Saddle-point von Hove singularity and dual topological insulator state in Pt$_2$HgSe$_3$

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Saddle-point von Hove singularities in the topological surface states are interesting because they can provide a new pathway for accessing exotic correlated phenomena in topological materials. Here, based on first-principles calculations combined with a k · p model Hamiltonian analysis, we show that the layered platinum mineral jacutingaite (Pt$_2$HgSe$_3$) harbours saddle-like topological surface states with associated von Hove singularities. Pt$_2$HgSe$_3$ is shown to host two distinct types of nodal lines without spin-orbit coupling (SOC) which are protected by combined inversion (I) and time-reversal (T) symmetries. Switching on the SOC gaps out the nodal lines and drives the system into a topological insulator state with nonzero weak topological invariant $Z_2 = (0;001)$ and mirror Chern number $n_{\text{M}} = 2$. Surface states on the naturally cleaved (001) surface are found to be nontrivial with a unique saddle-like energy dispersion with type II von Hove singularities. We also discuss how modulating the crystal structure can drive Pt$_2$HgSe$_3$ into a Dirac semimetal state with a pair of Dirac points. Our results indicate that Pt$_2$HgSe$_3$ is an ideal candidate material for exploring the properties of topological insulators with saddle-like surface states.

I. INTRODUCTION

Finding new topological materials with unique properties is currently drawing intense interest as an open research frontier in condensed matter physics and related fields.$^{1-3}$ Initial ideas of time-reversal symmetry (T) protected topological states have been generalized to incorporate crystal symmetries, leading to the identification of a variety of new topological states in insulators, semimetals, and metals.$^{4-8}$ Examples include mirror-symmetry protected topological crystalline insulators (TCIs), weak topological insulators (WTIs), Dirac/Weyl semimetals, nodal line semimetals, hourglass semimetals, triple-point semimetals, among others.$^{9-20}$ Theoretically predicted topological properties of a number of materials have been demonstrated experimentally via spectroscopic and transport measurements.$^{21-28}$ It has been recognized that a topological state can also be protected simultaneously by different crystal symmetries as is the case in Bi$_2$(Se, Te)$_3$ where the protection involves both T and crystalline mirror symmetries.$^{29,30}$ Such dual symmetry protected topological states can open up new possibilities for tuning topological properties via controlled symmetry breaking.

Topological surface states (TSSs) are the hallmark and source of numerous useful properties in topological quantum materials. Depending on the symmetries of their crystalline surfaces, the electronic dispersion ($E_k$) of TSSs can deviate substantially from the well-known Dirac-like form.$^{31}$ Specifically, when a surface lacks $C_{n\psi}$ with $n > 2$ rotational symmetry, the saddle-like $E_k$ dispersion with saddle points is allowed by symmetry constraints. These saddle points in k-space lead to Van Hove singularities (VHSs) where densities of states (DOSs) diverge logarithmically in two-dimensions (2D). The importance of VHSs has been revived recently in the theory of correlated twisted bilayer graphene and, in fact, the new concept of higher order VHSs has been proposed.$^{32-34}$ More generally, when VHSs lie close to the Fermi level, the increased DOS amplifies electron correlation effects that can drive various quantum many-body instabilities involving the lattice, charge and spin degrees of freedoms.$^{35-38}$ When these VHSs lie at generic k points, they favor an odd-parity pairing, which can lead to unconventional superconductivity in the topological materials.$^{39,40}$ Despite theoretical prediction of TSSs with VHSs, experimental evidence of such states is still lacking. The identification of new materials with saddle-like TSSs is thus of great importance.

In this paper, we investigate the topological electronic structure of layered platinum mineral jacutingaite Pt$_2$HgSe$_3$ and reveal a dual-symmetry-based protection of its topological state and the existence of saddle-point VHSs in the surface electronic spectrum. The monolayer Pt$_2$HgSe$_3$ has been predicted recently as a large band gap Kane-Mele quantum spin Hall (QSH) insulator.$^{41}$ A non-
trivial band gap of 0.53 eV was reported within the G0W0 approximation: its Fermiology under electron and hole doping suggests the existence of VHSs and unconventional superconductivity.\textsuperscript{42} The QSH state in Pt\textsubscript{2}HgSe\textsubscript{3} monolayer has been experimentally demonstrated using scanning tunneling microscopy (STM).\textsuperscript{43} Also, it is found that few nanometers thick as well as bulk jacutingaite is stable under ambient conditions on a timescale of months and even to a year.\textsuperscript{43} However, the bulk topological state and the associated TSSs with VHSs remain unexplored.

