Supplementary information: Three-dimensional all-dielectric photonic topological insulator

A. Derivation of the effective Hamiltonian from electromagnetic perturbation theory

First-order perturbation theory treatment of bianisotropy

It is known that a change in the material content of a resonator modifies the resonance frequency, which can be described within the framework of the perturbation theory [1, 2, 3]. Here, we apply a similar approach for a set of degenerate electromagnetic modes in all-dielectric metacrystal under consideration. A material permittivity change \( \varepsilon_r \rightarrow \varepsilon_r + \delta \varepsilon_r \) within the volume \( \Delta V \), inside a dielectric cylinder of volume \( V \) transforms an unperturbed resonant mode characterized by field components \( E, H \), and the resonance frequency \( \omega \), into a perturbed mode characterized by \( E', H' \), and \( \omega' \). Using the Maxwell’s equations, one can derive the following equation relating the unperturbed and perturbed modes:

\[
\frac{\omega' - \omega}{\omega'} = -\frac{\int_{\Delta V} d^3r \delta \varepsilon_r \varepsilon_0 E' \cdot E^*}{\int_V d^3r (\varepsilon_r \varepsilon_0 E' \cdot E^* + \mu_0 H' \cdot H^*)},
\]

which is an exact expression for the change in the resonant frequency due to the material’s permittivity change. Quite often, however, the perturbed mode profile, entering Eq. (1), is unknown, and, therefore, Eq. (1) is not particularly useful for calculating the resonance frequency shift. Equation (1) can be made more useable if one assumes that the set of the unperturbed modes forms a complete basis even for the perturbed system, and the perturbed modes are expanded in terms of the unperturbed ones. This approach is a good approximation for changes which are either small in amplitude \( \delta \varepsilon_r \), or take place in a relatively small volume \( \Delta V \).

By expanding the perturbed mode in terms of the unperturbed ones,

\[
E' = \sum_n a_n E_n \quad \text{and} \quad H' = \sum_n a_n H_n ,
\]

one can recast Eq. (1) into a generalized eigenvalue problem:

\[
\omega' \sum_n U_{mn} a_n = \omega_m \sum_n (U_{mn} + \Delta_{mn}) a_n ,
\]

where \( \Delta_{mn} = -\int d^3r \delta \varepsilon_r \varepsilon_0 E_n \cdot E_m^* \) and \( U_{mn} = \int_V d^3r (\varepsilon_r \varepsilon_0 E_n \cdot E_m^* + \mu_0 H_n \cdot H_m^*) \). Note that here we have replaced the left-hand-side denominator in Eq. (1) with \( \omega \), which does not affect the validity of our first-order approximation. By normalizing the arbitrary magnitude of the unperturbed eigenfunction so that \( U_{mn} = \delta_{mn} \), where \( \delta_{mn} \) is the Kronecker delta, Eq. (3) simplifies to
\[
\omega_m \sum_n (\delta_{mn} + \Delta_{mn}) a_n = \omega' a_m ,
\]  

(4)

which provides a description of the metacrystal with the part of the cylinders removed to induce the bianisotropic response. Eq. (4) allows retrieving an effective Hamiltonian with the spin-orbital interaction [4].

**Degenerate electromagnetic \( k \cdot p \) theory**

So far, we have studied the effect of bianisotropy of the first type caused by the change in the dielectric material. Next, we examine the effect of the second type of bianisotropy: out-of-plane propagation \( k_z \). Conventional electromagnetic \( k \cdot p \) perturbation theory is generally used to calculate the group velocity of nondegenerate dispersion bands [5, 6, 4]. Here, we develop a generalized version of electromagnetic \( k \cdot p \) theory for the case of degenerate modes, which will reproduce the Dirac dispersion found numerically.

With the assumption that the perturbed field components are \( \vec{E}' \) and \( \vec{H}' \) with the eigen-frequency \( \omega' \) and the unperturbed ones \( \vec{E} \) and \( \vec{H} \) with the eigen-frequency \( \omega \), and these fields have the exponential Bloch dependence, which implies \( \vec{E}' = E'(\vec{k}) \exp(-i\delta \vec{k} \cdot \vec{r}) \), the Maxwell’s equations can be written for Bloch amplitudes \( \vec{E} \) and \( \vec{H} \) as

\[
\begin{pmatrix}
0 \\
-\nabla \times \\
0
\end{pmatrix}
\begin{pmatrix}
\vec{E}' \\
\vec{H}'
\end{pmatrix}
- i \omega' \begin{pmatrix}
\varepsilon \\
0 \\
\mu
\end{pmatrix}
\begin{pmatrix}
\vec{E}' \\
\vec{H}'
\end{pmatrix}
= i \begin{pmatrix}
0 \\
-\delta \vec{k} \times \\
\mu
\end{pmatrix}
\begin{pmatrix}
\vec{E}' \\
\vec{H}'
\end{pmatrix}.
\]

Multiplying the above expression by the six component raw vector \( (\vec{E} \quad \vec{H}) \) from the left, and integrating it over the entire unit cell with volume \( V_0 \), we obtain the main equation of the degenerate \( k \cdot p \) perturbation theory:

\[
\omega' - \omega = \delta \vec{k} \cdot \int_{V_0} d^3r \left\{ \vec{E}' \times \vec{H}^* + \vec{E}^* \times \vec{H}' \right\}
= \int_{V_0} d^3r \left( \varepsilon_r \varepsilon_0 \vec{E}' \cdot \vec{E}^* + \mu_0 \vec{H}' \cdot \vec{H}^* \right).
\]

