite case with $t_d = 0$ and $t_H \neq 0$, the Haldane hopping leaves the structural C_{6z} symmetry intact. If both $t_d, t_H \neq 0$, then an effective C_{6z} symmetry cannot emerge in either AA or interlocked TBK through the combination of C_{3z} and $\mathcal{T}$. Nonetheless, due to deeper underlying symmetries present in the system, this does not prevent us from creating a sixfold singularity.

Both AA and interlocked TBK possess a C_3 point group symmetry when dimerization and complex NNN tunneling are included. By working in the twist-symmetric frame, the underlying moiré superlattice (i.e., neglecting dimerization and Haldane-type hopping) will always exhibit a dihedral symmetry along the x -axis, y -axis, or sometimes both. For AA TBK the underlying superlattice possesses dihedral symmetry along both axes for all commensurate twist angles: C_{2x} along the x -axis and C_{2y} along the y -axis. In contrast, the underlying superlattice of interlocked TBK will possess only C_{2x} (C_{2y}) for a zigzag (armchair) orientation. These symmetries produce the following mappings: $C_{2x} : (y, z; \phi) \rightarrow (-y, -z; -\phi)$ and $C_{2y} : (x, z; -\phi) \rightarrow (-x, -z; -\phi)$, which may be interpreted as $(k_y, \phi) \rightarrow (-k_y, -\phi)$ and $(k_x, \phi) \rightarrow (-k_x, -\phi)$, respectively, and an exchange of layers. Dimerization acts as a C_{2x} breaking mechanism, due to mapping of up triangles to down triangles upon a layer exchange. The topologically trivial part

of the Hamiltonian with $\Delta = 0$, H_0 , is therefore symmetric under time-reversal in all cases and C_{2y} for AA and armchair interlocked TBK when dimerization is present,

$$H_0 = \mathcal{T}H_0\mathcal{T}^{-1}, \quad H_0^{\text{AA}} = C_{2y}H_0^{\text{AA}}C_{2y}^{-1}, \\ H_0^{\text{Int}, \diamond} = C_{2y}H_0^{\text{Int}, \diamond}C_{2y}^{-1}, \quad (7)$$

where the superscript denotes the stacking configuration and MUC orientation ($\diamond$: armchair, $\circ$: zigzag). If dimerization is absent, $H_0 \rightarrow \bar{H}_0$, then up and down triangles are equivalent, and hence the topologically trivial piece of the Hamiltonian for zigzag interlocked TBK retains its dihedral symmetry:

$$\bar{H}_0^{\text{AA}} = C_{2x}\bar{H}_0^{\text{AA}}C_{2x}^{-1}, \quad \bar{H}_0^{\text{Int}, \diamond} = C_{2x}\bar{H}_0^{\text{Int}, \diamond}C_{2x}^{-1}. \quad (8)$$

The topological contribution to the Hamiltonian is not symmetric under any dihedral rotation or time-reversal ($C'_2 \in \{C_{2x}, C_{2y}\}$),

$$\mathcal{T}H_H\mathcal{T}^{-1} = H_H|_{\phi \rightarrow -\phi}, \quad C'_2H_HC'^{-1}_2 = H_H|_{\phi \rightarrow -\phi}, \quad (9)$$

but it is symmetric under their combined transformation,

$$H_H = \mathcal{T}C'_2H_H(\mathcal{T}C'_2)^{-1}. \quad (10)$$

This results in the total Hamiltonian exhibiting emergent dihedral time-reversal symmetries for AA TBK and interlocked TBK [Eqs. (7), (8), and (10)], $\mathcal{H}_0 = \mathcal{T}C'_2\mathcal{H}_0(\mathcal{T}C'_2)^{-1}$.

The combinations of $\mathcal{T}C_{2x}$ and $\mathcal{T}C_{2y}$ manifest as $k_x \rightarrow -k_x$ and $k_y \rightarrow -k_y$ symmetries, respectively, in the 2D MBZ. By expanding the energy of a given band about the origin, the $\mathcal{T}C'_2$ and C_{3z} symmetries of the Hamiltonian restrict the

TABLE I. A summary of the maximum number of simultaneous HOVHSs allowed around the high-symmetry points of the MBZ for AA and interlocked TBK. The entries in the left section of the table indicate which tuning parameters are present, while the middle section presents the magnetic point group for each case using international (left) and Schönflies (right) notation. We indicate the axes of dihedral symmetry explicitly in the superscripts of the crystallographic dihedral point groups when working in the twist-symmetric frame. The right section of the table lists the number of two- (second-order and fourth-order), three- (monkey saddle), and sixfold (sixth-order) singularities permitted to occur simultaneously at the MBZ high-symmetry points for that combination of parameters for the two stacking orders. The subscripts denote the MUC orientation ($\circ$: armchair, $\odot$: zigzag) and stacking order where their number of singularities differs.

t_d	t_H	Δ	Zigzag/Armchair AA		Zigzag interlocked		Armchair interlocked		HOVHSs (C_{2z} , C_{3z} , C_{6z})
$\times$	$\times$	$\times$	6 2 2	$D_6^{(x,y)} \cup \mathcal{T}$	3 2 1	$D_3^{(x)} \cup \mathcal{T}$	3 1 2	$D_3^{(y)} \cup \mathcal{T}$	(3,2,1)
$\checkmark$	$\times$	$\times$	3 1 2	$D_3^{(y)} \cup \mathcal{T}$	3	$C_3 \cup \mathcal{T}$	3 1 2	$D_3^{(y)} \cup \mathcal{T}$	(3,2,1)
$\times$	$\checkmark$	$\times$	6 2' 2'	$(1 + \mathcal{TC}_{2x})C_6$	3 2' 1	$(1 + \mathcal{TC}_{2x})C_3$	3 1 2'	$(1 + \mathcal{TC}_{2y})C_3$	(3,2,1)
$\checkmark$	$\checkmark$	$\times$	3 1 2'	$(1 + \mathcal{TC}_{2y})C_3$	3	C_3	3 1 2'	$(1 + \mathcal{TC}_{2y})C_3$	(3, 2, 1) $\odot$, (3, 1, 0) $\odot$
$\times$	$\times$	$\checkmark$	6	$C_6 \cup \mathcal{T}$	3	$C_3 \cup \mathcal{T}$	3	$C_3 \cup \mathcal{T}$	(3,2,1)
$\checkmark$	$\times$	$\checkmark$	3	$C_3 \cup \mathcal{T}$	3	$C_3 \cup \mathcal{T}$	3	$C_3 \cup \mathcal{T}$	(3,2,1)
$\times$	$\checkmark$	$\checkmark$	6	C_6	3	C_3	3	C_3	(3, 2, 1) $_{AA}$, (3, 1, 0) $_{Int}$
$\checkmark$	$\checkmark$	$\checkmark$	3	C_3	3	C_3	3	C_3	(3,1,0)

expansion to

$$E \simeq \tilde{a}_2 k^2 + \tilde{a}_4 k^4 + \tilde{a}_6 k^6 + a_3 k^3 \cos(3\varphi) + b_3 k^3 \sin(3\varphi) + a_6 k^6 \cos(6\varphi) + O(k^8), \quad (11)$$

where φ is the azimuthal angle, and $\tilde{a}_n$, a_n , and b_n are coefficients that are functions of the tuning parameters. Therefore, symmetry allows for the emergence of a sixfold HOVHS provided that $\mathcal{TC}'_2$ (an effective reflection symmetry in either the x - or y -axis) and C_{3z} symmetry is preserved.

Taking this symmetry analysis one step further, we determine how many singularities exist at the same energy. In the twist-symmetric frame, we note that the zigzag and armchair orientations of the MUC may yield different numbers of HOVHSs possessing the same energy due to the difference in their dihedral symmetries. Let us start by assuming that a monkey saddle exists at the K_M point of the MBZ. If $\mathcal{T}$ is preserved, K_M trivially maps onto K'_M , thereby yielding two simultaneous singularities. Introducing Haldane-type hopping breaks $\mathcal{T}$ and C'_2 symmetries, but it leaves the $\mathcal{TC}'_2$ symmetries in tact, allowing us to again connect the differing MBZ corners for zigzag (armchair) AA and interlocked TBK using $\mathcal{TC}_{2x}$ ($\mathcal{TC}_{2y}$). Only with both Haldane-type hopping and dimerization do the two orientations differ for both stacking orders, wherein $\mathcal{TC}_{2x}$ is broken in zigzag structures and $\mathcal{TC}_{2y}$ is preserved in armchair structures. Hence with both dimerization and complex NNN hopping, zigzag TBK will possess only a single HOVHS at a given MBZ corner energy, while armchair TBK will still exhibit two simultaneous singularities. Moving on to the case of twofold VHSs at the MBZ edges, the number of simultaneous singularities will always be three in AA and interlocked TBK due to possessing a C_{3z} symmetry. Only in AB TBK will the number of simultaneous singularities differ to become two instead of three due to its lack of C_{3z} symmetry. When dimerization is introduced, AB TBK will always exhibit a dihedral symmetry along one of three lines: the y -axis (i.e., the 90° line) or the $\pm 30^\circ$ lines. These will always act to map two differing MBZ edges onto one another while leaving one to map onto itself. We summarize the maximum number of singularities

occurring simultaneously for each possible combination of tuning parameters in Table I for AA and interlocked TBK.

IV. CREATING HIGHER-ORDER VAN HOVE SINGULARITIES

A. Monkey saddle singularities

Using a wide range of dimerizations, $0.05 \lesssim t_d/t \lesssim 0.7$, the linear band crossings at the MBZ corners are gapped out to create monkey saddles. This results in two types of singularities. Band 26 of dimerized AA TBK in Fig. 3(a) illustrates a *delocalized* monkey saddle characterized by energy contours connecting the singularities at K_M and K'_M . In contrast, band 18 [Fig. 3(b)] hosts *localized* HOVHS at the MBZ corners that are disconnected from each other. Both cases yield a divergence in the DOS that is well described by a $g(\varepsilon) \sim \varepsilon^{-1/3}$ power-law at leading order [bottom panels of Figs. 3(a) and 3(b)], where ε is the energy measured from the singularity. The fits shown here account for subleading-order corrections due to the HOVHS existing within a more complex energy landscape. The forms of these subleading corrections are discussed in Appendix C. Further examples of monkey saddles in other bands for AA and interlocked TBK can be found in Ref. [56].