Our analysis reveals that Pt\textsubscript{2}HgSe\textsubscript{3} supports two distinct types of nodal lines when spin-orbit coupling (SOC) effects are ignored. Including SOC effects in the computations gaps out the nodal lines and drives the system into a topological insulator state characterized by nonzero weak topological invariants $Z_2 = (0; 001)$, as well as the mirror Chern number $n_M = 2$. To highlight the nontrivial bulk band topology, we calculate the naturally cleavable (001) surface electronic structure and show the existence of a unique symmetry allowed saddle-like $E_k$ dispersion of topological surface state with saddle-point VHSs. Informed by our first-principles computations, we present a viable $k.p$ model Hamiltonian for the topological surface states. We also investigate the effect of hydrostatic pressure on bulk band topology and discuss a topological phase transition to a type-II Dirac semimetal.

The remainder of the paper is organized as follows. In Sec. II, we discuss computational details along with the crystal structure of Pt\textsubscript{2}HgSe\textsubscript{3}. The bulk topological properties are discussed in Sec. III. In section IV, we characterize the topological state and present surface electronic spectrum by constructing a ten layer thick slab with a vacuum region of 16 Å to avoid interactions between periodically repeated images using the VASP suite of codes.\textsuperscript{45,47,50}

functions and computed topological properties using the WannierTools package.\textsuperscript{48,49} We further calculated surface electronic spectrum by constructing a ten layer thick Pt\textsubscript{2}HgSe\textsubscript{3} slab with a vacuum region of 16 Å to avoid interactions between periodically repeated images using the VASP suite of codes.\textsuperscript{45,47,50}

![Diagram](image)

**FIG. 1:** (a) Side and (b) top view of the layered crystal structure of Pt\textsubscript{2}HgSe\textsubscript{3}. Pt(1) and Pt(2) denote two symmetry inequivalent Pt atoms in the unit cell. (c) Bulk and projected (100) and (001) surface Brillouin zones. Various high-symmetry points are marked.

Jacutingaite Pt\textsubscript{2}HgSe\textsubscript{3} forms a bipartite lattice (containing two sublattices) with the trigonal space group $P\overline{3}m1$ (No. 164).\textsuperscript{51} The crystal structure is layered which can be viewed as a $2 \times 2 \times 1$ supercell of 1T-PtSe\textsubscript{2} with additional Hg atoms that are placed in the anti-cuboctahedral voids of Se atoms [Figs. 1(a)-(b)]. There are two symmetry inequivalent Pt atoms in the primitive unit cell that form two distinct hexagonal sublattices. The Pt(1) atom connects to six nearest Se atoms and forms Pt(1)Se\textsubscript{6} local octahedral coordination while the Pt(2) atom constitutes Pt(2)Se\textsubscript{4} square structure.\textsuperscript{51,52} The Pt(1)-Se bond length is 2.55 Å which is slightly larger than the Pt(2)-Se bond length of 2.47 Å. This crystal structure has three-fold rotation symmetry around $z$-axis $\{C_3\}$, inversion symmetry $I$, and mirror symmetry $\{m_{100}\}$. Additionally, it respects $T$ symmetry.

II. COMPUTATIONAL DETAILS AND CRYSTAL STRUCTURE

Electronic structure calculations were performed within the framework of density functional theory (DFT) with the projector-augmented-wave (PAW) pseudopotentials and a plane wave basis set using Quantum Espresso package.\textsuperscript{44–46} We used an energy cut-off of 50 Ry for the plane wave basis set and a $9 \times 9 \times 8$ $k$ mesh for the bulk Brillouin zone integration. The generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof (PBE) was used to include the exchange-correlation effects.\textsuperscript{47} A tolerance of $10^{-8}$ Ry was used for electronic energy minimization. All the atomic positions were optimized until the residual forces on each atom become less than $10^{-3}$ Ry/au. We constructed a tight binding model Hamiltonian by deploying atom-centered Wannier functions and computed topological properties using the WannierTools package.\textsuperscript{48,49} We further calculated surface electronic spectrum by constructing a ten layer thick Pt\textsubscript{2}HgSe\textsubscript{3} slab with a vacuum region of 16 Å to avoid interactions between periodically repeated images using the VASP suite of codes.\textsuperscript{45,47,50}