(5)

Following the steps of the previous section, we expand the perturbed mode in terms of the unperturbed ones, \( \vec{E}' = \sum_n a_n \vec{E}_n \) and \( \vec{H}' = \sum_n a_n \vec{H}_n \), which allows rewriting Eq. (5) as

\[
(\omega' - \omega_m) \sum_n U_{mn} a_n = \sum_n \left( \delta k_x \tilde{s}_x + \delta k_y \tilde{s}_y + \delta k_z \tilde{s}_z \right) a_n,
\]

where \( \{S_i\}_{mn} = \int_{V_0} d^3r \left\{ \vec{E}_n^* \times \vec{H}_m + \vec{E}_m^* \times \vec{H}_n \right\} \), \( i = \{x, y, z \} \), and \( U_{mn} = \int_{V_0} d^3r \left( \varepsilon_r \varepsilon_0 \vec{E}_n \cdot \vec{E}_m^* + \mu_0 \vec{H}_n \cdot \vec{H}_m^* \right) \).

Finally, combining both perturbations [Eqs. (1) and (5)], and assuming the normalization \( U_{mn} = \delta_{mn} \), we arrive at the generalized effective Hamiltonian for the metacrystal near the K point, and describing the interaction of four modes which in the absence of perturbations are degenerate with the frequency of \( \omega_D \):
\[ \mathcal{H}' \mathbf{a} \equiv (\omega' - \omega_D) \mathbf{a} = (\omega_D \hat{\Delta} + \delta \mathbf{k} \cdot \hat{\mathbf{S}}) \mathbf{a}. \]  

The Hamiltonian Eq. (6) acts on the four-component vector of field amplitudes of the electric and magnetic modes \( \{ a_{E \text{ [lower]}}^{\text{lower}}, a_{E \text{ [upper]}}^{\text{upper}}, a_{M \text{ [upper]}}^{\text{upper}}, a_{M \text{ [lower]}}^{\text{lower}} \} \) forming the Dirac cone.

The perturbation theory allows capturing the effects of both a material change and a small wavevector change \( (\delta \mathbf{k}) \) on the dispersion and hybridization of these modes. Using the numerically solved electromagnetic unperturbed fields at the K point, we calculate the interaction terms among the modes. By changing the basis to that of circularly polarized modes as described in [4] this procedure yields the effective Hamiltonian of the form:

\[
\mathcal{H}_{4\times4}' = \omega_D \begin{pmatrix}
\Delta_0 & v_\parallel(\delta k_x - i \delta k_y) & M(1 + i \eta \delta k_z) & 0 \\
v_\parallel(\delta k_x + i \delta k_y) & \Delta_0 & 0 & -M(1 + i \eta \delta k_z) \\
M(1 - i \eta \delta k_z) & 0 & \Delta_0 & v_\parallel(\delta k_x - i \delta k_y) \\
0 & -M(1 - i \eta \delta k_z) & v_\parallel(\delta k_x + i \delta k_y) & \Delta_0
\end{pmatrix}.
\] (7)

**Figure S1** | Dispersion of the four modes as described by the effective Hamiltonian (7) after the perturbations are introduced. The calculation is done with the use of the numerically computed unperturbed field profiles.

The values of the parameters calculated from the numerically solved field profiles are \( \Delta_0 \approx 0.052, \eta \approx 0.051, M \approx 0.03, \) and the Dirac velocity \( v_\parallel \approx 1.9 \times 10^7 \text{ m/s} \). The modes dispersion as a function of the in-plane and out-of-plane wavevectors components is shown in the Fig. S1.
To understand the origin of the observed removal of degeneracy at K point, we first consider the in-plane propagation \((k_z = 0)\), where the unperturbed disks have mirror reflection symmetry \(\sigma_z\). Under this symmetry, the bands are classified as TE-like and TM-like modes, corresponding to electric and magnetic dipolar modes. Figure 2 of the main text shows this classification and the field profiles of all four bands at the K point of the Brillouin zone \(k = \left(\frac{4\pi}{3a_0} \times 0.999,0,0\right)\), where \(a_0\) is the lattice constant. As can be seen from the in-plane symmetries of the modes’ field profiles, a circular perturbation to the disk, like the one shown on the left bottom corner, mixes only the lower electric and upper magnetic unperturbed modes and also the upper electric and lower magnetic unperturbed modes. Interactions for all the other modes vanish. Another important consequence from the mirror reflection symmetry \(\sigma_z\) of the structure is that when the perturbation is introduced at the opposite side of the disks, the mass term, which is proportional to \(\Delta_{mn} = -\int d^3r \delta\epsilon \, E_n \cdot E_m\), flips its sign while maintaining its magnitude.

