Gate-tunable imbalanced Kane-Mele model in encapsulated bilayer jacutingaite

Louk Rademaker$^{1}$ and Marco Gibertini$^{2,3}$

$^{1}$Department of Theoretical Physics, University of Geneva, CH-1211 Geneva, Switzerland
$^{2}$Dipartimento di Scienze Fisiche, Informatiche e Matematiche, University of Modena and Reggio Emilia, IT-41125 Modena, Italy
$^{3}$Department of Quantum Matter Physics, University of Geneva, CH-1211 Geneva, Switzerland

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We study free, capped and encapsulated bilayer jacutingaite Pt$_2$HgSe$_3$ from first principles. While the free standing bilayer is a large gap trivial insulator, we find that the encapsulated structure has a small trivial gap due to the competition between sublattice symmetry breaking and sublattice-dependent next-nearest-neighbor hopping. Upon the application of a small perpendicular electric field, the encapsulated bilayer undergoes a topological transition towards a quantum spin Hall insulator. We find that this topological transition can be qualitatively understood by modeling the two layers as uncoupled and described by an imbalanced Kane-Mele model that takes into account the sublattice imbalance and the corresponding inversion-symmetry breaking in each layer. Within this picture, bilayer jacutingaite undergoes a transition from a 0+0 state, where each layer is trivial, to a 0+1 state, where an unusual topological state relying on Rashba-like spin orbit coupling emerges in only one of the layers.

I. INTRODUCTION

Topological insulators have a finite gap in their bulk energy spectrum, but differ from standard (trivial) insulators because a non-zero topological invariant is associated with the manifold of occupied states [1, 2]. In most cases, the non-trivial topological invariant results in the appearance of metallic states that cross the bulk gap close to the boundary of a finite-size system. The nature of the topological invariant depends on the dimensionality and the underlying fundamental symmetries of the system [3, 4], including crystal symmetries [5, 6]. A paradigmatic example is the integer quantum Hall state in two dimensions (2D), for which the topological invariant is a non-negative integer $C$ —known as Chern number— which provides the number of (chiral) states localized close to each edge and is related to the quantized Hall conductivity $\sigma_{xy} = C e^2/h$ [7, 8].

When time-reversal symmetry is preserved in 2D, although the Chern number vanishes identically, another topological invariant $\nu$ can be introduced [9–12], which is a $Z_2$ number that can assume only two values: 0 or 1, i.e. trivial or non-trivial. As a consequence of time-reversal symmetry, gapless states appear at the edges of the system in pairs of counter-propagating (helical) modes and a bulk-boundary correspondence relates $\nu$ to the parity of the number of such pairs. In particular, we have that an even number of helical pairs is topologically trivial ($\nu = 0$), as states belonging to different pairs can be mixed and adiabatically gapped out without breaking time-reversal symmetry. On the contrary, time-reversal-invariant topological insulators ($\nu = 1$), also known as quantum spin Hall insulators (QSHIs), have an odd number of pairs, so that the presence at each edge of at least one pair of helical gapless states is robust.

Experimental realizations of the QSHI phase have been reported in semiconductor quantum wells based on HgTe/CdTe [13–16] and InAs/GaSb [17, 18] heterostructures, as well as in 2D materials like WTe$_2$ [19–22]. In all these systems, the operating conditions where transport is dominated by edge states are limited to fairly low temperatures owing to their small bulk energy gap. A breakthrough could be represented by monolayer Pt$_2$HgSe$_3$, which has been predicted using first-principles simulations to be the first materials realization of the seminal Kane-Mele model [9, 10] for QSHIs, with a substantial energy gap of 0.5 eV [23]. Although monolayers of this material could be potentially exfoliated [24] from a bulk layered mineral called jacutingaite [25, 26], a clear experimental validation is still lacking [27].

When two QSHI monolayers are stacked together to form a bilayer, the system is expected to become trivial in the limit of weak interlayer coupling. Indeed, when the layers are almost independent, we inevitably have an overall even number of helical pairs that can hybridize and get gapped out, consistently with the fact that the bulk topological invariant is defined only modulo two, so that $\nu_{\text{bi}} = \nu_{\text{mono}} + \nu_{\text{mono}} = 1+1 = 0 \mod 2$. Analogously, a trilayer should be non-trivial, and for thicker layers we would expect an alternation of trivial and non-trivial topology that, in the bulk limit, would give rise to a weak topological phase [28] relying on the translational invariance along the stacking direction.