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Pt momenta points highlighted by gray boxes in the main fig-
K for bands near the Fermi energy. The inset in (a) and (b) show
tions at time-reversal invariant momentum points are marked
with spin-orbit coupling (SOC). The irreducible representa-
FIG. 2: Bulk band structure of Pt\(_2\)HgSe\(_3\) (a) without and (b)
with spin-orbit coupling (SOC). The irreducible representa-
tions at time-reversal invariant momentum points are marked
for bands near the Fermi energy. The inset in (a) and (b) show
the closeup of the in-plane energy dispersion near K and H
momentum points highlighted by gray boxes in the main fig-
ure. A clear gap emerges at K and H points with SOC in
(b). (c) and (d) show the orbital resolved band structure of
Pt\(_2\)HgSe\(_3\) without and with SOC, respectively.

III. BULK ELECTRONIC STRUCTURE AND
TOPOLOGICAL INVARIANTS

The bulk electronic spectrum of Pt\(_2\)HgSe\(_3\) without
SOC is shown in Fig. 2(a). It is semimetallic in charac-
ter where the \(A_u(A_g)\) symmetry band is seen to cross
with the \(B_g(B_u)\) band at the \(K(H)\) point in the bulk
BZ. These band crossings are linearly dispersed over a
substantial energy range along \(\Gamma M K\Gamma\) (ALHA) plane
directions. Similar Dirac-cone-like band features are also
there in the band structure of graphite and their origin is
attributed to the honeycomb lattice arrangements of the
constituents atoms.\(^{53}\) The orbital resolved band structure
in Fig. 2(c) shows that crossing bands are mainly
contributed by Hg s, Se p, and Pt \(d_{xz}\) and \(d_{yz}\) atomic
orbitals. The band structure with SOC is illustrated in
Fig. 2(b) and Fig. 2(d). The Dirac-cone-like band cross-
ings without SOC at \(K\) and \(H\) points are now gapped
and a continuous band gap appears between the valence
and conduction bands.

In order to characterize the nodal lines and their sym-
metry protection, we systematically examine the band
crossings in Fig. 3. A careful inspection of band cross-
ings in full bulk BZ reveals that Pt\(_2\)HgSe\(_3\) hosts two dis-
tinct types of nodal lines. The type I nodal lines (identi-
fied by NL\(_C\)) are generated by accidental band crossings
and form an inversion symmetric pair of closed loops at
generic \(k\) points around the \(\Gamma\) – \(A\) line inside the BZ.
Importantly, these nodal lines are not hooked to a fixed
momentum plane but trace an arbitrary path encircling the
\(\Gamma A\) line [see red and blue curves in Fig. 3(a)]. They
show considerable energy spread in the momentum space
as illustrated in Fig. 3(b) where the energies of the gap
closing points are plotted with color in the \(k_x – k_y – k_z\)
momentum space. We further demonstrate these nodal
crossing by plotting the band structure along the in-plane
directions for a fixed \(k_z = 0.27(\frac{2\pi}{a})\) plane in Fig. 3(e).

The type II nodal lines (NL\(_{KH}\)) stretch along the \(K – H\)
high symmetry directions at the hinges of hexagonal BZ
[green lines in Fig. 3(a)]. These nodal lines are essen-
tial and enforced by little group symmetries of the
KH line. Notably, \(KH\) line is invariant under three-
fold rotational symmetry \(C_{3z}\) and anti-unitary operator
\(\mathcal{I}T\). For a spinless system, the eigenvalues of \(C_{3z}\) are
1, \(e^{i\frac{2\pi}{3}}\), and \(e^{-i\frac{2\pi}{3}}\). The conjugate symmetry operator
\(\mathcal{I}T\) however enforces a double degeneracy between states
with \(e^{i\frac{2\pi}{3}}\) and \(e^{-i\frac{2\pi}{3}}\) eigenvalues. We have verified these
symmetry states based on the first-principles wavefunc-
tion analysis. We find that the symmetry adapted basis
\(\Psi = (\psi_+, \psi_-)^T\) of the degenerate bands can be expressed
as \(\psi_\pm = w_1|p_x \pm i p_y\rangle + w_2|d_{xz} \pm id_{yz}\rangle + w_3|d_{x^2-y^2} \mp 2id_{xy}\rangle\)
where \(w_{i=1,2,3}\) are normalized coefficients. We further
explore the nodal line energy dispersion in Figs. 3(c)
and 3(g). We emphasize that similar type-II nodal lines
have also been reported in AA stacked graphite, the high-
temperature superconductor MgB\(_2\) and it’s isostructural
counterparts like AlB\(_2\).\(^{54–56}\)