### B. Derivation of Dirac Hamiltonian in 3D Topological Insulator: Effective Medium Approach

Maxwell equations for a bi-anisotropic medium have the form

\[
\begin{align*}
\nabla \times \mathbf{E} &= \imath k_0 (\hat{\mu} \mathbf{H} + \hat{\chi} \mathbf{E}), \\
\nabla \times \mathbf{H} &= -\imath k_0 (\hat{\epsilon} \mathbf{E} + \hat{\chi} \mathbf{H}),
\end{align*}
\]

where material response for the system of interest is described by effective parameters

\[
\hat{\mu} = \begin{pmatrix} \mu_\perp & 0 & 0 \\ 0 & \mu_\perp & 0 \\ 0 & 0 & \mu_{zz} \end{pmatrix}, \hat{\epsilon} = \begin{pmatrix} \epsilon_\perp & 0 & 0 \\ 0 & \epsilon_\perp & 0 \\ 0 & 0 & \epsilon_{zz} \end{pmatrix}, \hat{\chi} = \begin{pmatrix} 0 & i\Delta & 0 \\ -i\Delta & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.
\]

The requirements imposed by the energy conservation and time-reversal symmetry result in the Hermitian effective Hamiltonian, \(\hat{\chi} = \hat{\chi}^\dagger\) [7, 8].

From Maxwell equations (8.a) one can get a reduced set of equations for TE-like and TM-like modes coupled to each other by either bianisotropy or out-of-plane propagation \((\partial_z \mathbf{E} \neq 0, \partial_z \mathbf{H} \neq 0)\)

\[
\begin{align*}
\partial_x \mu_\perp^{-1} \partial_x + \partial_y \mu_\perp^{-1} \partial_y + k_0^2 \epsilon_{zz} \right) E_x &= \partial_x \mu_\perp^{-1} (\partial_z - k_0 \Delta) E_x + \partial_y \mu_\perp^{-1} (\partial_z - k_0 \Delta) E_y, \\
(\partial_x \epsilon_\perp^{-1} \partial_x + \partial_y \epsilon_\perp^{-1} \partial_y + k_0^2 \mu_{zz}) H_z &= \partial_x \epsilon_\perp^{-1} (\partial_z + k_0 \Delta) H_x + \partial_y \epsilon_\perp^{-1} (\partial_z + k_0 \Delta) H_y.
\end{align*}
\]

Here we are interested in dispersion characteristics in the proximity of K (K’) point of the 3D hexagonal lattice and assume \(k_z \ll k_0\), so that the first-order approximation holds. In this approximation, one can find from Maxwell equations, \(E_x \cong -\frac{\epsilon_\perp}{ik_0} \partial_y H_z, E_y \cong \frac{\epsilon_\perp}{ik_0} \partial_x H_z\).
\[ \frac{\mu_\perp^{-1}}{ik_0} \partial_y E_Z, H_y \approx \frac{\mu_\perp^{-1}}{ik_0} \partial_x E_Z. \]

Substituting these expressions into (9), and introducing compact notations
\[ q = \frac{k_z}{k_0 \mu_\perp \epsilon_\perp}, \delta = \frac{\Delta}{\mu_\perp \epsilon_\perp}, \]
we obtain a closed form equations coupling z-components of electric and magnetic fields only [6]
\[ \left( \partial_x \mu_\perp^{-1} \partial_x + \partial_y \mu_\perp^{-1} \partial_y + k_0^2 \epsilon_{zz} \right) E_x = -i[\partial_x(\delta - iq) \partial_y - \partial_y(\delta - iq) \partial_x] H_z, \] (10a)
\[ \left( \partial_x \epsilon_\perp^{-1} \partial_x + \partial_y \epsilon_\perp^{-1} \partial_y + k_0^2 \mu_{zz} \right) H_z = -i[\partial_x(\delta + iq) \partial_y - \partial_y(\delta + iq) \partial_x] E_z. \] (10b)

The topological phase of the proposed metacrystal relies on the electromagnetic duality symmetry, thus, we impose the condition \( \hat{\mu} = \hat{\epsilon} \). By using the fact of periodicity of the system we apply the Bloch theorem, and Fourier transform the material parameters and expand the wave-fields into plane-waves,
\[ E_z(\mathbf{r}; \mathbf{k}) = \sum_G E_G e^{i(\mathbf{k} + \mathbf{G}) \cdot \mathbf{r}}, H_z(\mathbf{r}; \mathbf{k}) = \sum_G H_G e^{i(\mathbf{k} + \mathbf{G}) \cdot \mathbf{r}}, \]
\[ \mu_\perp^{-1}(\mathbf{r}) = \epsilon_\perp^{-1}(\mathbf{r}) = \sum_G \epsilon_G e^{i\mathbf{G} \cdot \mathbf{r}}, \delta(\mathbf{r}) - iq(\mathbf{r}) = \sum_G \theta_G^- e^{i\mathbf{G} \cdot \mathbf{r}}, \delta(\mathbf{r}) + iq(\mathbf{r}) = \sum_G \theta_G^+ e^{i\mathbf{G} \cdot \mathbf{r}}. \]