Both types of singularities are of particular relevance to metals exhibiting non-Fermi-liquid behavior in their transport coefficients and thermodynamic properties. The presence of remote regions where the Fermi velocity vanishes (i.e., localized singularities) has been shown to alter the electrical resistivity of materials by acting as reservoirs for current-carrying electrons to scatter to and from [6] and heat capacity [5]. Similarly, the appearance of singularities on a single Fermi surface that has both dispersive and flat regions (i.e., delocalized singularities) has been shown to dominate the interaction-induced electron self-energy, thus governing the electronic contribution to thermal transport [66].

B. Sixfold singularities

Due to its high-order nature, a sixfold singularity is very sensitive to the tuning parameters and may require several

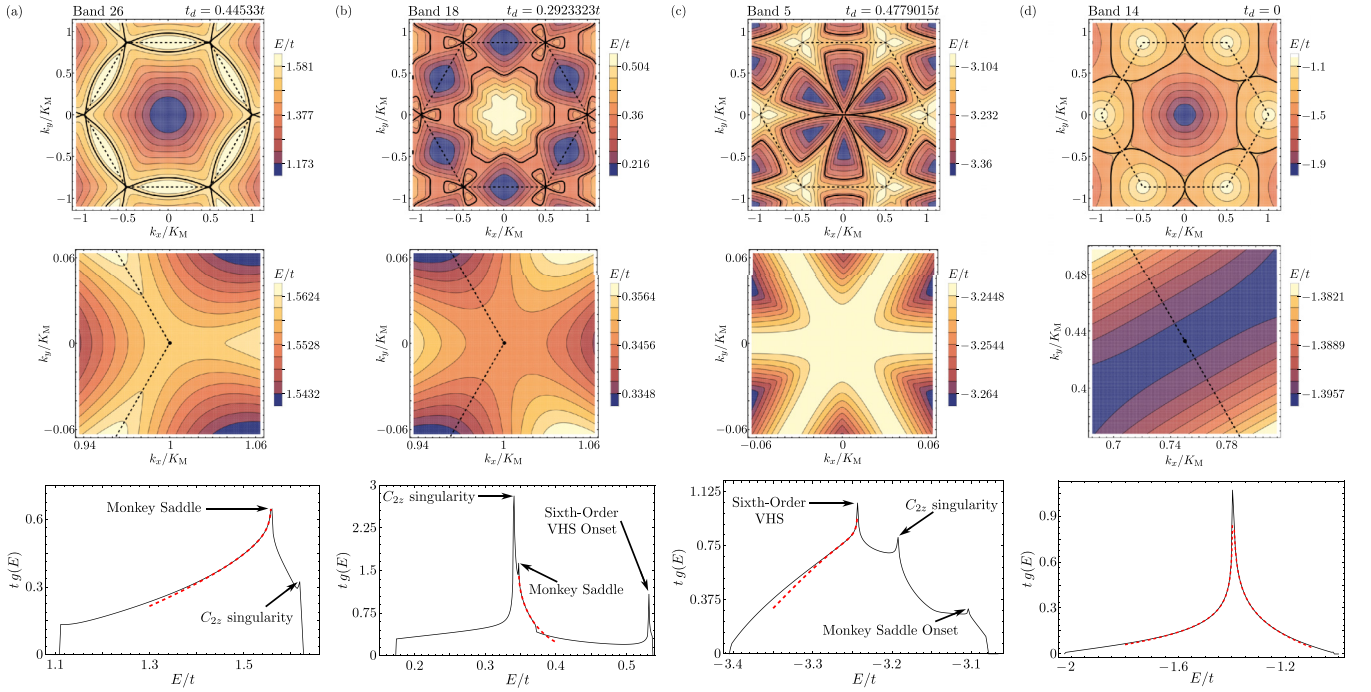


FIG. 3. Energy contours of bands tuned to host HOVHSs around the MBZ high-symmetry points and their corresponding DOS. Here we present the contours of bands hosting HOVHSs at K_M in (a) and (b), Γ_M in (c), and M_M in (d) due to dimerization, with the thick contour indicating the critical contour of the singularity. The momentum is scaled to the K_M point, and the black dashed line indicates the boundary of the first MBZ. The top row shows the energy surfaces over the entire MBZ, while the second row focuses on the relevant HOVHS. The bottom row shows the corresponding single-spin DOS per unit volume for the band. The red dashed lines are fittings of the expected HOVHS behavior in the vicinity of the divergence (more details are provided in Ref. [56]). The AA TBK system considered here takes $\theta_c = 38.2^\circ$, $a = 0.5338$ nm, $d_\perp = 0.6596$ nm, $t_H = 0$, and $\gamma = 20$ [30,50], with $t_\perp = 0.3t$ in (a)–(c) and $t_\perp = 0.267t$ in (d). The band number and choice of t_d are given at the top of each column.

to achieve an exact HOVHS. However, symmetry can reduce the number of tuning parameters necessary to yield an effective sixth-order singularity from the perspective of experiment. Figure 3(c) presents an example of a sixfold singularity achieved using only dimerization. Our analysis of the expansion coefficients in Eq. (11) reveals that band 5 has a vanishing second-order coefficient ($\tilde{c}_2 = 0$) and a fourth-order coefficient we infer to be small in comparison to the sixth-order term, $\tilde{c}_4 \ll c_6$: we obtain $\tilde{c}_4$ to be nonzero but observe an extremely small minimum in the band $[E(\mathbf{0}) - E(0.01K_M)]/E(\mathbf{0}) \sim 10^{-7}$. Moreover, the divergence of the DOS at the HOVHS energy is easily fitted by the $g(\varepsilon) \sim \varepsilon^{-2/3}$ scaling at leading order characteristic of a sixth-order singularity [13,16]; see Fig. 3(c). The onset of a sixfold singularity can also be seen in other bands. The third peak in the DOS of band 18 [Fig. 3(b)] can be attributed to a set of six closely packed twofold singularities: closer inspection reveals a small minimum at the origin. We provide additional examples of effective sixfold HOVHSs in Ref. [56] for AA and interlocked TBK, with the latter being tuned via an interlayer potential.

C. Twofold singularities

The appearance of singularities (either localized or delocalized) with a twofold symmetry at the M_M points is expected in TBK given the VHSs that exist at the BZ edges of the monolayer. We immediately note that fourth-order singularities of the form $\varepsilon \sim k_x^2 - k_y^4$ can be acquired without the need

for sophisticated hoppings to break inversion or time-reversal symmetry as illustrated by band 14 in Fig. 3(d). Here we set $t_d = t_H = 0$ and tune the interlayer hopping amplitude to $t_\perp = 0.267t$ to produce a DOS scaling of $g(\varepsilon) \sim D_\pm |\varepsilon|^{-1/4}$ at the MBZ edge. Moreover, the prefactors D_+ and D_- for $\varepsilon > 0$ and $\varepsilon < 0$, respectively, yield a ratio of $D_-/D_+ \simeq \sqrt{2}$, matching the expected value for this type of HOVHS [16]. This demonstrates that HOVHSs can be achieved in layered systems purely through twisting. We note that even with dimerization included, twofold singularities can persist as in band 26, which hosts extremely flat singularities at its MBZ edges, yielding the second peak in the DOS plot of Fig. 3(a), and in band 5, also yielding the second peak in the DOS in Fig. 3(c). Twofold singularities may also form away from the MBZ edges, as seen in Fig. 3(b) for band 18 (first DOS peak) hosting C_{2z} singularities close to the Γ_M - K_M high-symmetry line. Finally, we note that it may also be possible to engineer fourth-order singularities around the MBZ edges through dimerization and additional parameters beyond those considered here, which we discuss in Ref. [56].

D. Topological monkey saddles

Complex NNN hopping is an alternative way to gap out the Dirac cones that appear at MBZ corners, creating monkey saddle singularities through the breaking of $\mathcal{T}$. We show in Fig. 4 the electronic structure for AA TBK with a purely imaginary NNN hopping tuned to yield a delocalized monkey saddle

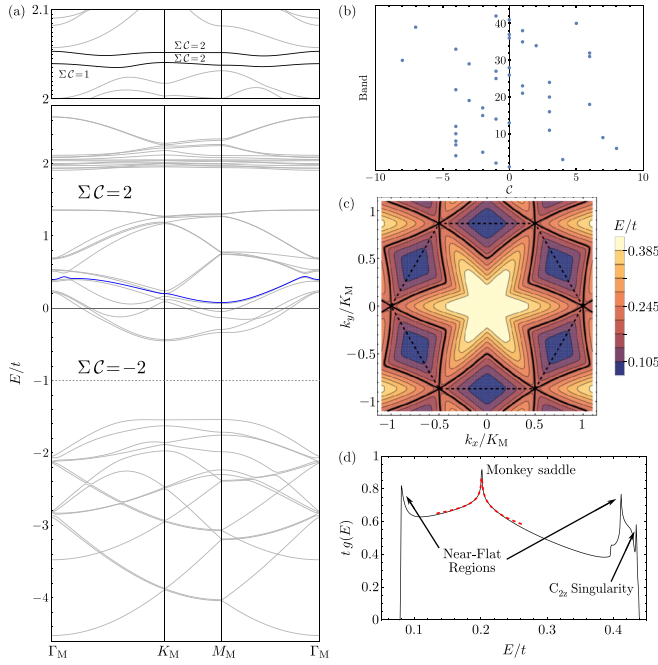


FIG. 4. Band structure and Chern numbers for AA TBK tuned to a topological monkey saddle singularity, alongside the DOS of the topological band hosting the singularity. Parameters: $\theta_c = 38.2^\circ$, $a = 0.5338$ nm, $d_\perp = 0.6596$ nm, $t_H = 0.18147t$, $\phi = \pi/2$, $t_\perp = 0.3t$, and $\gamma = 20$ [30,50]. (a) Band structure with the monkey saddle host band highlighted (band 20). The sums of the Chern numbers in the insulating gaps are indicated. The top panel focuses on bands 35 and 36 (highlighted in black). (b) The set of Chern numbers for each band. We note that all degeneracies are lifted. Reference [56] provides details on checking the numerical convergence of the Chern numbers. (c) Energy contours of band 20 across the entire MBZ (boundary marked by the dashed line) with the HOVHS energy contour highlighted by the bold line. (d) Single-spin DOS per unit volume for band 20. The red dashed line marks our fitting of the monkey saddle divergence whose leading-order behavior is $g(\varepsilon) \propto \varepsilon^{-1/3}$.