We present the Fermi surface of Pt\(_2\)HgSe\(_3\) in Fig. 3(d)
with unique electron and hole pockets. These pockets
originate from both NL\(_C\) and NL\(_{KH}\) nodal lines and can
lead to unique transport properties solely governed by
nontrivial pockets.

Figures 3(f) and 3(h) show the energy bands with SOC
along the selective \(k\) path of NL\(_C\) and NL\(_{KH}\), respec-
tively. Clearly, the SOC opens an energy gap at the nodal
crossing points, making valence and conduction band
separated locally at each \(k\) point. This band gap opening
facilitates the calculation of symmetry-based indicator
(SI) to determine the topological state. Following Ref.\(^{7}\),
the band insulators in space group \(P\overline{3}m1\) are defined by
three \(Z_2\) and a single \(Z_4\) indicator i.e. \((Z_2, Z_2, Z_2, Z_4)\).
By explicitly calculating the irreducible representations
of the occupied bands at different time-reversal invariant
momentum points, we find \((Z_2, Z_2, Z_2, Z_4) = (0,0,1,2)\).
Such SI leads to two distinct scenarios for the existence
of a dual topological phase characterized by weak invari-
ants along with either a nonzero mirror Chern number
\(n_M = 2\), or a nonzero rotation invariant, \(n_{2s,00} = 1.7\)
In both the cases, the inversion invariant has non-zero
value \(n_i = 1\). In order to pin down the exact topologi-
cal state, we further calculate the mirror Chern number,
\(n_M\) and find it to be 2. The calculated SI and topologi-
cal invariants are listed in Table I. Thus, the topological
phase of Pt\(_2\)HgSe\(_3\) is characterized by both \((001)\) weak
topological invariants and a non-zero mirror Chern num-
ber \(n_M = 2\).
Two distinct types of nodal lines are shown. Type-I nodal lines (NL$_C$) are located inside the bulk BZ and marked in red and blue colors. Type-II nodal lines (NL$_{KH}$) are located along the hinges and shown in solid green color. (b) Energy-momentum spread of NL$_C$ in the BZ. (c) Schematics of NL$_{KH}$ structure in the BZ. (d) Fermi surface with electron and hole pockets without SOC. Band structure at $k_z = 0.27(\pi/c)$ plane (e) without and (f) with SOC. The nodal band crossings are clearly resolved along $\Gamma_1 - M_1$ and $\Gamma_1 - K_1$ in (e). (g) and (h) show energy dispersion of NL$_{KH}$ nodal line without and with SOC, respectively.

TABLE I: Calculated symmetry indicator and topological invariants for Pt$_2$HgSe$_3$.

| $\{Z_3 Z_4 Z_5\}$ ($\nu_0; \nu_1, \nu_2, \nu_3$) | n$_M$ | n$_{2100}$ | n$_i$ |
|---------------------------------|-------|------------|-------|
| $\{0.0 1.2\}$                  | 2     | 0          | 1     |

IV. SURFACE ELECTRONIC STRUCTURE

We present the electronic spectrum of various surfaces of Pt$_2$HgSe$_3$ in Fig. 4. The NL$_C$ nodal lines projection on (001) surface forms two closed loops whereas NL$_{KH}$ nodal lines project at the corner points of (001) surface BZ. The topological surface states appearing due to NL$_C$ are therefore more obvious over the (001) surface as found in Fig. 4(a) without SOC. The two drumhead surface states (DSSs) nested outside the nodal line are clearly visible, consistent with the calculated nontrivial character of the nodal lines. Interestingly, the DSSs are more dispersive and have opposite band curvature along $\overline{\Gamma} - \overline{T}$ and $\overline{M} - \overline{K}$ directions. They form unique saddle-like $E_k$ dispersion with $\overline{M}$ being the saddle point. When SOC is included in the computations, the DSSs split away from $\overline{T}$ symmetric $\overline{M}$ point, evolving into topological Dirac-cone-like states with a saddle-like energy dispersion [see Fig. 4(b)].