This procedure results into a set of linear equations for the Fourier components of the fields
\[ k_0^2 \epsilon_{zz} E_G - \sum_{\mathbf{G}'} \epsilon_{G-G'}(\mathbf{k} + \mathbf{G}) \cdot (\mathbf{k} + \mathbf{G}') E_{G'} = -i \sum_{\mathbf{G}'} \theta_{G-G'}^- (\mathbf{k} + \mathbf{G}) \times (\mathbf{k} + \mathbf{G}') H_{G'}, \]
\[ k_0^2 \epsilon_{zz} H_G - \sum_{\mathbf{G}'} \epsilon_{G-G'}(\mathbf{k} + \mathbf{G}) \cdot (\mathbf{k} + \mathbf{G}') H_{G'} = -i \sum_{\mathbf{G}'} \theta_{G-G'}^+ (\mathbf{k} + \mathbf{G}) \times (\mathbf{k} + \mathbf{G}') E_{G'}. \] (11)

We describe the modes near the K-point which corresponds to the Bloch wave-vector \( \mathbf{K}=\mathbf{K}(1,0,0) \), where \( \mathbf{K} = \frac{4\pi}{3a_0} \). We assume that there is no mode entering the frequency range of interest due to the diffraction in z-direction, which allows us to cut off the basis [5, 6] and consider only following in-plane reciprocal lattice vectors \( \mathbf{G}_0=(0,0,0), \mathbf{G}_1=\mathbf{K}(\frac{3}{2},-\frac{\sqrt{3}}{2},0), \mathbf{G}_2=\mathbf{K}(-\frac{3}{2},\frac{\sqrt{3}}{2},0) \), so that we only have three points in the reciprocal space \( \mathbf{k}_1=\mathbf{K}+\mathbf{G}_0, \mathbf{k}_2=\mathbf{K}+\mathbf{G}_1, \mathbf{k}_3=\mathbf{K}+\mathbf{G}_2 \) contributing to the formation of bands
\[ \sum_{n=1}^3 (\mathbf{k}_n \cdot \mathbf{k}_m \epsilon_{n-m} H_n - i \mathbf{k}_n \times \mathbf{k}_m \theta_{n-m}^+ E_n) = k_0^2 \epsilon_{zz} H_m. \] (12)

In order to keep a simpler form, index \( \mathbf{G}_n \) is abbreviated to an index \( n \) from now on. Finally, to obtain 3D spatial dispersion, we apply \( \mathbf{k} \cdot \mathbf{p} \) approximation near the K point, and neglect terms of the 2\(^{nd} \) and higher orders, which results in
\[ \mathcal{H} \begin{pmatrix} E_n \\ H_n \end{pmatrix} = \begin{pmatrix} \Omega & -i\Omega \\ i\Omega^* & \Omega \end{pmatrix} \begin{pmatrix} E_n \\ H_n \end{pmatrix} = k_0^2 \epsilon_{zz} \begin{pmatrix} E_m \\ H_m \end{pmatrix}, \] (13)
where
\[ \Omega = \begin{pmatrix}
    \mathbf{k}_1 \cdot \mathbf{k}_1 \varepsilon_0 & \mathbf{k}_1 \cdot \mathbf{k}_2 \varepsilon_1 & \mathbf{k}_1 \cdot \mathbf{k}_3 \varepsilon_1 \\
    \mathbf{k}_2 \cdot \mathbf{k}_1 \varepsilon_1 & \mathbf{k}_2 \cdot \mathbf{k}_2 \varepsilon_0 & \mathbf{k}_2 \cdot \mathbf{k}_3 \varepsilon_1 \\
    \mathbf{k}_3 \cdot \mathbf{k}_1 \varepsilon_1 & \mathbf{k}_3 \cdot \mathbf{k}_2 \varepsilon_1 & \mathbf{k}_3 \cdot \mathbf{k}_3 \varepsilon_0 
\end{pmatrix} + \delta \mathbf{k} \begin{pmatrix}
    2\mathbf{k}_1 \varepsilon_0 & (\mathbf{k}_1 + \mathbf{k}_2) \varepsilon_1 & (\mathbf{k}_1 + \mathbf{k}_3) \varepsilon_1 \\
    (\mathbf{k}_2 + \mathbf{k}_1) \varepsilon_1 & 2\mathbf{k}_2 \varepsilon_0 & (\mathbf{k}_2 + \mathbf{k}_3) \varepsilon_1 \\
    (\mathbf{k}_3 + \mathbf{k}_1) \varepsilon_1 & (\mathbf{k}_3 + \mathbf{k}_2) \varepsilon_1 & 2\mathbf{k}_3 \varepsilon_0 
\end{pmatrix}, \]

\[ \Xi = \begin{pmatrix}
    0 & \mathbf{k}_1 \times \mathbf{k}_2 \theta_1^- & \mathbf{k}_1 \times \mathbf{k}_3 \theta_1^- \\
    \mathbf{k}_2 \times \mathbf{k}_1 \theta_1^- & 0 & \mathbf{k}_2 \times \mathbf{k}_3 \theta_1^- \\
    \mathbf{k}_3 \times \mathbf{k}_1 \theta_1^- & \mathbf{k}_3 \times \mathbf{k}_2 \theta_1^- & 0 
\end{pmatrix}, \]

\[ \delta \mathbf{k} = (\delta k_x + \delta k_y), \text{ and } \varepsilon_0, \varepsilon_1 \text{ and } \theta_1^- \text{ are Fourier components of the dielectric parameters,} \]

\[ \varepsilon_0 = \frac{f}{\varepsilon_{a\perp}} + \frac{1-f}{\varepsilon_{a\parallel}} \varepsilon_1 = 2f \left( \frac{1}{\varepsilon_{a\perp}} - \frac{1}{\varepsilon_{a\parallel}} \right) J_1(\frac{\varepsilon_{nm} \alpha_0}{|\varepsilon_{nm} \alpha_0|}) (n \neq m), \]

\[ \theta_1^- = 2f \left( \frac{1}{(\delta - iq)_{a\perp}} - \frac{1}{(\delta - iq)_{a\parallel}} \right) J_1(\frac{\varepsilon_{nm} \alpha_0}{|\varepsilon_{nm} \alpha_0|}) (n \neq m). \]

where \( f \) is the filling factor, \( J_1(x) \) is the Bessel function of the first kind.