in band 20. We find that all degeneracies are lifted to result in the majority of bands becoming topologically nontrivial, with Chern numbers as large as $|C| = 8$ being observed in bands 6 and 30 [Fig. 4(b)]. Two major gaps ($\Delta E \sim 0.5t$ to t) open in the band structure and split the bands into three equal sets of 14 bands [Fig. 4(a)], with the lowest energy set giving a total Chern number of -2 while the middle energy set possesses a total Chern number of 4. Therefore, the AA TBK system will also become a Chern insulator exhibiting topologically protected edge states yielding an intrinsic anomalous Hall conductivity of $\sigma_{yx}^{\text{int}} = \pm 2e^2/h$ in these gaps. Closer inspection of the near-flat band region for this particular case reveals three more, albeit smaller, insulating gaps ($\Delta E \sim 0.01t$) around bands 35 and 36; see Fig. 4(a). However, band 36 is topologically trivial and so we only observe $\sigma_{yx}^{\text{int}} = e^2/h$ below band 35 and $\sigma_{yx}^{\text{int}} = 2e^2/h$ above bands 35 and 36. Regarding band 20, it acts as a host to a delocalized topological HOVHS with a Chern number of $C = 3$. The DOS for this band [Fig. 4(d)] reveals multiple singularities: a set of six closely situated second-order VHSs near the origin approaching a sixth-order singularity near the top of the band,

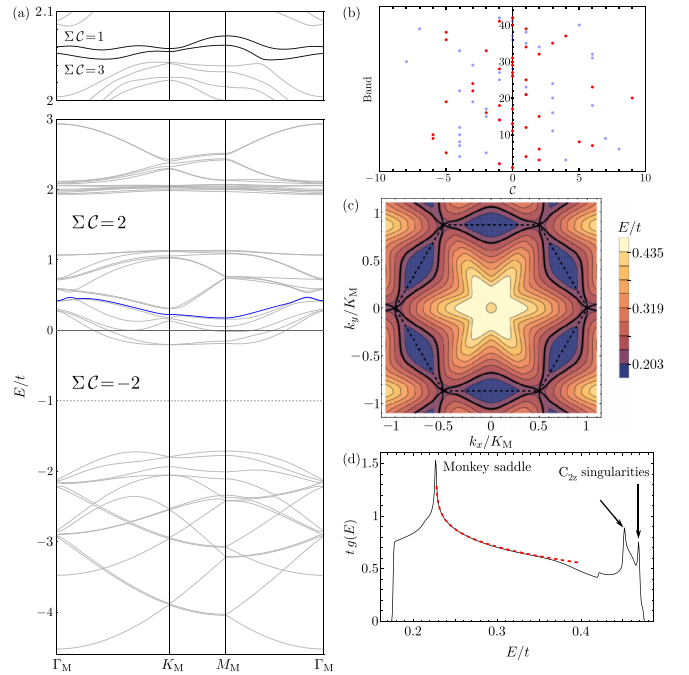


FIG. 5. Band structure and Chern numbers for interlocked TBK tuned to a topological monkey saddle singularity, alongside the DOS of the topological band hosting the singularity. Parameters: $\theta_c = 38.2^\circ$, $a = 0.5338$ nm, $d_\perp = 0.6596$ nm, $t_H = 0.26589t$, $\phi = \pi/2$, $t_\perp = 0.3t$, and $\gamma = 20$ [30,50]. (a) Band structure with the monkey saddle host band highlighted (band 20). The sums of the Chern numbers for the first and second sets of 14 bands are indicated. The top panel focuses on bands 35 and 36 (highlighted in black). (b) The set of Chern numbers for each band for interlocked (red) and AA TBK (pale blue) when tuned to host a monkey saddle in band 20, respectively. Again, all degeneracies are lifted. (c) Energy contours of band 20 across the entire MBZ (boundary marked by the dashed line), with the HOVHS energy contour highlighted by the bold line. (d) Single-spin DOS per unit volume for band 20. The red dashed line marks our fitting of the monkey saddle divergence, whose leading-order behavior is $g(\varepsilon) \propto \varepsilon^{-1/3}$.

and two regions where the band becomes extremely flat. The monkey saddle peak is well fitted by a DOS with a leading-order correction that scales as $g(\varepsilon) \propto \varepsilon^{-1/3}$.

Changing the stacking from AA to interlocked, another delocalized topological monkey saddle in band 20 is revealed with a larger choice of t_H ; see Fig. 5. However, the topology of all bands is altered drastically in comparison to the AA system with a Chern number of $C = 9$ now being associated with the monkey saddle band [Fig. 5(b)]. Moreover, the minor insulating gaps above band 36 and below band 35 remain and appear larger than in the AA system. Likewise, the two major insulating gaps also persist, again splitting the bands into three groups of 14 bands and allowing for a quantum anomalous Hall response of $\sigma_{yx}^{\text{int}} = \pm 2e^2/h$ equivalent to the AA stacked system. In contrast, the insulating gap between bands 35 and 36 has now become an indirect gap preventing a fifth region of Chern insulator behavior for this tuning of the electronic structure. Nonetheless, we note that it may be possible to tune the system to open this gap and encourage a giant anomalous Hall conductivity with $\sigma_{yx}^{\text{int}} = \pm 6e^2/h$ due to

the sum of Chern numbers from bands 35 and below giving $\Sigma C = 6$. Further examples of topological monkey saddles are provided in Ref. [56].

E. The role of sublattice interference

Nesting vectors act to enhance particle-hole fluctuations by connecting large parallel sections of the Fermi surface, and they can play a crucial role in the formation of different phases [67]. However, sublattice interference in a kagome monolayer can greatly affect these vectors by requiring that they further connect sections of the Fermi surface with the same sublattice projection [68]. Specifically, it has been shown that the critical contour associated with the VHS at 5/12 filling has six nesting vectors, as opposed to the three we might expect akin to graphene tuned to its VHS, which connect the BZ corners to the opposing edge M points [68]. This results in a preference for f -wave superconductivity in a kagome Hubbard system. However, the energy contours associated with the various HOVHSs are not simple hexagons due to their nature of curving the Fermi surface, and thus they naturally suppress nesting effects [69]. Nonetheless, due to HOVHSs tending to enhance the transition temperatures of ordered phases, thermal broadening of the Fermi surface should be accounted for to yield *diffusive nesting* vectors that may connect regions of the thermally broadened Fermi surface [70]. Specifically, for AA TBK, we may identify diffusive nesting vectors that connect sections of the Fermi surface that are related to each another by a π rotation about the z -axis; see Fig. 6(a). The precise diffusive nesting vectors depend on the filling and the associated shape of the Fermi surface, but from the symmetry point of view, it is possible for them to survive. The symmetries of the Fermi surface respect at least those of the BZ as defined here.

By projecting the eigenstates for TBK onto the A , B , and C sublattices of the first and second layers, we observe a similar sublattice polarization pattern across the entire MBZ that matches with that seen for monolayer kagome in Ref. [68]. Specifically, the Fermi surface sections that possess the same sublattice polarization form a C_{2z} symmetry, see Fig. 6, thus matching the natural nesting vectors that can be inferred directly from the Fermi surface contour. This would suggest that sublattice interference around the full Fermi surface is unlikely to have as large an effect as in the monolayer for these cases. However, other singularities exist within the TBK band structure with vastly different Fermi surface shapes, meaning we cannot rule out sublattice interference as a means to restrict the nesting vectors beyond the requirements of the Fermi surface geometry. Moreover, sublattice interference may play a significant role in constructing the effective interaction channels through connecting pairs of electrons situated close to a HOVHS [14,71]. The sublattice projections of the bands reveal that the eigenstates can either be localized primarily on a single sublattice or between two sublattices. Band 20 in Fig. 6(a) shows the former case, while band 8 in Fig. 6(b) exhibits the latter with admixing between sublattices. Finally, we note that the dihedral symmetry along the x -axis is clearly illustrated by the sublattice projections of the two layers in Fig. 6, with A and A' mapping onto one another, while B (C) maps onto C' (B') for the $\theta_c = 38.2^\circ$

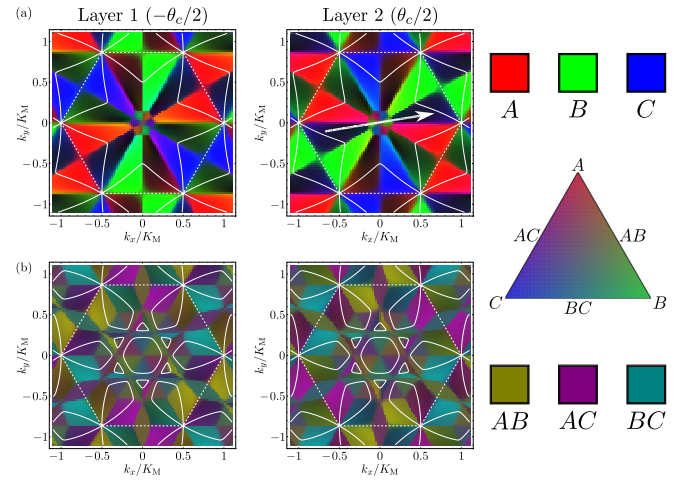


FIG. 6. Sublattice polarization for different bands tuned to host a monkey saddle singularity. Color maps for two bands in AA TBK tuned to host monkey saddle singularities at the MBZ corners indicating their sublattice projection throughout the MBZ within the bottom (left) and top (right) layers. If the eigenstate is completely localized to a single sublattice, it is given a color of red (A), green (B), or blue (C). However, if the state is equally localized between two sublattices, it is given by equal mixing of their respective colors. The white contours highlight the Fermi surface at the critical energy of the HOVHS, and the white dashed hexagon indicates the MBZ boundary. The white arrow is an example of a possible nesting vector between Fermi surface regions related by a π rotation. In both cases, we use $\theta_c = 38.2^\circ$, $a = 0.5338$ nm, $d_\perp = 0.6596$ nm, $t_\perp = 0.3t$, and $\gamma = 20$ [30,50]. (a) Band 20 with $t_H = 0.18147t$ and $\phi = \pi/2$. (b) Band 8 with $t_d = 0.0862t$.