Generally the tight-binding based methods for calculating surface spectrum neglect possible surface potential caused by charge redistribution near the surface area and provide only an approximate representation of the surface states. To showcase the robustness of saddle-like topological states, we calculate 10 layers slab band structure by considering the self-consistent surface potential effects within DFT computations and present results in Figs. 4(c) and 4(d). We find that these results are in reasonable agreement with the ones obtained using semi-infinite tight-binding slab calculations. More importantly, the saddle-like energy dispersion of the DSSs is preserved in DFT computations. Since (001) surface is a natural cleavable surface of Pt$_2$HgSe$_3$ due to the presence of weakly coupled pair of layers, these state can be easily accessed in spectroscopic experiments.

The (100) surface band structure is presented in Figs. 4(e) and 4(f) without and with SOC effects, respectively. Over the (100) surface, NL$_{KH}$ nodal lines projection connects $\overline{\Gamma} - \overline{\Gamma}$ and $\overline{Z} - \overline{U}$ symmetry lines as shown in Fig. 3(a). The topological DSSs connect these projections which are seen clearly in Fig. 4(e). On considering SOC effects, the DSSs evolve into the Dirac-cone like states with Dirac points at $\overline{U}$ and $\overline{Y}$ points, in accordance with the calculated topological invariants.
FIG. 4: Surface band structure of (001) semi-infinite slab calculated using Green’s function method (a) without and (b) with SOC. The sharp yellow lines represent surface states. Surface band structure of 10L thick Pt$_3$HgSe$_3$ slab obtained by DFT calculations (c) without and (d) with SOC. The shaded green region highlights the projected bulk bands and solid yellow lines mark the surface states. (e) and (f) are same as (a) and (b) but for the (100) surface. The yellow line on the surface states connecting bulk NL nodal line projections are clearly visible. They evolve to topological Dirac cone states with SOC at Γ and U point of (100) surface BZ.

V. $\mathbf{k} \cdot \mathbf{p}$ MODEL HAMILTONIAN

We now discuss a minimal low-energy $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian for the topological surface states that capture essential features of these states. Based on our first-principles calculations, the TSSs spread around $\overline{M}$ point on the (001) surface. Therefore, a $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian around $\overline{M} = (0, \pi)$ point is sufficient to describe the TSSs. On the (001) surface at $\overline{M}$, the little group $C_s$ contain a mirror plane symmetry. In the presence of SOC, the symmetry operators are given as $M_1 = -i\sigma_2 \tau_1$ and $T = -i\sigma_2 \tilde{K}$, where $\sigma$ and $\tau$ are Pauli matrices in spin and sublattice spaces, respectively. The associated symmetry allowed basis functions for TSSs $\Psi = (\psi^A_{\alpha,\uparrow}, \psi^A_{\alpha,\downarrow}, \psi^B_{\alpha,\uparrow}, \psi^B_{\alpha,\downarrow})^T$, where $A$ and $B$ represent two sublattice of bipartite lattice, can be expressed as

$$|\psi_{\alpha,\sigma}\rangle = \lambda_\alpha |s,\sigma\rangle + \lambda_{d_{yz}} |d_{yz},\sigma\rangle + \lambda_{d_{x^2-y^2}} |d_{x^2-y^2},\sigma\rangle + \lambda_{d_{z^2}} |d_{z^2},\sigma\rangle.$$  