In bulk jacutingaite, the layers can not be considered as nearly independent, so that this scenario is expected to break down. Indeed, first-principles simulations have shown that nearby layers are strongly hybridized, giving rise to a large second-nearest layer hopping [29]. This strong coupling drives bulk jacutingaite into a semimetallic state endowed with a dual topology [29–31] that combines a non-zero mirror Chern number with a weak topology. Recent experiments have verified both the semimetallic nature of bulk Pt$_2$HgSe$_3$ [32] and the presence of surface states protected by the crystalline mirror symmetry [33].

Here we consider bilayer jacutingaite and predict us-
ing first-principles simulations that it is trivial, although
in an unexpected way, with \( \nu_{\text{bi}} = 0 + 0 \). The trivial
gap arises from an inversion-symmetry breaking in each
layer, with competing contributions from a structural
distortion that makes the two Hg atoms inequivalent and
the different environment affecting intra-sublattice hop-
ping. As a result of this sublattice imbalance, the Kane-
Mele term that drives the topological nature of mono-
layer jacutingaite\cite{23} is replaced by a spin-orbit coupling
that has the same sign on the two sublattices. When en-
capsulated in hexagonal boron nitride (h-BN), the trivial
gap is strongly reduced and can be turned topological by
a small perpendicular field, promoting bilayer Pt\(_2\)HgSe\(_3\)
into a promising system for experimental explorations.

II. BILAYER STRUCTURES

Jacutingaite comprises AA-stacked honeycomb lattices
of Hg atoms, where the A (B) sublattice is positioned
above (below) a plane of Pt atoms (see Fig. 1). In the ab-
sence of spin-orbit coupling, the electronic band structure
of monolayer jacutingaite contains gapless Dirac cones at
the corners \( K \) and \( K' \) of the hexagonal Brillouin zone \cite{23},
similarly to what happens in graphene. These cones can
be gapped in two different ways. The first is by break-
ning the sublattice (inversion) symmetry, e.g. by making
the Hg distance to the Pt planes different on the two
sides, leading to a trivial insulator. The second way to
open a gap is via Kane-Mele spin-orbit coupling, making
monolayer jacutingaite a quantum Hall insulator.

In bilayer jacutingaite, although a global inversion
symmetry connecting the two layers is still present, there
is no inversion symmetry \textit{per layer}, i.e. the two sublat-
tices in each layer are no longer equivalent. This means
that Hg atoms can be displaced to make each layer by
itself trivial \( \nu_{\text{bi}} = 0 + 0 = 0 \). If no or only small displace-
ments occur and the two layers are almost independent,
however, the combination of two topological monolayers
together makes the bilayer trivial - following the heuristic
rule \( \nu_{\text{bi}} = 1 + 1 = 0 \). In either case, bilayer jacutingaite
is expected to be a trivial insulator.

To confirm this, we perform first principles density-
functional theory (DFT) calculations of various
few-layered jacutingaite structures using QUANTUM
ESPRESSO \cite{34,35}, with a Coulomb cut-off \cite{36} to
reproduce the correct open boundary conditions in the
vertical direction and the van-der-Waals compliant func-
tional vdw-DF-cx \cite{37,38,39} that gives the best agreement
with Raman experiments for the vibrational frequencies
of bulk jacutingaite \cite{32} (for further details of the
calculations see App. A). The unit cell is hexagonal
(point group \( D_{3d} \) or \( 3m \)) with in-plane lattice constant
fixed to the bulk relaxed value \( a = 7.384 \text{ Å} \).