By explicitly separating contributions of bianisotropy and out-of-plane propagation, \( \theta_1^- = \theta_r - i\theta_1 \delta k_z \), and changing the basis through a linear transformation \( \mathcal{H}' = U_1 \mathcal{H} U_1^{-1} \) [5, 6], where

\[ U_1 = \frac{1}{\sqrt{3}} \begin{pmatrix}
    1 & 1 & 1 \\
    e^{-\frac{2i\pi}{3}} & e^\frac{2i\pi}{3} & e^{-\frac{2i\pi}{3}} \\
    e^{\frac{2i\pi}{3}} & e^{-\frac{2i\pi}{3}} & e^{\frac{2i\pi}{3}} 
\end{pmatrix} \otimes \begin{pmatrix}
    1 & 0 \\
    0 & 1 
\end{pmatrix}, \]

we eliminate singlet TE and TM states which do not couple with the doublet TE and TM states and obtain the effective Hamiltonian

\[ \mathcal{H}'_{4 \times 4} = \]

\[ \begin{pmatrix}
    \frac{1}{2} K^2 (2\varepsilon_0 + \varepsilon_1) & K(\varepsilon_0 - \varepsilon_1)(\delta k_x - i\delta k_y) & \frac{3}{2} K^2 (\theta_r + i\theta_1 \delta k_z) & 0 \\
    K(\varepsilon_0 - \varepsilon_1)(\delta k_x + i\delta k_y) & \frac{1}{2} K^2 (2\varepsilon_0 + \varepsilon_1) & 0 & -\frac{3}{2} K^2 (\theta_r + i\theta_1 \delta k_z) \\
    \frac{3}{2} K^2 (\theta_r - i\theta_1 \delta k_z) & 0 & \frac{1}{2} K^2 (2\varepsilon_0 + \varepsilon_1) & K(\varepsilon_0 - \varepsilon_1)(\delta k_x + i\delta k_y) \\
    0 & -\frac{3}{2} K^2 (\theta_r - i\theta_1 \delta k_z) & K(\varepsilon_0 - \varepsilon_1)(\delta k_x + i\delta k_y) & \frac{1}{2} K^2 (2\varepsilon_0 + \varepsilon_1) 
\end{pmatrix}, \]

which acts in the subspace of the doublet states \( \mathbf{E}_d = [E_1^Z, E_2^Z], \mathbf{H}_d = [H_1^Z, H_2^Z] \).

By applying an additional linear transformation [6],

\[ U_2 = \begin{pmatrix}
    I & I \\
    I & -I 
\end{pmatrix}, \]

where \( I \) is 2 \times 2 identity matrix, we obtain the 3D massive Dirac Hamiltonian

\[ H = H_0 + v \mathbf{n} \cdot (\delta k_x \hat{x} + \delta k_y \hat{y}) \hat{s}_0 + v \mathbf{n} \cdot \delta k_z \hat{z} \hat{s}_0 + m \hat{z} \hat{s}_0, \]

\[ v = v_1 (\delta k_x \hat{x} + \delta k_y \hat{y}) \hat{s}_0 + v \mathbf{n} \cdot \delta k_z \hat{z} \hat{s}_0 + m \hat{z} \hat{s}_0, \]
where \( H_0 = \frac{1}{2} K^2(2\epsilon_0 + \epsilon_1 + 3\theta_r) \), \( v|| = K(\epsilon_0 - \epsilon_1) \), \( m_r = \frac{3}{2} K^2 \theta_r \), \( v_\perp = -\frac{3}{2} K^2 \theta_i \), \( \hat{s}_i \) and \( \hat{\sigma}_i \) are Pauli matrices acting in the pseudo-spin and orbital subspaces, respectively.

As expected, the effective Hamiltonian (15) is identical to that obtained in Section A with the use of the electromagnetic perturbation theory.

C. Tolerance to the duality violation

Our studies suggest that the violation of the duality leading to the removal of the degeneracy, which can be viewed as the mixing of the pseudo-spins, can be tolerated to some degree, which has also been studied by some of us before in the case of 2D systems (the \( \beta \)-term in Eq.(4) in Ref. [4]). Interestingly, that in solid state physics similar behaviour may occur and, for instance, it is well-known that the \( Z_2 \) phase can survive perturbations that do not conserve spin (e.g. the Rashba term as in [9], and which is also a general situation in 3D topological insulators [10]).