AA TBK system; see Fig. 8 in Appendix B for the MUCs. In both cases, the sublattice polarization around the HOVHSs is highly nontrivial, so we leave interaction considerations and the interplay of HOVHSs and sublattice interference to future works.

V. DISCUSSION

In this article, we have presented a detailed analysis of the symmetries and band structure for twisted bilayer kagome vdW heterostructures for a large commensurate twist angle, and we identified its potential to host exotic topological HOVHSs. Specifically, we encountered three types of Van Hove singularity in the band structure: monkey saddles around the K_M point, sixfold singularities around Γ_M , and twofold singularities at the M_M point. These singularities could be achieved through the use of dimerization, an applied out-of-plane electric field, and complex NNN hopping. The monkey saddle singularities were found to occur in several bands and for a large range of tuning parameters, making them relatively accessible as they can be expected to occur in a plethora of TBK systems. In studying this type of singularity, we classified them into two categories: delocalized and localized. Both types of singularity can be expected to have significant effects on the electric and thermal transport coefficients, shifting them from the typical Fermi liquid behavior. Through complex NNN hopping, we also found them to emerge in topological bands, creating topological HOVHSs. Moreover,

we observed the emergence of five insulating gaps enabling quantum anomalous Hall behavior. This suggests that TBK hosts a rich landscape of transport phenomena ranging from non-Fermi-liquid behavior to topologically protected edge states. Furthermore, we found that the TBK system hosted bands with large Chern numbers with a magnitude of order 10 when tuned to host a HOVHS. This is of particular interest in searching for systems with a giant quantum anomalous Hall response and systems hosting a large number of active edge states. Our work, therefore, serves as a demonstration that such strong topological signatures may be achievable in twisted heterostructures.

Symmetry analysis identified the combination of dihedral rotation and time reversal, TC'_2 , to play a central role in determining the number of possible HOVHSs that may occur simultaneously due to the breaking of time-reversal symmetry changing the symmetry from a trivial lattice point group to a nontrivial magnetic point group. The application of an out-of-plane electric field acts to break this symmetry and reduce the number of HOVHSs. We expect that the AA and interlocked stackings will have similar properties and phase diagrams when they possess the same symmetries. This is not the case when Haldane tunneling is included while dimerization is absent. In contrast, the AB system is likely to exhibit the most unique phase diagram because it only hosts singularities with C_2 symmetry. If we consider a scenario where AB TBK is in the same phase as the AA and interlocked systems, then we would still expect unique signatures in the transport coefficients and electron self-energy courtesy of the different types of HOVHS [6,66].

The results presented here act as a guide to how topological HOVHSs can be achieved when constructing vdW heterostructures with kagome patterns. Currently, there are several candidate systems in which to probe these ideas: the largest class of candidate materials are MOFs, but recently N-doped kagome graphene and 2D π -conjugated polymers have been synthesized, realizing kagome patterns formed predominantly of triangular carbon atom islands [72,73]. There is intensive research being done for more materials of kagome structure, where the results of this work are relevant. For the case of small twist angles, while the treatment of a breathing kagome lattice as a dimerized lattice is no longer applicable, the symmetry analysis of the HOVHSs presented here remains true in general for all commensurate angles. Additionally, the two types of HOVHSs identified here—localized and delocalized—should also appear at small twist angles for both commensurate and incommensurate angles handled via Bistritzer-MacDonald-type analysis. Such low-energy continuum models would introduce topological HOVHSs characterized by valley Chern numbers instead, which may lead to an interesting interplay between valley-polarized phases and topology. Regarding other lattices, the same symmetries occur in hexagonal and triangular lattices. The dense flat band region of the kagome bilayer, though, which led to the rich structure of HOVHSs, is the reason that we took this lattice as an example. Future work will focus on the role of interactions in the TBK system to discover how the flat bands and the plethora of topological HOVHSs influence phase formation.

ACKNOWLEDGMENTS

We thank Claudio Chamon, Andrey Chubukov, Naëmi Leo, Natalia Perkins, and Ioannis Rouschatzakis for useful discussions, and especially Titus Neupert and Luiz Santos for reading the manuscript and providing insightful comments and questions. The work has been supported by the UK Engineering and Physical Sciences Research Council Grants No. EP/T034351/1 and No. EP/X012557/1.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX A: TWO CLASSES OF MOIRÉ SUPERLATTICES

The set of commensurate angles are defined by a pair of unique coprime integers (m, n) , such that $m > n > 0$. The commensurate angle θ_c associated with (m, n) is given by Eq. (1). These commensurate angles can be split into two classes: those with n divisible by 3 and those with n not divisible by 3. If θ_c is defined by a choice of n that is divisible by 3, then it has a partner commensurate angle that is associated with a choice of n that is not divisible by 3, $\theta'_c = \pi/3 - \theta_c$ [65]. When constructing a commensurate twisted bilayer, we may choose to work in the twist-symmetric frame where layer 1 is rotated clockwise by $\theta_c/2$ and layer 2 is rotated anticlockwise by $\theta_c/2$. We can relate the two classes of superlattices yielded by θ_c and θ'_c in the twist-symmetric frame by reflection in the line of $y = x$, as we prove below.

Let us start by considering a kagome hexagon centered on the origin and label each of the sublattices around the corners; see the first line of Fig. 7. We can choose to rotate this layer anticlockwise by $\theta_c/2$ to acquire one of its orientations in the twist-symmetric frame for one of the superlattice classes. To reflect this in the line of $y = x$, we rotate the whole system anticlockwise by 45° , reflect it in the y -axis ($x \rightarrow -x$), and then rotate the system clockwise by 45° , as illustrated in Fig. 7. The other superlattice class would be given by choosing to rotate this layer by $\theta'_c/2 = (\pi/3 - \theta_c)/2$ anticlockwise; see the second line of Fig. 7. By comparing the first and second lines of Fig. 7, we immediately see that the θ_c moiré pattern is mapped onto the θ'_c moiré pattern with a swapping of sublattices. From the perspective of geometry there is no difference, but for the Hamiltonian this can have consequences due to the relative orientation of the sublattices determining the topological contribution.

Alternatively, we can instead choose to rotate this layer clockwise by either $\theta_c/2$ or $\theta'_c/2$ to consider the other layer in the twisted bilayer, as shown in the third and fourth lines of Fig. 7, respectively. By transforming the $\theta_c/2$ layer by reflection in the line of $y = x$, see the third line of Fig. 7, we again acquire the same geometry as the $\theta'_c/2$ layer. However, unlike the anticlockwise rotation, not only is there a swapping of sublattices, but the orientation of up and down triangles is also swapped, as shown by the switching of highlighted and blank regions in Fig. 7. Therefore, while the geometries of the two classes are connected by a simple reflection, the topological

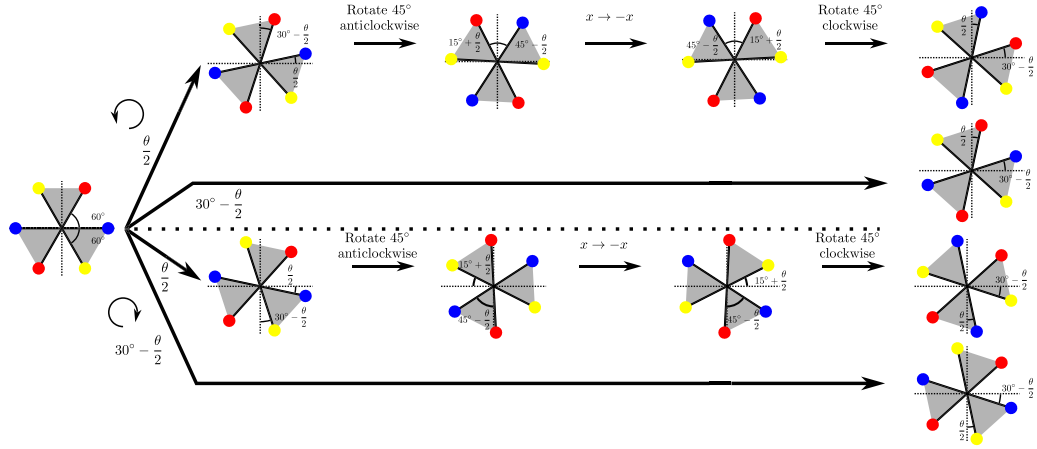


FIG. 7. Schematic representation for the relation of layers rotated by an arbitrary angle of $\theta/2$ and $\theta'/2 = \pi/6 - \theta/2$ by reflection in the line of $y = x$. We start with the hexagon center of a kagome lattice at the origin and label the three sublattices using red, blue, and yellow colored dots. We connect these to the origin and shade down triangles while leaving up triangles blank. The first line shows the hexagon rotated anticlockwise by $\theta/2$ and then transformed by reflection in $y = x$. The second line shows the hexagon rotated anticlockwise by $\theta'/2$. Similarly, the third line shows the hexagon rotated clockwise by $\theta/2$ and then transformed by reflection in $y = x$, while the fourth line shows the hexagon rotated clockwise by $\theta'/2$.

aspect of the Hamiltonian will once again be flipped, and the nature of the dimerization will also be reversed.