We first relax the structure of a free-standing bilayer,
which shows a large shift in the vertical position of the
outer Hg atoms. The distance of the Hg atoms to the Pt
planes increases from 1.73 Å in the monolayer to 2.02 Å
for the outer Hg atoms. The sublattice asymmetry is re-
sponsible for a large trivial \( \nu_{\text{bi}} = 0 + 0 = 0 \) band-gap of
290 meV at the \( K \) point. The same level of displacement
is found in trilayer jacutingaite, however, the trilayer is
semimetallic owing to a large second-nearest layer hop-
ping between the outer layers, similarly to what happens
in the bulk \cite{29}. See Table I for an overview of the Hg po-
sitions and bandgaps of the different studied structures.

The bandgap in free bilayer jacutingaite is so large
that a topological transition cannot be obtained using
reasonable perpendicular external electric fields (up to
1 V/Å), unlike monolayer jacutingaite which has a trans-
ition at \( E_{\text{ext}} = 0.36 \text{ V/Å} \). This is because the external
electric field is never sufficient to reduce the sublattice
asymmetry. We note in passing that these values do not
 correspond to a potential drop across the system (e.g.\( E_{\text{ext}} = 1 \text{ V/Å} \) does not correspond to 1 V over 1 Å),
as in first-principles simulations we can set only the ex-
ternal electric field (related the dielectric displacement
\( D \) through \( E_{\text{ext}} = 4\pi D \)), and not the total electric field
as in experiments (through the gate voltages applied to

egin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1}
\caption{Top and lateral views of the crystal structure of h-BN encapsulated bilayer jacutingaite. In the top view, the green shaded area highlights the hexagonal Wigner-Seitz unit cell and the (buckled) honeycomb lattice formed by Hg atoms. Notice that the two sublattices are above/below a plane of Pt atoms. Two Wannier functions associated with the two sublattices of the upper layer are also reported as isosurfaces for both positive (blue) and negative (red) values. The Wannier functions associated with the bottom layer can be simply obtained by inversion symmetry.}
\end{figure}
TABLE I. Main properties of various layered jacutingaite structures. Monolayer and bulk have been studied before, here we show new results for free, capped, and encapsulated bilayers, as well as for trilayer Pt\textsubscript{2}HgSe\textsubscript{3}. The second column contains the gap at $\mathbf{K}$ obtained using DFT. The third column contains the $z$-position of the Hg atoms relative to the nearest Pt plane (see Fig. 1). Notice that in capped, encapsulated, and the trilayer case the position depends on the layer (abbreviated “l.”).

| System      | Gap at $\mathbf{K}$ | $\Delta z$ Hg-Pt |
|-------------|---------------------|------------------|
| Bulk        | < 1 meV             | 1.84 Å           |
| Monolayer   | 168 meV             | 1.73 Å           |
| Bilayer     | 290 meV             | 1.81 Å (inner Hg) |
|             |                     | 2.02 Å (outer Hg) |
| BN/Bilayer  | 44 meV              | 1.78 Å (outer Hg, capped l.) |
|             |                     | 1.80 Å (inner Hg, capped l.) |
|             |                     | 1.78 Å (inner Hg, free l.) |
|             |                     | 1.90 Å (outer Hg, free l.) |
| BN/Bilayer/BN | 27 meV          | 1.80 Å (inner Hg) |
|             |                     | 1.78 Å (outer Hg) |
| Trilayer    | < 1 meV             | 1.84 Å (middle l.) |
|             |                     | 1.81 Å (inner Hg, outer l.) |
|             |                     | 2.02 Å (outer Hg, outer l.) |

electrodes at the two sides of the system).

A possible way to restore sublattice symmetry, and thus to make a topological transition more feasible—at least in one layer, is to suppress the lattice distortion by encapsulating one side of bilayer jacutingaite with h-BN. As can be seen in Table I, this indeed reduces the sublattice asymmetry in one of the layers and reduces the gap. However, the system is still $0 + 0 = 0$ trivial and fields up to 1 V/Å do not induce a topological transition - instead they make the system metallic, with a charge transfer from the bilayer to h-BN.

On the other hand, the reduction in gap size suggests that fully encapsulating bilayer jacutingaite with h-BN might bring us to the regime where we can induce a topological transition via an electric field. We indeed find that the Hg positions are nearly symmetrical in h-BN encapsulated bilayers. Furthermore, the gap is reduced to only 27 meV, which brings us in the regime that allows for a topological transition.