![Figure S2](https://example.com/figure_s2.png)

**Figure S2**} Robustness of the topological phase and of the edge states to violation of the duality symmetry/detuning in the Dirac cones. **a** Bulk photonic band structure of one unit cell without bianisotropy. **b** Photonics band structure with bianisotropy and the topological band gap shown by green shaded region. **c,d** Band structure for in-plane and out of plane (cut through the Dirac cone) directions, respectively, calculated for the supercell of 24 unit cells and revealing the presence of gapless edge states with duality violated. The spectral detuning due to duality violation is 25MHz and the gap open by the bianisotropy at the Dirac cone is 40MHz.

To confirm such robustness of the proposed all-dielectric photonic metacrystal we performed a set of large scale full-wave simulation with the duality symmetry violated by the suboptimal
design of the meta-atoms and the degeneracy between the Dirac cones removed. We observe that the surface states maintain their gapless character as long as the spectral detuning between the Dirac cones remains smaller than the topological gap open by the bianisotropy (the synthetic gauge field). Example of some of the most extreme case with the highly detuned Dirac cones is shown in Fig. S2, where the gapless character of the edge states is clearly maintained. This case demonstrates the robustness of the proposed structure even to the perturbations in the meta-atoms design and geometry.

In addition to the robustness against uniform violation of the duality we have performed a set of large scale simulations with randomized distribution of such symmetry reduction introduced over the entire supercell. As can be seen from Fig. S3, we found that, while the bulk band gap narrows expectedly, the surface states maintain their gapless character even for the magnitudes of dispersion in the diameters of the dielectric disks as large as 5%. In fact, the only modification to the surface band diagram is the slightly different dispersion of the surface states localized to the two opposite domain walls (shown by red and blue lines in Fig. S3) of the supercell which perceive different dielectric environments.

Figure S3| Effect of disorder on topological surface states. The disorder in duality achieved through random distribution of the diameter of the dielectric cylinders. The disorder is increasing progressively from left to right as indicated by the captions to the subplots. a and b show in-plane and out-of-plane (cut through the Dirac cone) supercell band diagrams, respectively.
D. Jackiw-Rebbi-like edge states and spin-locking in the 3D topological metacrystal

Within our analytical description, given by Hamiltonian (1) of the main text, a 2D domain wall with the flip of bianisotropy can be described as an interface across which the effective mass reverses its sign. In 2D systems, such as graphene and quantum spin Hall effect (QSHE) systems [11, 12, 5, 13], which are described by the 2D version of the Dirac equation, the mass term is known to open the band gap, and the reversal of the mass term across the interface gives rise to the emergence of the edge states. The system described by the effective Hamiltonian displays analogous behaviour in 3D, and exhibits emergence of gapless surface states within the bandgap induced by the mass term, which was confirmed by finding the eigenmodes of the effective Hamiltonian for the two half-spaces and matching the solutions at the domain wall with the use of continuity boundary condition.

In this section, we demonstrate that the effective Hamiltonian predicts topological surface states on the domain wall between two domains with opposite effective masses \(m_r\), which are classical analogues of Jackiw-Rebbi surface states existing on the boundary between two relativistic Dirac half-spaces with opposite masses of particles [14, 15, 16, 17]. Indeed, the effective Hamiltonian can be brought to a form identical to the Dirac equation by unitary linear transformation [16].

The effective Hamiltonian describing our system in the basis of the circularly polarized electric and magnetic dipoles has the form

\[
H = \begin{pmatrix}
0 & v_{\|}(k_x - ik_y) & m_r + iv_{\perp}k_z & 0 \\
v_{\|}(k_x + ik_y) & 0 & 0 & -m_r - iv_{\perp}k_z \\
m_r - iv_{\perp}k_z & 0 & 0 & v_{\|}(k_x + ik_y) \\
0 & -m_r + iv_{\perp}k_z & v_{\|}(k_x - ik_y) & 0
\end{pmatrix},
\]

and it acts on the four-component wavefunctions \(\Psi' = (e_1, e_2, h_1, h_2)^T\). After partial block diagonalization using the transformation

\[
U_2 = \begin{pmatrix}
I & I \\
I & -I
\end{pmatrix},
\]

this Hamiltonian is transformed to the pseudo-spin basis of spin-up and spin-down states characterized by the wavefunctions \(\Psi' = (e_1 + h_1, e_2 + h_2, e_1 - h_1, e_2 - h_2)^T\) and takes the form given in the main text Eq. (1)

\[
H' = v_{\|}(k_x \hat{x} + k_y \hat{y}) + v_{\perp}k_z \hat{y} \hat{z} + m_r \hat{z} \hat{z}.
\]

Considering first the homogeneous case, \(m_r = \text{const}\) and solving the eigenvalue problem \(H'\psi' = \Omega(k)\psi'\), we find the dispersion relation for propagating waves \(\psi' \sim \exp[i(k_x x + k_y y + k_z z)]\). The characteristic equation
\[(\Omega^2 - m_r^2 - v_{\parallel}^2(k_x^2 + k_y^2) - v_{\perp}^2k_z^2)^2 = 0\]
yields the bulk spectrum of two doubly degenerate bands shown in Fig. S4

\[\Omega_{\pm} = \pm \sqrt{m_r^2 + v_{\parallel}^2(k_x^2 + k_y^2) + v_{\perp}^2k_z^2}.\]