APPENDIX B: DERIVATION OF THE TBK TIGHT-BINDING HAMILTONIAN

Let us start by considering a moiré unit cell due to an arbitrary commensurate twist angle of θ_c . Each monolayer

contributes N^M triangular lattice sites to the unit cell, and hence $3N^M$ sublattice sites, thus leaving us with $6N^M$ sublattice sites within the moiré unit cell. We may then introduce $c_{il\alpha}^\dagger$ ($c_{il\alpha}$) creation (annihilation) operators to describe the addition (removal) of an electron from sublattice α of layer l in the moiré unit cell centered on $\mathbf{R}_i$, where $\{\alpha | \alpha \in \mathbb{Z}, 1 \leq \alpha \leq 3N^M\}$. We prescribe $\delta_\alpha^{(l)}$ as the position of sublattice site α in layer l within the moiré unit cell. The general Hamiltonian for this system may then be written as

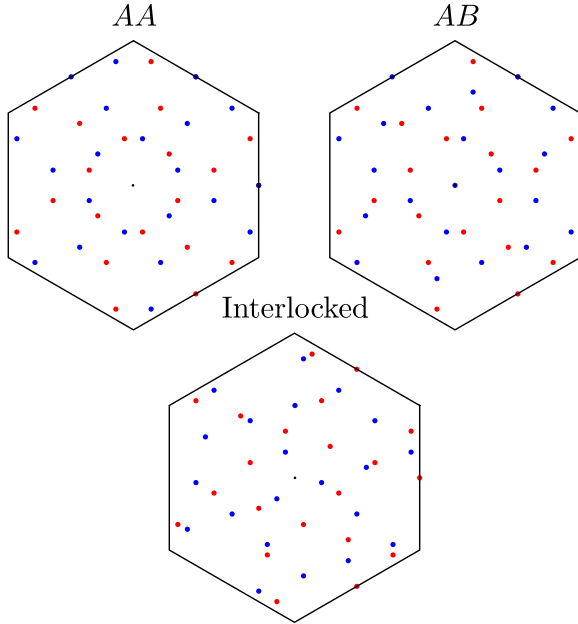


FIG. 8. Wigner-Seitz constructed moiré unit cells for the three possible stacking choices with a $\theta = 38.2^\circ$ twist applied about the hexagon center of layer 1. The red and blue dots belong to layers 1 and 2, respectively, while the small black dot indicates the twist origin and Wigner-Seitz lattice site. We show the MUCs in the twist symmetric frame.

$$\begin{aligned}
 H = & - \sum_i \sum_l \sum_{\alpha \neq \beta} t_{l,ii}^{\alpha\beta} c_{il\alpha}^\dagger c_{il\beta} \\
 & - \sum_{\langle i,j \rangle, l} \sum_{\alpha, \beta} t_{l,ij}^{\alpha\beta} c_{il\alpha}^\dagger c_{jl\beta} \\
 & - \sum_i \sum_{\alpha, \beta} t_{\perp,ii}^{\alpha\beta} (c_{i1\alpha}^\dagger c_{i2\beta} + c_{i2\beta}^\dagger c_{i1\alpha}) \\
 & - \sum_{\langle i,j \rangle, \alpha, \beta} t_{\perp,ij}^{\alpha\beta} (c_{i1\alpha}^\dagger c_{j2\beta} + c_{j2\beta}^\dagger c_{i1\alpha}), \quad (B1)
 \end{aligned}$$

assuming that the tunneling is real and decays sufficiently quickly to only allow tunneling up to NNN moiré unit cells. The first and second lines represent intralayer tunneling, while the third and fourth lines account for the interlayer tunneling. In writing this Hamiltonian, we noted that the tunneling energy should not depend on the direction of tunneling, $t_{\perp,ij}^{\alpha\beta} = t_{\perp,ji}^{\beta\alpha}$. Furthermore, we define the MUC as the Wigner-Seitz constructed unit cell centered on the twist origin, see Fig. 8, and we use $\langle i, j \rangle$ and $\langle\langle i, j \rangle\rangle$ to denote NN and NNN unit cells, respectively.

For simplicity, let us assume that the tunneling elements may be written as $t_{l,ij}^{\alpha\beta} = t^{\alpha\beta} f(|\mathbf{R}_i + \delta_\alpha^{(l)} - \mathbf{R}_j - \delta_\beta^{(l)}|)$ and $t_{\perp,ij}^{\alpha\beta} = t_{\perp 0}^{\alpha\beta} f_\perp(|\mathbf{R}_i + \delta_\alpha^{(1)} - \mathbf{R}_j - \delta_\beta^{(2)}|)$, with $t^{\alpha\beta} = t^{\beta\alpha}$ and $t_{\perp 0}^{\alpha\beta} = t_{\perp 0}^{\beta\alpha}$ (the superscripts remain to allow different orbital

overlaps between sublattices), where $f(r)$ and $f_{\perp}(r)$ are functions that decay as r increases. Now we can move to momentum space,

$$\begin{aligned}
H = & - \sum_{\mathbf{k}} \sum_l \sum_{\alpha \neq \beta} t^{\alpha\beta} f(|\delta_{\beta\alpha}^{(l)}|) e^{i\mathbf{k} \cdot \delta_{\beta\alpha}^{(l)}} c_{\mathbf{k}l\alpha}^{\dagger} c_{\mathbf{k}l\beta} \\
& - \sum_{\mathbf{k}} \sum_l \sum_{\alpha, \beta} t^{\alpha\beta} \tilde{\Gamma}_l^{\alpha\beta}(\mathbf{k}) c_{\mathbf{k}l\alpha}^{\dagger} c_{\mathbf{k}l\beta} \\
& - \sum_{\mathbf{k}} \sum_{\alpha, \beta} t_{\perp 0}^{\alpha\beta} [(f_{\perp}(|\delta_{\beta\alpha}^{(21)}|) e^{i\mathbf{k} \cdot \delta_{\beta\alpha}^{(21)}} + \tilde{\Gamma}_{\perp}^{\alpha\beta}(\mathbf{k})) c_{\mathbf{k}1\alpha}^{\dagger} c_{\mathbf{k}2\beta} \\
& + (f_{\perp}(|\delta_{\beta\alpha}^{(21)}|) e^{-i\mathbf{k} \cdot \delta_{\beta\alpha}^{(21)}} + \tilde{\Gamma}_{\perp}^{\alpha\beta}(\mathbf{k})^*) c_{\mathbf{k}2\beta}^{\dagger} c_{\mathbf{k}1\alpha}], \quad (\text{B2})
\end{aligned}$$

with $\delta_{\beta\alpha}^{(l)} = \delta_{\beta}^{(l)} - \delta_{\alpha}^{(l)}$, $\delta_{\beta\alpha}^{(21)} = \delta_{\beta}^{(2)} - \delta_{\alpha}^{(1)}$,

$$\begin{aligned}
\tilde{\Gamma}_l^{\alpha\beta}(\mathbf{k}) &= \sum_{i=1}^{18} f(|\delta_{\beta\alpha}^{(l)} + \mathbf{c}_i^M|) e^{i\mathbf{k} \cdot (\delta_{\beta\alpha}^{(l)} + \mathbf{c}_i^M)}, \\
\tilde{\Gamma}_{\perp}^{\alpha\beta}(\mathbf{k}) &= \sum_{i=1}^{18} f_{\perp}(|\delta_{\beta\alpha}^{(21)} + \mathbf{c}_i^M|) e^{i\mathbf{k} \cdot (\delta_{\beta\alpha}^{(21)} + \mathbf{c}_i^M)}, \quad (\text{B3})
\end{aligned}$$

and

$$\begin{aligned}
\{\mathbf{c}_i^M\} = & \{ \pm \mathbf{a}_1^M, \pm \mathbf{a}_2^M, \pm (\mathbf{a}_2^M - \mathbf{a}_1^M), \\
& \pm 2\mathbf{a}_1^M, \pm 2\mathbf{a}_2^M, \pm 2(\mathbf{a}_2^M - \mathbf{a}_1^M), \\
& \pm (\mathbf{a}_2^M + \mathbf{a}_1^M), \pm (2\mathbf{a}_2^M - \mathbf{a}_1^M), \pm (2\mathbf{a}_1^M - \mathbf{a}_2^M) \}, \quad (\text{B4})
\end{aligned}$$

being the set of moiré lattice vectors connecting NN and NNN moiré unit cells. We can further simplify the Hamiltonian in Eq. (B2) by introducing

$$\begin{aligned}
\Gamma_l^{\alpha\beta}(\mathbf{k}) &= f(|\delta_{\beta\alpha}^{(l)}|) e^{i\mathbf{k} \cdot \delta_{\beta\alpha}^{(l)}} (1 - \delta_{\alpha\beta}) + \tilde{\Gamma}_l^{\alpha\beta}(\mathbf{k}), \\
\Gamma_{\perp}^{\alpha\beta}(\mathbf{k}) &= f_{\perp}(|\delta_{\beta\alpha}^{(21)}|) e^{i\mathbf{k} \cdot \delta_{\beta\alpha}^{(21)}} + \tilde{\Gamma}_{\perp}^{\alpha\beta}(\mathbf{k}), \quad (\text{B5})
\end{aligned}$$

which yields

$$\begin{aligned}
H = & - \sum_{\mathbf{k}} \sum_{\alpha, \beta} \left(\sum_l t^{\alpha\beta} \Gamma_l^{\alpha\beta}(\mathbf{k}) c_{\mathbf{k}l\alpha}^{\dagger} c_{\mathbf{k}l\beta} \right. \\
& \left. + t_{\perp 0}^{\alpha\beta} [\Gamma_{\perp}^{\alpha\beta}(\mathbf{k}) c_{\mathbf{k}1\alpha}^{\dagger} c_{\mathbf{k}2\beta} + \Gamma_{\perp}^{\alpha\beta}(\mathbf{k})^* c_{\mathbf{k}2\beta}^{\dagger} c_{\mathbf{k}1\alpha}] \right). \quad (\text{B6})
\end{aligned}$$

We include complex NNN tunneling as a purely intralayer process. Written in real space, this mechanism contributes

$$\begin{aligned}
H_H = & -t_H \sum_l \sum_i'' \sum_{\alpha \neq \beta} e^{iS_{\alpha\beta}\phi} c_{il\alpha}^{\dagger} c_{il\beta} \\
& -t_H \sum_l \sum_{\langle i,j \rangle}'' \sum_{\alpha, \beta} e^{iS_{\alpha\beta}\phi} c_{il\alpha}^{\dagger} c_{jl\beta} \quad (\text{B7})
\end{aligned}$$

to the Hamiltonian, where the double primes indicate the restriction of the sum to NNN sites. Moving to momentum space yields

$$H_H = -t_H \sum_{\mathbf{k}} \sum_l \sum_{\alpha, \beta} \Gamma_H^{\alpha\beta}(\mathbf{k}) e^{iS_{\alpha\beta}\phi} c_{\mathbf{k}l\alpha}^{\dagger} c_{\mathbf{k}l\beta}, \quad (\text{B8})$$

with

$$\Gamma_H^{\alpha\beta}(\mathbf{k}) = \left[\delta_{\langle\alpha, \beta\rangle} + \sum_{i=1}^6 \delta_{\langle\alpha, \beta\rangle}^i e^{i\mathbf{k} \cdot \mathbf{c}_i^M} \right], \quad (\text{B9})$$

where $\delta_{\langle\alpha, \beta\rangle}$ is unity when α and β are NNN within the same unit cell and zero otherwise. Similarly, $\delta_{\langle\alpha, \beta\rangle}^i$ is unity when α and β are NNN while located in NN unit cells, such that their separation is $\delta_{\alpha} - \delta_{\beta} - \mathbf{c}_i^M$, and zero otherwise.