III. BAND STRUCTURE AND WANNIERIZATION

We will now discuss in-depth the properties of the encapsulated bilayer structure. For simplicity, we locate the h-BN layers on the two sides of the bilayer so that, in the absence of an external electric field, the total system again contains inversion symmetry, and we let only the vertical position of the h-BN layers relax. The full band structure is shown in the top panel of Fig. 2 for $E_{\text{ext}} = 0$, where all bands are doubly degenerate as a consequence of time-reversal and inversion symmetry. Whereas the bandwidth of the four main bands is about 1 eV, the bandgap is only 27 meV.

When a finite external electric field $E_{\text{ext}}$ is applied, the gap at $\mathbf{K}$ reduces, until it closes at about $E_{\text{ext}} = 0.3$ V/Å, as shown in the lower central panel of Fig. 2. At larger fields, the gap opens again with clear signatures of band inversion. Note that at zero field all bands are double degenerate due to inversion symmetry, whereas at nonzero fields this degeneracy is lifted.

To elucidate if the band inversion is associated with a topological phase transition, we map first-principles eigenstates for the bands facing the energy gap into a set of maximally-localized Wannier functions (WFs) [40] using Wannier90 [41]. The Hg s-orbitals are used as first projections to initialize the Wannierization procedure. We thus end up with four WFs (eight by including spin), two per layer, that are depicted in Fig. 1 for the top layer when $E_{\text{ext}} = 0$. While for the external sublattice the WF is similar to the one of the monolayer [23] and it is well localized on just one layer, the inner WF has significant contributions from orbitals in the opposite layer, signaling a strong hybridization between the layers similarly to what happens in bulk jacutingaite [29]. As a result, the center of the inner WFs is significantly shifted in the z-direction such that the center of the top WF of
the bottom layer is higher than the one of the bottom WF of the top layer.

From the knowledge of the WFs, we can easily compute the \(Z_2\) topological invariant using WannierTools [42] by monitoring the evolution of the Wannier charge centers (WCCs) over half of the Brillouin zone [43, 44], i.e. the expectation value of the coordinate along one direction of hybrid WFs [45] as a function of momentum in the remaining direction, along which they are delocalized. The \(Z_2\) invariant \(\nu\) can be then obtained by considering the parity of the number of times an arbitrary curve going from \(k = 0\) to \(k = 0.5\) (in units of the primitive reciprocal lattice vector in that direction) crosses the WCC lines [43, 44]. As shown in Fig. 3, this confirms the presence of a topological transition as a function of the external electric field (see Fig. 4d and e for the WCC evolution at small and large fields). In particular, while the system is trivial (\(\nu = 0\)) in the absence of external fields (confirmed also using a parity approach [46]), it becomes a QSHI (\(\nu = 1\)) when \(E_{\text{ext}} > 0.3 \text{ V/Å}\), showing that the topological state of bilayer jactungaïte can be easily manipulated.

The mapping of the first-principles results into WFs can be beneficial also to extract an effective tight-binding model that describes the behavior of bilayer jactungaïte, helping to gain additional physical insight into the mechanisms underlying the topological transition. The resulting eight-band model (including spin) involves the sites of two buckled honeycomb lattices—one for each layer—with one orbital per site and spin (given by the WFs in Fig. 1). We find that even though the WFs associated with the inner sublattices are delocalized over the two layers (see Fig. 1 and the discussion above), the effective tight-binding model is still dominated by intralayer terms.

In Table II we summarize the most important terms of the effective tight-binding model when \(E_{\text{ext}} = 0\). The two largest contributions are by far the intralayer nearest-neighbor (NN) hopping \(t = 233 \text{ meV}\) and the sublattice symmetry breaking on-site term \(m = 135 \text{ meV}\). The absence of layer inversion symmetry allows a NN (Rashba-like) spin-orbit coupling \(\lambda_R\) that is vanishing in isolated monolayers.

The most important contribution that couples the two layers is a NN hopping \(t_1 \sim 50 \text{ meV}\), which—together with the other relevant interlayer term \(t_2\) in Table II—plays a minor role on the band structure. To verify this, we calculated the band-structure using the full tight-binding model with and without interlayer coupling. The result is shown in Fig. 4. In the absence of a perpendicular field, the band-structure is marginally changed: removing the interlayer coupling mainly reduces the gap at \(\textbf{K}\). The interlayer coupling can therefore be neglected for a qualitative understanding of the topological transition.