Next, we study the case of the domain wall hosting surface states along yz plane between two half-spaces with the mass terms of the opposite signs \(m_r(x) = m_r \text{sgn}(x)\), \(m_r > 0\), induced by the bianisotropy. We decompose the Hamiltonian as \(H' = H_x + H_{yz}\), where \(H_x = v_{\parallel}k_x \hat{\sigma}_x + m_r \hat{\sigma}_z\), \(H_{yz} = v_{\parallel}k_y \hat{\sigma}_y + v_{\perp}k_z \hat{\sigma}_z\). Note, for the states localized at surface \(x=0\) we have \(H_x \psi'(r)|_{x=0} = 0\), and \(k_x = \pm \frac{im_r}{v_{\parallel}}\). Thereby, the surface modes are given by

\[\psi_s'(r) = u_0 e^{i(k_y y + k_z z) - \kappa |x|},\]

where \(\kappa = \frac{m_r}{v_{\parallel}}, u_0\) is the polarization vector, and the surface waves dispersion \(\Omega_{s\pm}(k_y, k_z) = \pm \sqrt{v_{\parallel}^2k_y^2 + v_{\perp}^2k_z^2}\) is formed of two cones (see Fig. S4) touching at the Dirac point, where the sign \(\pm\) indicates the upper/lower cone.

By utilizing the relation \((\hat{\sigma}_x - i \hat{\sigma}_z \hat{\sigma}_y)u_0 = 0\) and the property \((\hat{\sigma}_x + i \hat{\sigma}_y \hat{\sigma}_z)(\hat{\sigma}_x - i \hat{\sigma}_y \hat{\sigma}_z) = 2(1 - \hat{\sigma}_z \hat{\sigma}_y)\), we obtain

\[\hat{\sigma}_z \hat{\sigma}_y u_0 = u_0.\]

Substituting Eq. (16) in \(H_{yz}\), which governs the behavior of surface states in \(x=0\) plane in accord with the equation

\[H_{yz} \psi' = \Omega_{s\pm} \psi',\]

the eigenvalue problem (17) for the surface is rewritten as

\[(v_{\parallel}k_y \hat{\sigma}_z + v_{\perp}k_z \hat{\sigma}_y)u_0 = \Omega_{s\pm}u_0.\]

In this way, we find the expression for the normalized surface states with the spin components \((e_1 \pm h_1)\) in the circularly polarized pseudo-spin basis as follows

\[\psi_{s\pm}^{(1)}(x, y, z) = \frac{1}{A} \left(\frac{iv_{\perp}k_z}{v_{\parallel} k_y - \Omega_{s\pm}}\right) e^{i(k_y y + k_z z) - \kappa |x|},\]

where \(A = i\sqrt{2\Omega_{s\pm} - \Omega_{s\pm} v_{\parallel} k_y}\) is the normalization factor, and where we use redundancy of the four-component basis on the surface and reduced it to the two-component basis. This redundancy leads to the pairwise equivalency of the solutions, expressed as \(\psi_{s\pm}^{(1)} = \psi_{s\mp}^{(2)}(k_y \rightarrow -k_y)\), where the superscripts "(1)" and "(2)" refer to \((e_1 \pm h_1)\) and \((e_2 \pm h_2)\), components of the
basis, respectively. The wavefunction of the surface state can be written in the spin-up/spin-down basis in terms of the electromagnetic field

\[ \psi_{s\pm}^{(1)} \sim i v_\perp k_z |e_1 + h_1 > + (v_{||} |k_y - \Omega_{s\pm}) |e_1 - h_1 >, \]

which clearly shows how the out-of-plane propagation results in mixing of the up/down pseudo-spins and the spin-locking.

When the pseudo-spin \( \vec{s} \) is projected onto the coordinate basis of the surface, it shows locking to the wavevector, as illustrated by color arrows in Fig. 3e

\[ \psi_{s\pm}^{(1)\dagger} \vec{s} \psi_{s\pm}^{(1)} = \frac{v_\perp k_z}{\Omega_{s\pm}} \hat{y} + \frac{v_{||} k_y}{\Omega_{s\pm}} \hat{z}. \]

As expected, if \( k_z = 0 \), surface basis reduces to the case of spin-up and spin-down states \( |e_1 \pm h_1 > \) and \( |e_2 \pm h_2 > \), and the expectation value for the spin \( \vec{s} \) becomes the unit vector along \( z \) direction, in agreement with the previous results for 2D systems. For the case of the surface wave propagating in the vertical direction (understood in terms of the mode group velocity and corresponding to \( k_y = 0 \)) the spin is aligned along the wall in the horizontal direction. For all other values of \( k_z \) the eigenstates have their spin rotated with respect to their propagation direction so that the spins corresponding to opposite \( k \) are orthogonal to each other [18].

**Figure S4**| Band structure of bulk and surface states obtained from the eigenvalue problems for bulk and the boundary, respectively. The bulk bands are gapped due to the non-vanishing mass term and the gapless surface states lie within the bulk gap.
The band diagrams for the bulk and surface states calculated from the above analytical equations, are depicted in Fig. S4, where the surface bands represent two cones touching at the Dirac point within a band gap of the bulk states.