APPENDIX C: OBTAINING MONKEY SADDLE SINGULARITIES

The presence of a monkey saddle singularity can be determined by checking the vanishing of all second-order terms in the expansion of the band energy about the K_M point. Expanding a given band around the K_M point that hosts a critical point yields

$$\begin{aligned}
\varepsilon = & \varepsilon_0 + c_0^{(2)} p_x^2 + c_1^{(2)} p_x p_y + c_2^{(2)} p_y^2 \\
& + c_0^{(3)} p_x^3 + c_1^{(3)} p_x^2 p_y + c_2^{(3)} p_x p_y^2 + c_3^{(3)} p_y^3 + O(p^4) \quad (\text{C1})
\end{aligned}$$

for the local dispersion where $\mathbf{p} = \mathbf{k} - \mathbf{K}_M$, $c_i^{(j)}$ are generic expansion constants, and ε_0 is the band's energy at the K_M point. A regular VHS will manifest when the second-order coefficients are nonzero. The point group symmetry of AA TBK is D_6 while for interlocked TBK it is D_3 [54]. When dimerization is added, they are both D_3 . If an out-of-plane electric field is applied to induce an interlayer potential, then the dihedral symmetry is broken due to one layer acquiring an on-site energy of $\Delta/2$ and the other $-\Delta/2$, reducing the point group symmetry to C_{3z} . The threefold rotational symmetry of this system ensures that the MBZ corners must also exhibit C_{3z} symmetry, requiring $c_0^{(2)} = c_2^{(2)}$, $c_2^{(3)} = -3c_0^{(3)}$, $c_1^{(3)} = -3c_3^{(3)}$, and $c_1^{(2)} = 0$, to yield

$$\begin{aligned}
\varepsilon = & \varepsilon_0 + c_0^{(2)} p^2 + p^3 [c_1^{(3)} \cos(3\varphi) - c_4^{(3)} \sin(3\varphi)] \\
& + O(p^4), \quad (\text{C2})
\end{aligned}$$

where φ is the local azimuthal angle.

Let us now restrict the above scenario to one where dihedral symmetry is preserved along the x -axis (i.e., no interlayer potential) with a choice of θ_c such that $n/3 \in \mathbb{Z}$. In this case, the dihedral symmetry manifests as a reflection $k_y \rightarrow -k_y$ symmetry in momentum space within the twist symmetric frame courtesy of the system's effective 2D nature: the dihedral symmetry can be thought of as a reflection in the x -axis ($y \rightarrow -y$) followed by a reflection in the xy plane ($z \rightarrow -z$, i.e., swapping the layers). The out-of-plane reflection has no effect on the dispersion since the layers are identical. Hence, C_{2x} dihedral symmetry sets $c_4^{(3)} = 0$, resulting in

$$\varepsilon = \varepsilon_0 + c_0^{(2)} p^2 + c_1^{(3)} p^3 \cos(3\varphi) + O(p^4). \quad (\text{C3})$$

This effective $k_y \rightarrow -k_y$ symmetry is seen in all cases of Fig. 3, Fig. S3 of Ref. [56], aside from Fig. S3c, where an interlayer potential is present. Figure S3c demonstrates how this effective reflection symmetry is broken through the application of an out-of-plane electric field. If there were instead a dihedral symmetry along the y -axis through a choice of n such

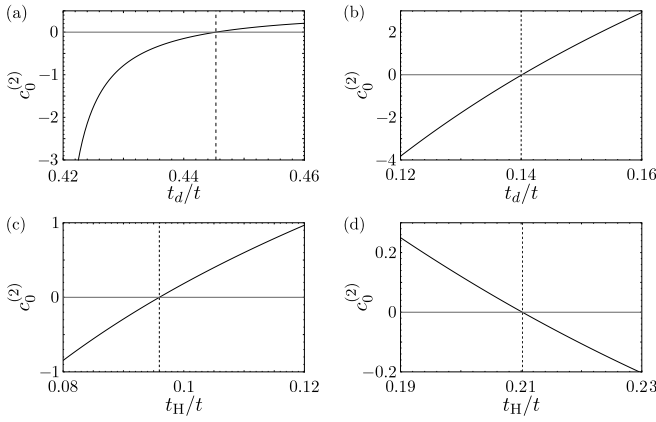


FIG. 9. Variation of the second-order coefficient, $c_0^{(2)}$, with dimerization and Haldane hopping. (a) Band 26 with AA stacking. (b) Band 8 with interlocked stacking. (c) Band 18 with AA stacking. (d) Band 12 with interlocked stacking.

that $n/3 \notin \mathbb{Z}$, then symmetry would instead require $c_1^{(3)} = 0$ and allow for $c_4^{(3)} \neq 0$.

Nonetheless, whether dihedral symmetry is preserved or not, we can demonstrate the existence of an exact monkey saddle simply by studying how $c_0^{(2)}$ changes as the tuning parameters are varied. If $c_0^{(2)} = 0$ at some point while some third-order coefficients are nonzero, then that choice of parameters will yield a monkey saddle singularity. We present the dependence of $c_0^{(2)}$ on the dimerization and Haldane hopping in Fig. 9 to illustrate this in various bands of AA and interlocked TBK.

Higher-order corrections to the DOS

The DOS for a band with dispersion $E(\mathbf{k})$ is given by

$$g(\varepsilon) = \int_{\text{BZ}} \frac{d^2k}{(2\pi)^2} \delta(E(\mathbf{k}) - \varepsilon), \quad (\text{C4})$$

where the integral is over the BZ. If $E(\mathbf{k})$ has the form of a pure HOVHS, we can obtain the power-law behavior of the DOS by scaling $k_x \rightarrow |\varepsilon|^\alpha p_x$ and $k_y \rightarrow |\varepsilon|^\beta p_y$ for some appropriate α and β in this integral. For example, for the HOVHS $k_x^4 - k_y^2$, we need to set $\alpha = 1/4$, $\beta = 1/2$ so that

$$\begin{aligned} g(\varepsilon) &\approx \int_{\mathbb{R}^2} \frac{d^2k}{(2\pi)^2} \delta(k_x^4 - k_y^2 - \varepsilon) \\ &= \int_{\mathbb{R}^2} \frac{|\varepsilon|^{\frac{1}{4} + \frac{1}{2}} d^2p}{(2\pi)^2} \delta(|\varepsilon| p_x^4 - |\varepsilon| p_y^2 - \varepsilon) \end{aligned}$$

$$\begin{aligned} &= |\varepsilon|^{-\frac{1}{4}} \int_{\mathbb{R}^2} \frac{d^2p}{(2\pi)^2} \delta(p_x^4 - p_y^2 - \text{sgn}(\varepsilon)) \\ &= D_\pm |\varepsilon|^{-\frac{1}{4}}, \end{aligned} \quad (\text{C5})$$

where we have extended the integral over the entire real plane (introducing a finite error in comparison to the divergence of the DOS) and used the scaling property of the delta function: $\delta(ax) = \delta(x)/|a|$. The final integral is independent of the magnitude of ε and depends only on the sign, evaluating, respectively, to D_+ for $\varepsilon > 0$ and D_- for $\varepsilon < 0$. The ratio D_+/D_- is a characteristic feature of each HOVHS, alongside the exponent of the power-law DOS. In particular, the power-law DOS for the $k_x^4 - k_y^2$ singularity is $|\varepsilon|^{-1/4}$. When there are higher-order terms that correct the HOVHS (as happens for the series expansion of a realistic band dispersion), we are guaranteed to have a smooth coordinate transformation with a smooth inverse $\psi : (\tilde{k}_x, \tilde{k}_y) \rightarrow (k_x, k_y)$ that maps the full dispersion to the exact form of the HOVHS in some neighborhood of the critical point. That is, with $(k_x, k_y) = \psi(\tilde{k}_x, \tilde{k}_y)$ we have $E(k_x, k_y) = E(\psi(\tilde{k}_x, \tilde{k}_y)) = \tilde{k}_x^4 - \tilde{k}_y^2$ (or the equivalent form for the other HOVHS). The DOS integral then takes the form

$$g(\varepsilon) \approx \int_{\mathbb{R}^2} \frac{d^2\tilde{k}}{(2\pi)^2} J(\tilde{k}_x, \tilde{k}_y) \delta(\tilde{k}_x^4 - \tilde{k}_y^2 - \varepsilon), \quad (\text{C6})$$

where $J(\tilde{k}_x, \tilde{k}_y)$ is the Jacobian determinant for ψ that is necessary to effect the change of variables in a multiple integral. Since ψ is a local diffeomorphism, $J_0 = J(0, 0)$ has to be nonzero. We can then series expand $J(\tilde{k}_x, \tilde{k}_y)$ around $(0, 0)$, and scale $\tilde{k}_x$ and $\tilde{k}_y$ in each integral in the resultant series appropriately to obtain the power-law DOS at leading order, which is corrected by subleading terms [16]

$$g(\varepsilon) \approx |\varepsilon|^{-\gamma} \left(J_0 D_\pm + \sum_{n=1}^{\infty} \sum_{m=0}^n c_{mn} |\varepsilon|^{m\alpha + (n-m)\beta} \right), \quad (\text{C7})$$

where the leading-order exponent $\gamma = 1 - \alpha - \beta$. Since $0 < \alpha, \beta < 1$, and $m \leq n$, we have $m\alpha + (n-m)\beta > 0$, which ensures that terms in the sum are subleading in the $\varepsilon \rightarrow 0$ limit. While fitting for the power law DOS arising from a realistic dispersion with HOVHS, we may have to include a few terms in this series to get an accurate description for the chosen energy range near the critical energy. Notice that the leading-order terms for $\varepsilon > 0$ and $\varepsilon < 0$, respectively, have the coefficients $J_0 D_+$ and $J_0 D_-$ ensuring that the universal ratio of prefactors D_+/D_- is preserved.

- [1] L. Classen and J. J. Betouras, High-order Van Hove singularities and their connection to flat bands, *Annu. Rev. Condens. Matter Phys.* **16**, 229 (2025).
- [2] L. Van Hove, The occurrence of singularities in the elastic frequency distribution of a crystal, *Phys. Rev.* **89**, 1189 (1953).
- [3] S. A. Grigera, R. S. Perry, A. J. Schofield, M. Chiao, S. R. Julian, G. G. Lonzarich, S. I. Ikeda, Y. Maeno, A. J. Millis, and A. P. Mackenzie, Magnetic field-tuned quantum criticality in the metallic ruthenate $\text{Sr}_3\text{Ru}_2\text{O}_7$, *Science* **294**, 329 (2001).