An external field now reduces the gap further in the top layer whereas it increases the gap in the bottom layer (Fig. 4). This is indicative of the topological transition that goes from \(\nu = 0 + 0\) to \(\nu = 0 + 1\) state. Indeed, Fig. 4d (e) shows the evolution of the WCCs at small (large) external field. In both cases the WCCs of the full model (black) are consistent with the WCC computed for the separate layers (blue and red), thus justifying the assumption that the topological invariant can be expressed as the sum of the invariants in the two layers, \(\nu_{\text{total}} = \nu_1 + \nu_2\). Moreover, while at small fields both layers are trivial (and related by inversion symmetry), at large fields the layers are no longer equivalent and the top layer (red) is non-trivial after the gap re-opens at \(\textbf{K}\).

Within each layer, the inequivalence of the two sublattices not only makes the on-site energy very different (as expressed by \(m\)), but also introduces a large imbalance in the intralayer next-nearest neighbor (NNN) hopping terms. This arises as a result of the different (de)localization of the Wannier orbitals for the inner and

| Coupling          | Proportional to          | Value [meV] |
|-------------------|--------------------------|-------------|
| Onsite potential  | \(\sigma^z \tau^z\)      | 135         |
| NN intralayer     | \(\sigma^{3\text{NN}}\)  | 233         |
| NN Rashba \(\lambda_R\) | \(s^{z\text{NN}} \sigma^z \tau^z\) | 10          |
| NN interlayer     | \(\sigma^z \sigma^{2\text{NN}}\) | 53          |
| NNN intralayer    | \((1 - \sigma^z \tau^z)\) | -34 (outer) |
| NNN interlayer    | \((1 + \sigma^z \tau^z)\) | 32 (inner)  |
| NNN Rashba \(\lambda_R\) | \(s^{z\text{NN}}(\sigma^z - \tau^z)\) | -20 (inner) |
| NNN Kane-Mele \(\lambda_{\text{KMN}}\) | \(\sigma^z \sigma^{2\text{NN}}(1 - \sigma^z \tau^z)\) | -16 (outer) |
| NNN interlayer    | \(\tau^{z\text{NN}}\)    | -20         |
FIG. 4. Bilayer jacutingaita can be qualitatively understood as two decoupled layers. a: To verify this, we calculated the gap at $K$ as a function of external field for the individual layers using the tight-binding model with interlayer couplings set to zero. Though the gap is quantitatively underestimated (compare Fig. 3, we still find a topological transition in the top layer. b: The dispersion close to $K$ changes only subtly when we have interlayer coupling (black) or not (red/blue dashed lines), at zero field. c: At a finite external field of $E_{\text{ext}} = 0.46$ V/Å, the dispersion for just the top layer (red) and bottom layer (blue) has still a large overlap with the full bilayer band-structure. d: The WCCs (in units of the lattice parameter $a$) computed for the full tight-binding model (black) are the same as the WCCs computed per layer (red and blue). e: Same calculation as in d, but now at a finite field $E_{\text{ext}} = 0.46$ V/Å. We clearly see the topological nature of the bands in the top layer (red).

outer sublattice sites. A first important example of NNN term is the hopping energy $t_2$ that takes approximately opposite values for the inner and outer sublattices. In particular, we find that $t_2$ is positive for the outer sites similarly to what happens in monolayer $Pt_2HgSe_3$, while it is negative for inner sites in complete analogy with bulk jacutingaita. This effectively staggered NNN hopping term gives rise to a trivial gap at $K$ that is found to compete with the trivial gap associated with the on-site $m$ (see also below). This compensation is almost perfect in h-BN encapsulated bilayers (contrary to the free-standing case), thus explaining the very small trivial gap at $K$.