Here, the subscript $s = \uparrow / \downarrow$ denotes spin-up/spin-down, respectively, and $\lambda_\alpha, \lambda_{d_{yz}}, \lambda_{d_{x^2-y^2}}, \text{and} \lambda_{d_{z^2}}$ describe normalization coefficients. Using the above basis, the minimal four band Hamiltonian around the surface Dirac point (up to second order in momentum) can be written as

$$H_{TSS}(\mathbf{p}) = \frac{1}{2m^*} (p_x^2 + \eta p_y^2) + v_R (p_x \sigma_2 - p_y \sigma_1)$$
$$+ v_{33} p_x \tau_3 \sigma_3 + \lambda_{23} p_x p_y \tau_3 \sigma_3$$
$$+ \delta_{30} \tau_3 \sigma_0 + \delta_{21} \tau_2 \sigma_1.$$  

where $\eta, v_R, v_{33}, \lambda_{23}$ and $\delta_{12}$ are real numbers and $v_R$ denotes Rashba parameter. The corresponding eigenenergies of $H_{TSS}(\mathbf{p})$ are

$E_{TSS}(\mathbf{p}) = \frac{1}{2m^*} (p_x^2 + \eta p_y^2) + \xi \sqrt{v_R^2 p_x^2 + \delta_{21}^2} + p_x^2 (v_{33}^2 + \lambda_{23}^2 p_y^2) + \xi' \sqrt{v_R^2 p_y^2 + v_{33}^2 p_x^2}$

with $p_x^2 = p_x^2 + p_y^2$ and $\xi(\xi') = \pm 1$. Equation (2) shows that the lower branch of conduction band cross with the top branch of valence band at $(p_x, p_y) = (0, \pm \delta_{21})$ along mirror invariant $\overline{M} - \Gamma$ line. This gives rise to the Dirac cones states protected by mirror symmetry, as shown explicitly in Figs. 5(a) and 5(b). In addition, for $\eta < 0$, we find a pair of type II saddle-point VHSs, $^{31}$ as illustrated in Fig. 5(c).

VI. TOPOLOGICAL PHASE TRANSITION

We now demonstrate the possibility of tuning the topological order of Pt$_3$HgSe$_3$ and realizing a Dirac semimetal by modulating the unit cell volume in Fig. 6. For this purpose, it is useful to define the SOC induced gap as $\Delta_K = E_{K1}^\lambda - E_{K2}^\lambda$ at $K$ and $\Delta_H = E_{H1}^\lambda - E_{H2}^\lambda$ at $H$ between the $\Lambda_1$ and $\Lambda_2$ states that form a nodal line without SOC along $KH$ direction (see Fig. 6 for details). The evolution of $\Delta_K$ and $\Delta_H$ with relative unit cell volume $V/V_0$ where $V_0$ denotes equilibrium unit cell vol-
In contrast to this, in Pt\(_2\)HgSe\(_3\) the gap \(\Delta_K \Delta_H > 0\) show a topological insulator state whereas \(\Delta_K \Delta_H < 0\) identify a Dirac semimetal state. Band structure along the \(KH\) line for different relative cell volume (b) \(\frac{V}{V_0} = 0.83\), (c) \(\frac{V}{V_0} = 1.00\), and (d) \(\frac{V}{V_0} = 1.19\). Panels (e)-(g) illustrate the corresponding atomic displacements with respect to the equilibrium structure. The length of the arrows is proportional to the magnitude of displacement.

**VII. CONCLUSION**

In conclusion, based on our first-principles calculations combined with a \(k\mathbf{p}\) model Hamiltonian analysis, we identify and characterize the dual-symmetry-protected topological state of Pt\(_2\)HgSe\(_3\). The material is shown to harbor two distinct types of nodal lines when SOC effects are neglected in the computations. Inclusion of SOC gaps out the nodal lines and drives the system into a topological insulator state which is characterized by both the weak topological invariant \(Z_2 = 0\) and the mirror Chern number \(\eta_M = 2\). The (001) surface band structure reveals the existence of unique saddle-like topological surface states with saddle-point VHSs. We further discuss the tenability of the topological state of Pt\(_2\)HgSe\(_3\) by modulating its crystal structure. In this way, the system is shown to undergo a unique topological phase transition where a topological insulator state exists as an intermediate phase between gapless Dirac semimetal states. Our analysis suggests that the naturally cleaved (001) surface of Pt\(_2\)HgSe\(_3\) presents an ideal testbed for exploring saddle-like topological surface states with VHSs and the
associated physics in topological materials.

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