- [4] A. Tamai, M. P. Allan, J. F. Mercure, W. Meevasana, R. Dunkel, D. H. Lu, R. S. Perry, A. P. Mackenzie, D. J. Singh, Z.-X. Shen, and F. Baumberger, Fermi surface and van Hove singularities in the itinerant metamagnet $\text{Sr}_3\text{Ru}_2\text{O}_7$, *Phys. Rev. Lett.* **101**, 026407 (2008).
- [5] D. V. Efremov, A. Shtyk, A. W. Rost, C. Chamon, A. P. Mackenzie, and J. J. Betouras, Multicritical Fermi surface topological transitions, *Phys. Rev. Lett.* **123**, 207202 (2019).

- [6] C. H. Mousatov, E. Berg, and S. A. Hartnoll, Theory of the strange metal $\text{Sr}_3\text{Ru}_2\text{O}_7$, *Proc. Natl. Acad. Sci. USA* **117**, 2852 (2020).
- [7] L. Wei, Q. Xu, Y. He, Q. Li, Y. Huang, W. Zhu, K. Watanabe, T. Taniguchi, M. Claassen, D. A. Rhodes, D. M. Kennes, L. Xian, A. Rubio, and L. Wang, Linear resistivity at van Hove singularities in twisted bilayer WSe_2 , *Proc. Natl. Acad. Sci. USA* **121**, e2321665121 (2024).
- [8] Y. Cao, V. Fatemi, S. Fang, K. Watanabe, T. Taniguchi, E. Kaxiras, and P. Jarillo-Herrero, Unconventional superconductivity in magic-angle graphene superlattices, *Nature (London)* **556**, 43 (2018).
- [9] H. Zhou, T. Xie, T. Taniguchi, K. Watanabe, and A. F. Young, Superconductivity in rhombohedral trilayer graphene, *Nature (London)* **598**, 434 (2021).
- [10] J. M. Park, Y. Cao, L.-Q. Xia, S. Sun, K. Watanabe, T. Taniguchi, and P. Jarillo-Herrero, Robust superconductivity in magic-angle multilayer graphene family, *Nat. Mater.* **21**, 877 (2022).
- [11] D. Guerci, P. Simon, and C. Mora, Higher-order Van Hove singularity in magic-angle twisted trilayer graphene, *Phys. Rev. Res.* **4**, L012013 (2022).
- [12] Y. Cao, D. Chowdhury, D. Rodan-Legrain, O. Rubies-Bigorda, K. Watanabe, T. Taniguchi, T. Senthil, and P. Jarillo-Herrero, Strange metal in magic-angle graphene with near Planckian dissipation, *Phys. Rev. Lett.* **124**, 076801 (2020).
- [13] A. Shtyk, G. Goldstein, and C. Chamon, Electrons at the monkey saddle: A multicritical Lifshitz point, *Phys. Rev. B* **95**, 035137 (2017).
- [14] Y.-C. Lee, D. V. Chichinadze, and A. V. Chubukov, Crossover from ordinary to higher order Van Hove singularity in a honeycomb system: A parquet renormalization group analysis, *Phys. Rev. B* **109**, 155118 (2024).
- [15] H. Isobe and L. Fu, Supermetal, *Phys. Rev. Res.* **1**, 033206 (2019).
- [16] A. Chandrasekaran, A. Shtyk, J. J. Betouras, and C. Chamon, Catastrophe theory classification of Fermi surface topological transitions in two dimensions, *Phys. Rev. Res.* **2**, 013355 (2020).
- [17] N. F. Q. Yuan and L. Fu, Classification of critical points in energy bands based on topology, scaling, and symmetry, *Phys. Rev. B* **101**, 125120 (2020).
- [18] A. Chandrasekaran and J. J. Betouras, Effect of disorder on density of states and conductivity in higher-order Van Hove singularities in two-dimensional bands, *Phys. Rev. B* **105**, 075144 (2022).
- [19] A. Chandrasekaran, L. C. Rhodes, E. A. Morales, C. A. Marques, P. D. C. King, P. Wahl, and J. J. Betouras, On the engineering of higher-order Van Hove singularities in two dimensions, *Nat. Commun.* **15**, 9521 (2024).
- [20] A. Chandrasekaran and J. J. Betouras, A practical method to detect, analyze, and engineer higher order Van Hove singularities in multi-band Hamiltonians, *Adv. Phys. Res.* **2**, 2200061 (2023).
- [21] E. H. Lieb, Two theorems on the Hubbard model, *Phys. Rev. Lett.* **62**, 1201 (1989).
- [22] A. J. Kollár, M. Fitzpatrick, P. Sarnak, and A. A. Houck, Line-graph lattices: Euclidean and non-Euclidean flat bands, and implementations in circuit quantum electrodynamics, *Commun. Math. Phys.* **376**, 1909 (2020).
- [23] D.-S. Ma, Y. Xu, C. S. Chiu, N. Regnault, A. A. Houck, Z. Song, and B. A. Bernevig, Spin-orbit-induced topological flat bands in line and split graphs of bipartite lattices, *Phys. Rev. Lett.* **125**, 266403 (2020).
- [24] B. R. Ortiz, L. C. Gomes, J. R. Morey, M. Winiarski, M. Bordelon, J. S. Mangum, I. W. H. Oswald, J. A. Rodriguez-Rivera, J. R. Neilson, S. D. Wilson, E. Ertekin, T. M. McQueen, and E. S. Toberer, New kagome prototype materials: Discovery of KV_3Sb_5 , RbV_3Sb_5 , and CsV_3Sb_5 , *Phys. Rev. Mater.* **3**, 094407 (2019).
- [25] M. Kang, S. Fang, J.-K. Kim, B. R. Ortiz, S. H. Ryu, J. Kim, J. Yoo, G. Sangiovanni, D. Di Sante, B.-G. Park, C. Jozwiak, A. Bostwick, E. Rotenberg, E. Kaxiras, S. D. Wilson, J.-H. Park, and R. Comin, Twofold van Hove singularity and origin of charge order in topological kagome superconductor CsV_3Sb_5 , *Nat. Phys.* **18**, 301 (2022).
- [26] S.-W. Kim, H. Oh, E.-G. Moon, and Y. Kim, Monolayer kagome metals AV_3Sb_5 , *Nat. Commun.* **14**, 591 (2023).
- [27] Y. Luo, Y. Han, J. Liu, H. Chen, Z. Huang, L. Huai, H. Li, B. Wang, J. Shen, S. Ding, Z. Li, S. Peng, Z. Wei, Y. Miao, X. Sun, Z. Ou, Z. Xiang, M. Hashimoto, D. Lu, Y. Yao *et al.*, A unique van Hove singularity in kagome superconductor $\text{CsV}_{3-x}\text{Ta}_x\text{Sb}_5$ with enhanced superconductivity, *Nat. Commun.* **14**, 3819 (2023).
- [28] H. Li, S. Cheng, B. R. Ortiz, H. Tan, D. Werhahn, K. Zeng, D. Johrendt, B. Yan, Z. Wang, S. D. Wilson, and I. Zeljkovic, Electronic nematicity without charge density waves in titanium-based kagome metal, *Nat. Phys.* **19**, 1591 (2023).
- [29] H. Yang, Y. Ye, Z. Zhao, J. Liu, X.-W. Yi, Y. Zhang, H. Xiao, J. Shi, J.-Y. You, Z. Huang, B. Wang, J. Wang, H. Guo, X. Lin, C. Shen, W. Zhou, H. Chen, X. Dong, G. Su, Z. Wang *et al.*, Superconductivity and nematic order in a new titanium-based kagome metal CsTi_3Bi_5 without charge density wave order, *Nat. Commun.* **15**, 9626 (2024).
- [30] L. Ye, M. Kang, J. Liu, F. von Cube, C. R. Wicker, T. Suzuki, C. Jozwiak, A. Bostwick, E. Rotenberg, D. C. Bell, L. Fu, R. Comin, and J. G. Checkelsky, Massive Dirac fermions in a ferromagnetic kagome metal, *Nature (London)* **555**, 638 (2018).
- [31] J.-X. Yin, W. Ma, T. A. Cochran, X. Xu, S. S. Zhang, H.-J. Tien, N. Shumiya, G. Cheng, K. Jiang, B. Lian, Z. Song, G. Chang, I. Belopolski, D. Multer, M. Litskevich, Z.-J. Cheng, X. P. Yang, B. Swidler, H. Zhou, H. Lin *et al.*, Quantum-limit Chern topological magnetism in TbMn_6Sn_6 , *Nature (London)* **583**, 533 (2020).
- [32] M. Li, Q. Wang, G. Wang, Z. Yuan, W. Song, R. Lou, Z. Liu, Y. Huang, Z. Liu, H. Lei, Z. Yin, and S. Wang, Dirac cone, flat band and saddle point in kagome magnet YMn_6Sn_6 , *Nat. Commun.* **12**, 3129 (2021).
- [33] L. Wang, E.-M. Shih, A. Ghiotto, L. Xian, D. A. Rhodes, C. Tan, M. Claassen, D. M. Kennes, Y. Bai, B. Kim, K. Watanabe, T. Taniguchi, X. Zhu, J. Hone, A. Rubio, A. N. Pasupathy, and C. R. Dean, Correlated electronic phases in twisted bilayer transition metal dichalcogenides, *Nat. Mater.* **19**, 861 (2020).
- [34] T. Devakul, V. Crépel, Y. Zhang, and L. Fu, Magic in twisted transition metal dichalcogenide bilayers, *Nat. Commun.* **12**, 6730 (2021).
- [35] C. G. Péterfalvi, A. David, P. Rakytá, G. Burkard, and A. Kormányos, Quantum interference tuning of spin-orbit coupling in twisted van der Waals trilayers, *Phys. Rev. Res.* **4**, L022049 (2022).