Even more compelling, the imbalance affects also two additional NNN spin-orbit terms: a Kane-Mele [9, 10] and in-plane Rashba-like [47] spin-orbit coupling. Also in this case, these terms retain values very close to the one in the monolayer for the outer sublattices, while they are strongly suppressed for the inner sublattices, in analogy with bulk jacutingaita where the effect of spin-orbit coupling is almost negligible [29–31]. Traditionally, topological transitions were understood in terms of spin-orbit couplings that were identical on both sublattices [9, 10]. In bilayer jacutingaita, however, the fact that the spin-orbit coupling is different on the two sublattices requires an extension of the original Kane-Mele model.

IV. IMBALANCED KANE-MELE MODEL

As argued in the previous section, the topological transition can be qualitatively understood by decoupling the two layers and focusing on the top layer only. We will now explore the question of whether we can understand the transition purely in terms of a short-ranged hopping model. To this end, we introduce the so-called imbalanced Kane-Mele model, which contains nearest ($t$) and a staggered next-nearest neighbor hopping ($t_2$), a sublattice symmetry breaking potential ($m$) and two spin-orbit terms, see Fig. 5. In addition to the regular Kane-Mele (KM) term $\lambda_{\text{KM}} \sum_{\langle ij \rangle} \nu_{ij} c_{i}^{\dagger} s^z c_{j}$, which has oppo-
site sign on the two sublattices, we include a sublattice-symmetric Kane-Mele term $\lambda_{KM}$,
\[ i\lambda_{KM} \sum_{\langle ij \rangle} \nu_{ij} c_i^\dagger \sigma^z s^z c_j. \]  
This term, as is shown in Fig. 5, has the same sign of the spin-orbit coupling term on the two sublattices. As a consequence, the effective spin-orbit coupling on the two sublattices given by $\lambda_{KM} \pm \nu_{KM}$.

In momentum space, the regular KM term is proportional to $\lambda_{KM} d(k) \sigma^z s^z$ where $d(k) = 2 \sin(k_x a) - 4 \sin(k_x a/2) \cos(\sqrt{3} k_y a/2)$, if we define the honeycomb lattice with lattice vectors $\mathbf{a}_{1,2} = \frac{1}{2} (\pm 1, \sqrt{3})$. Consequently, the sublattice-symmetric KM term is proportional to $\lambda_{KM} d(k) s^z$. As a result, at the $K$ and $K'$ points, the Hamiltonian reads
\[ H = (m - 3t_2) \sigma^z + 3\sqrt{3} \lambda_{KM} \kappa \sigma^z s^z + 3\sqrt{3} \lambda_{KM} \kappa s^z \]  
where $\kappa = \pm 1$ for the $K/K'$ valley. In the absence of spin-orbit coupling, the trivial gap at $K$ is determined by the sublattice potential reduced by the staggered nearest-neighbor hopping, $m - 3t_2$. For $\lambda_{KM} > \lambda_{KM}' > 0$, the gap is insensitive to the sublattice-symmetric KM term, and given by $\Delta = |m - 3t_2| - 3\sqrt{3} \lambda_{KM}$. As long as this parameter $\Delta$ is positive, the system is trivial, and for $\Delta < 0$ the model is a quantum spin Hall insulator with $\nu = 1$. When the two spin-orbit terms are exactly equal, $\lambda_{KM} = \lambda_{KM}'$, the system realizes a semimetal with quadratic band-touching as long as $\Delta < 0$. If the sublattice-symmetric KM term dominates, $\lambda_{KM} < \lambda_{KM}'$, the system is either metallic ($\Delta' < 0$) or a trivial insulator ($\Delta' > 0$), with $\Delta = |m - 3t_2| - 3\sqrt{3} \lambda_{KM}'$.

When also the NN Rashba spin-orbit coupling
\[ i\lambda_{R} \sum_{\langle ij \rangle} c_i^\dagger (s \times d_{ij}) \sigma^z c_j \]  
(arising from the inversion symmetry breaking in each layer) is included, not only a finite gap is opened in the semimetallic phase when $\lambda_{KM} < \lambda_{KM}'$, but also a nontrivial topological phase emerges for $m - 3t_2 < \lambda_{KM}$. When $m - 3t_2$ further decreases the gap closes again (away from $K/K'$ at 3 Dirac cones around each corner of the Brillouin zone) and the system enters a trivial phase adiabatically connected to the one for $\Delta' > 0$ when $\lambda_{R} = 0$. The topological phase thus survives over a finite interval of values of $m - 3t_2$, whose extension increases with $\lambda_{R}$ and is non-vanishing only when $m - 3t_2$ has the same sign as $\lambda_{KM}'$, even in the limit $\lambda_{KM} \to 0$.