**E. Topological surface states with a single surface at Γ point**

In addition to the case of domain wall hosting two sets of surfaces (Dirac cones) in the dispersion of the surface states, we also were able to obtain a topological surfaces state with dispersion in the form of a single isolated surface at Γ point. In this case the full-wave simulation was conducted for a 3D crystal made out of disks composed of a dual material $\hat{\varepsilon} = \hat{\mu} = \text{diag}[15, 15, 16]$ and with the gauge field induced by the bianisotropy $\chi_{xy} = 5$ in the disks [13]. To ensure that the edge state does not leak into the radiative continuum, a specially designed impedance boundary condition was used to emulate the medium with dielectric parameters $\hat{\varepsilon} = \hat{\mu} = \text{diag}[1, 1, -1000]$, essentially a dual hyperbolic metamaterial, one unit cell away from the crystal. The choice of such bounding material is required to preserve the duality symmetry responsible for the topological phase on the interface that is required to ensure the gapless character of the surface state. The calculated band diagram in two cross-sections of the dispersion surface, $k_{||} - \omega$ and $k_z - \omega$, respectively, is shown in Fig. S5. While practical implementation of such material would be hardly feasible, the presence of the surface band of the form of the single surface simulation confirms the topological nature of the 3D metacrystals where the duality generates the pseudo-spin degree of freedom and the bianisotropy produces the synthetic spin-orbit coupling and indices the topological transition.

![Figure S5](image_url)

**Figure S5** Photonic band structure of the topological surface state in the form of a single surface (red line) within the photonic band gap of the bulk band structure (blue shaded areas). **a** and **b** show two cuts of the surface in the horizontal and vertical directions.
F. Topologically trivial gapless surface states confined to the horizontal domain walls

One major distinction of the proposed 3D photonic structure from its 2D counterparts is related to the possibility of having domain walls facing any direction in 3D space. As an example, here we consider the domain wall in the horizontal (along the $z$-axis) direction, which is formed by stacking the all-dielectric metacrystals so that upper and lower domains have wider sections of the disks facing each other, as shown in Fig. S6(a), with the projected 2D BZ plotted in Fig. S6(b).

The results of the numerical simulations for the all-dielectric metacrystal for the case of such horizontal domain wall are presented in Fig. S6 and also reveal the presence of the surface mode. The corresponding field profile of such surface mode is shown in Fig. S6(c) and the photonic band diagrams are plotted in Fig. S6(d,e). The corresponding ($xy$) domain wall has hexagonal symmetry and effectively represents a quasi-2D lattice with the modes confined in the vertical direction due to the presence of the complete band gap in the upper and lower metacrystals. For a given configuration of the domain wall this symmetry results in the presence of the isolated Dirac-like conical bands, which extends over the entire gapped region [Fig. S6(e)]. However, as one could expect for the weak topological structure formed by stacking planar QSHE layers, these modes are topologically trivial by their nature. They exist solely due to the domain wall playing the role of a high index defect, which facilitates the field localization, and the in-plane hexagonal symmetry, which ensures the presence of the Dirac points at the $K$ and $K'$ valleys. Nonetheless, it is indeed a noteworthy property of our system that, while representing a weak photonic topological insulator, it may exhibit gapless surface modes along both horizontal and vertical cuts.
Figure S6| Surface states of two-dimensional x-y-domain wall in three-dimensional all-dielectric metacrystal. (a) The schematics of the domain wall formed by the reversal of the bianisotropy in the middle. (b) The field profile indicating localization of the surface state to the domain wall at K point. (c,d) Band diagrams of topological surface states supported by the domain wall in (a). (c) Two-dimensional band diagram $\omega$ vs. $k_\parallel$, with $k_\parallel$ changing along the high symmetry directions of the 2D hexagonal Brillouin zone of the domain wall, and (d) the conical Dirac-like dispersion of the surface states near the K-point of the 2D hexagonal Brillouin zone.

G. Dielectric materials for the realization of the metacrystal

While in the design we have used meta-atoms with high dielectric permittivity $\epsilon_d = 81$ embedded into the matrix with $\epsilon_b = 3$, the only purpose of high dielectric contrast was to allow strong localization of the surface modes, which reduces the size of the geometrical domain used in numerical modelling. Nonetheless, in the microwave frequency range materials with high permittivity and low loss are easy to find. For example, the dielectric constant for water is $\epsilon = 81$, for ceramic MgO-CaO-TiO$_2$ it ranges from $\epsilon \approx 20$ to $\epsilon \approx 140$, and for ceramic TiO$_2$-ZrO$_2$ lies within the range $95 - 100$, depending on the composition. Any type of plastics can be involved in order to realize the matrix, for example polyethylene, to host the disks. In the optical domain, the realization of the structure is more challenging, but still possible with the use of
high-index materials, Ge$_2$Sb$_2$Te$_5$ $\varepsilon \approx 30$ [19] and tellurium (Te) $\varepsilon \approx 23$ in infrared [20], and silicon (Si) $\varepsilon \approx 12$ and germanium (Ge) $\varepsilon \approx 16$ in near-infrared, which can be patterned by 3D nanofabrication techniques such as NanoScribe®. We have found that to implement a practical design for optical domain the lack of a very high permittivity can be compensated by reduction of the matrix permittivity. Although the surface states tend to be less localized to the domain walls due to the reduction in the width of the topological bandgap, they remain to be well defined.

References