- [36] A. Veneri, D. T. S. Perkins, C. G. Péterfalvi, and A. Ferreira, Twist angle controlled collinear Edelstein effect in van der Waals heterostructures, *Phys. Rev. B* **106**, L081406 (2022).
- [37] L. Sun, L. Rademaker, D. Mauro, A. Scarfato, A. Pásztor, I. Gutiérrez-Lezama, Z. Wang, J. Martinez-Castro, A. F. Morpurgo, and C. Renner, Determining spin-orbit coupling in graphene by quasiparticle interference imaging, *Nat. Commun.* **14**, 3771 (2023).
- [38] Q. Rao, W.-H. Kang, H. Xue, Z. Ye, X. Feng, K. Watanabe, T. Taniguchi, N. Wang, M.-H. Liu, and D.-K. Ki, Ballistic transport spectroscopy of spin-orbit-coupled bands in monolayer graphene on WSe₂, *Nat. Commun.* **14**, 6124 (2023).
- [39] D. T. S. Perkins, A. Veneri, and A. Ferreira, Spin Hall effect: Symmetry breaking, twisting, and giant disorder renormalization, *Phys. Rev. B* **109**, L241404 (2024).
- [40] H. Yang, B. Martín-García, J. Kimák, E. Schmoranzzerová, E. Dolan, Z. Chi, M. Gobbi, P. Němic, L. E. Hueso, and F. Casanova, Twist-angle-tunable spin texture in WSe₂/graphene van der Waals heterostructures, *Nat. Mater.* **23**, 1502 (2024).
- [41] A. Abouelkomsan, E. J. Bergholtz, and S. Chatterjee, Multiferroicity and topology in twisted transition metal dichalcogenides, *Phys. Rev. Lett.* **133**, 026801 (2024).
- [42] N. Regnault, Y. Xu, M.-R. Li, D.-S. Ma, M. Jovanovic, A. Yazdani, S. S. P. Parkin, C. Felser, L. M. Schoop, N. P. Ong, R. J. Cava, L. Elcoro, Z.-D. Song, and B. A. Bernevig, Catalogue of flat-band stoichiometric materials, *Nature (London)* **603**, 824 (2022).
- [43] M. G. Yamada, T. Soejima, N. Tsuji, D. Hirai, M. Dincă, and H. Aoki, First-principles design of a half-filled flat band of the kagome lattice in two-dimensional metal-organic frameworks, *Phys. Rev. B* **94**, 081102(R) (2016).
- [44] T. Takenaka, K. Ishihara, M. Roppongi, Y. Miao, Y. Mizukami, T. Makita, J. Tsurumi, S. Watanabe, J. Takeya, M. Yamashita, K. Torizuka, Y. Uwatoko, T. Sasaki, X. Huang, W. Xu, D. Zhu, N. Su, J.-G. Cheng, T. Shibauchi, and K. Hashimoto, Strongly correlated superconductivity in a copper-based metal-organic framework with a perfect kagome lattice, *Sci. Adv.* **7**, eabf3996 (2021).
- [45] B. Field, A. Schiffrin, and N. V. Medhekar, Correlation-induced magnetism in substrate-supported 2D metal-organic frameworks, *npj Comput. Mater.* **8**, 227 (2022).
- [46] S. Kang and J. Yu, Electronic structure and magnetic properties of transition metal kagome metal-organic frameworks, *Phys. Chem. Chem. Phys.* **24**, 22168 (2022).
- [47] B. Lowe, B. Field, J. Hellerstedt, J. Ceddia, H. L. Nourse, B. J. Powell, N. V. Medhekar, and A. Schiffrin, Local gate control of Mott metal-insulator transition in a 2D metal-organic framework, *Nat. Commun.* **15**, 3559 (2024).
- [48] M. Fuchs, P. Liu, T. Schwemmer, G. Sangiovanni, R. Thomale, C. Franchini, and D. Di Sante, Kagome metal-organic frameworks as a platform for strongly correlated electrons, *J. Phys. Mater.* **3**, 025001 (2020).
- [49] A. Consiglio, T. Schwemmer, X. Wu, W. Hanke, T. Neupert, R. Thomale, G. Sangiovanni, and D. Di Sante, Van Hove tuning of AV₃Sb₅ kagome metals under pressure and strain, *Phys. Rev. B* **105**, 165146 (2022).
- [50] F. Crasto de Lima, R. H. Miwa, and E. Suárez Morell, Double flat bands in kagome twisted bilayers, *Phys. Rev. B* **100**, 155421 (2019).
- [51] T. Neupert, M. M. Denner, J.-X. Yin, R. Thomale, and M. Z. Hasan, Charge order and superconductivity in kagome materials, *Nat. Phys.* **18**, 137 (2022).
- [52] P. Fontana, M. Burrello, and A. Trombettoni, Topological van Hove singularities at phase transitions in Weyl metals, *Phys. Rev. B* **104**, 195127 (2021).
- [53] E. Wang, L. Pullasserri, and L. H. Santos, Higher-order Van Hove singularities in kagome topological bands, *Phys. Rev. B* **111**, 075114 (2025).
- [54] D. T. S. Perkins, Symmetry preservation in commensurate twisted bilayers, *Phys. Rev. B* **112**, 035410 (2025).
- [55] E. J. Mele, Commensuration and interlayer coherence in twisted bilayer graphene, *Phys. Rev. B* **81**, 161405(R) (2010).
- [56] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/8y2v-kx2w> for a summary of the Hamiltonian and electronic structure for monolayer and bilayer kagome. We demonstrate how the choice of stacking can greatly influence the electronic structure of TBK, and we present further examples of the various HOVHSs that may be engineered in TBK for both topologically trivial and nontrivial cases. We also provide details behind our numerical calculation of the Chern numbers, which required large grid sizes to accurately capture narrow avoided crossings, which also includes Ref. [74].
- [57] Y. Sheffer, R. Queiroz, and A. Stern, Symmetries as the guiding principle for flattening bands of Dirac fermions, *Phys. Rev. X* **13**, 021012 (2023).
- [58] H.-M. Guo and M. Franz, Topological insulator on the kagome lattice, *Phys. Rev. B* **80**, 113102 (2009).
- [59] R. Ciola, K. Pongsangangan, R. Thomale, and L. Fritz, Chiral symmetry breaking through spontaneous dimerization in kagome metals, *Phys. Rev. B* **104**, 245138 (2021).
- [60] S. Regmi, A. P. Sakhya, T. Fernando, Y. Zhao, D. Jeff, M. Sprague, F. Gonzalez, I. Bin Elius, M. I. Mondal, N. Valadez, D. Jarrett, A. Agosto, J. Yang, J.-H. Chu, S. I. Khondaker, X. Xu, T. Cao, and M. Neupane, Observation of flat and weakly dispersing bands in the van der Waals semiconductor Nb₃Br₈ with breathing kagome lattice, *Phys. Rev. B* **108**, L121404 (2023).
- [61] H. Zhang, Z. Shi, Z. Jiang, M. Yang, J. Zhang, Z. Meng, T. Hu, F. Liu, L. Cheng, Y. Xie, J. Zhuang, H. Feng, W. Hao, D. Shen, and Y. Du, Topological flat bands in 2D breathing-kagome lattice Nb₃TeCl₇, *Adv. Mater.* **35**, 2301790 (2023).
- [62] F. D. M. Haldane, Model for a quantum Hall effect without Landau levels: Condensed-matter realization of the “parity anomaly”, *Phys. Rev. Lett.* **61**, 2015 (1988).
- [63] S. Shallcross, S. Sharma, and O. A. Pankratov, Quantum interference at the twist boundary in graphene, *Phys. Rev. Lett.* **101**, 056803 (2008).
- [64] S. Shallcross, S. Sharma, E. Kandelaki, and O. A. Pankratov, Electronic structure of turbostratic graphene, *Phys. Rev. B* **81**, 165105 (2010).
- [65] M. G. Scheer, K. Gu, and B. Lian, Magic angles in twisted bilayer graphene near commensuration: Towards a hypermagic regime, *Phys. Rev. B* **106**, 115418 (2022).
- [66] V. C. Stangier, E. Berg, and J. Schmalian, Breakdown of the Wiedemann-Franz law at the Lifshitz point of strained Sr₂RuO₄, *Phys. Rev. B* **105**, 115113 (2022).
- [67] A. Zervou, D. V. Efremov, and J. J. Betouras, Fate of density waves in the presence of a higher-order van Hove singularity, *Phys. Rev. Res.* **5**, L042006 (2023).

- [68] M. L. Kiesel and R. Thomale, Sublattice interference in the kagome Hubbard model, *Phys. Rev. B* **86**, 121105(R) (2012).
- [69] P. K. Nag, R. Batabyal, J. Ingham, N. Morali, H. Tan, J. Koo, A. Consiglio, E. Liu, N. Avraham, R. Queiroz, R. Thomale, B. Yan, C. Felser, and H. Beidenkopf, Pomeranchuk instability induced by an emergent higher-order van Hove singularity on the distorted kagome surface of $\text{Co}_3\text{Sn}_2\text{S}_2$, [arXiv:2410.01994](#).
- [70] J. Beck, J. Bodky, M. Dürrnagel, R. Thomale, J. Ingham, L. Klebl, and H. Hohmann, Kekulé order from diffuse nesting near higher-order van Hove points, [arXiv:2410.01994](#).
- [71] L. Classen, A. V. Chubukov, C. Honerkamp, and M. M. Scherer, Competing orders at higher-order Van Hove points, *Phys. Rev. B* **102**, 125141 (2020).
- [72] G. Galeotti, F. De Marchi, E. Hamzehpoor, O. MacLean, M. Rajeswara Rao, Y. Chen, L. V. Besteiro, D. Dettmann, L. Ferrari, F. Frezza, P. M. Sheverdyaeva, R. Liu, A. K. Kundu, P. Moras, M. Ebrahimi, M. C. Gallagher, F. Rosei, D. F. Perepichka, and G. Contini, Synthesis of mesoscale ordered two-dimensional π -conjugated polymers with semiconducting properties, *Nat. Mater.* **19**, 874 (2020).
- [73] R. Pawlak, X. Liu, S. Ninova, P. D'Astolfo, C. Drechsel, J.-C. Liu, R. Häner, S. Decurtins, U. Aschauer, S.-X. Liu, and E. Meyer, On-surface synthesis of nitrogen-doped kagome graphene, *Angew. Chem. Int. Ed.* **60**, 8370 (2021).
- [74] T. Fukui, Y. Hatsugai, and H. Suzuki, Chern numbers in discretized Brillouin zone: Efficient method of computing (spin) Hall conductances, *J. Phys. Soc. Jpn.* **74**, 1674 (2005).