From Table II it follows that in bilayer jactatingaite the sublattice-symmetric KM term dominates: $\lambda_{KM} = 9$ meV while $\lambda_{KM} = 7$ meV (their sum is the ‘outer’ sublattice Kane-Mele term while their difference the inner). In the absence of a field, the sublattice potential $m$ controls the physics and we expect a trivial insulator. A perpendicular electric field affects the value of $m$ and $t_2$, because of the different z-positions of the Wannier orbitals. In particular, by wannierizing the electronic structure at different $E_{ext}$, we find that the onsite potential and the staggered hopping $t_2$ change linearly with field, approximately as $\Delta m = - 135$ meV per V/$\text{Å}$ and $\Delta t_2 = 9$ meV per V/$\text{Å}$. This change has opposite sign in the two layers, making the bottom layer having a larger trivial gap upon the application of a field, whereas the top layer reduces the gap.

Consistently with the results above, the imbalanced Kane-Mele thus predicts that the bottom layer remains trivial with just an increasing gap at $K$, while in the top layer the gap decreases and closes at a critical value when the field is such that $m - 3t_2 = \lambda_{KM}'$, in qualitative agreement with Fig. 4a). When $E_{ext}$ is further increased, the gap re-opens and the top layer is in a topologically non-trivial state ($\nu = 1$), protected by the NN Rashba $\lambda_{R}$. This prediction is validated by the fact that without spin-flipping inter-sublattice hopping terms (such as $\lambda_{R}$), no topological transition occurs even in the full WF tight-binding model. Of course, longer-range and inter-layer hopping terms in the full model play a role in the quantitative determination of energy gaps and transition fields, but the imbalanced Kane-Mele is sufficient to describe the essential physical features of the topological transition occurring in encapsulated bilayer jactatingaite.

V. OUTLOOK

We predict that h-BN encapsulated bilayer Pt$_2$H$_2$Se$_3$ undergoes a topological transition under the application of an electric field, from a trivial insulator at zero field to a quantum spin Hall insulator. The transition can be qualitatively understood by considering the layers as decoupled and described by an imbalanced Kane-Mele model, with a new, sublattice-symmetric next-nearest-neighbor spin-orbit coupling. This additional term emerges from the inversion-symmetry breaking in each layer associated with the inequivalence of the two sublattices. This imbalance also allows for a non-zero Rashba spin-orbit coupling that plays an essential role in stabilizing the topological phase at large fields.

Jactatingaite has been predicted to be potentially exfoliable [23, 24], and consequently bilayer jactatingaite can also appear during an exfoliation process. Recently, experiments have shown that this is possible [27], although the quality of the exfoliated samples needs to be improved. If encapsulated, this could lead to the construction of a gate-switchable topological insulator (off at zero field, on at finite field), which is complementary to the monolayer case (on at zero field, off at finite field) [23].

VI. ACKNOWLEDGEMENTS

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Appendix A: Calculation details

As mentioned in the main text, all first-principles DFT calculations were performed using the QUANTUM ESPRESSO suite of codes [34, 35]. Structural relaxations were carried out using the van-der-Waals compliant vdW-DF-cx [37–39] functional without spin-orbit coupling, with pseudopotentials from the Standard Solid State Pseudopotential library [48] (efficiency version 1.0), with an energy cutoff of 60 Ry for wavefunctions and 480 Ry for the density. The Brillouin zone was sampled with \(8 \times 8 \times 1\) k-points of a uniform \(\Gamma\)-centered Monkhorst-Pack grid with a cold smearing of 0.015 Ry [49]. Band structures were computed by including spin-orbit coupling through fully-relativistic pseudopotentials of the Pseudo-Dojo family [50] with a wavefunction cutoff of 80 Ry on top of self-consistent calculations with \(12 \times 12 \times 1\) k-points within the generalized gradient approximation [51].

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