Three-dimensional all-dielectric photonic topological insulator

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The discovery of two-dimensional topological photonic systems has transformed our views on the propagation and scattering of electromagnetic waves, and the quest for similar states in three dimensions is open. Here, we theoretically demonstrate that it is possible to design symmetry-protected three-dimensional topological states in an all-dielectric platform, with the electromagnetic duality between electric and magnetic fields being ensured by the structure design. Magneto-electrical coupling plays the role of a synthetic gauge field that determines a topological transition to an ‘insulating’ regime with a complete three-dimensional photonic bandgap. We reveal the emergence of surface states with conical Dirac dispersion and spin-locking, and we numerically confirm robust propagation of the surface states along two-dimensional domain walls with first-principles studies. The proposed system represents a table-top platform capable of emulating the relativistic dynamics of massive Dirac fermions and the surface states can be interpreted as Jackiw–Rebbi states bound to the interface separating domains with particles of opposite masses.

Following in the footsteps of condensed-matter topological systems, significant progress has recently been made in understanding and realizing topological states in classical systems1–25. Unlike fermionic systems, achieving topological states for bosons meets several limitations. While fermions can support topological phases protected by time-reversal (TR) symmetry, in bosonic and classical systems TR symmetry cannot result in any nontrivial topological phase26. Consequently, the traditional approach to engineering topological phase in classical systems relies on removal of TR symmetry. This approach requires either using magnetic materials, which was successfully realized in 2D27–29 and studied theoretically in 3D30, or temporal modulation emulating the effect of an external magnetic field31–33. Recently, a new class of topological states of condensed matter characterized by symmetry-protected topological (SPT) phases has expanded the traditional topological classification based on TR symmetry. Topological properties of the SPT systems originate in crystalline or intrinsic symmetries of the wave fields, which result in a ‘symmetry-restricted’ topological state, and numerous demonstrations have been reported34–36,37. Thus, SPT phases represent attractive means to engineer photonic topological phases without the need to break TR symmetry38,39. The TR symmetry breaking can be a very restrictive requirement in the optical domain, where magneto-optical effects are weak and cannot yield a topological phase from a practical viewpoint. Even in the microwave frequency region, where magneto-optical effects can be strong, the need for magnets and magnetic materials—which are hard to integrate into practical devices—makes SPT phases an appealing alternative.

Three-dimensional SPT systems were predicted to exist in condensed-matter systems34–36, yet have so far not been emulated in photonics. Although a 3D photonic topological insulator (TI) without TR symmetry has been recently discussed40, the suggested design is challenging due to the requirement of non-uniform magnetization of ferrite constituents. The possibility to engineer the topological state of light in 3D while relying on a fabrication-friendly platform is of significant fundamental interest, as it may allow emulating exotic states of matter described by the relativistic Dirac equation in 3D. Such realization may also usher in a broad range of practical applications enabled by topologically robust routing of photons in 3D. This could lead to novel photonic technologies based on the integration of photonic elements and 3D topologically robust optical circuitry.

In the following, we demonstrate a 3D topological photonic metacrystal based on an all-dielectric metamaterial platform41, which for this reason is free from the restrictive requirements characterizing earlier concepts (such as TR-violating systems)9,19,38,39, and at the same time avoids lossy metal-based components9,38. The suggested design could thus be implemented across the electromagnetic spectrum, from the microwave to the visible domain. To our knowledge, this design is also the first to be based on the concept of ‘weak’ 3D TIs, originally proposed in solid-state physics42–44, which now takes advantage of a versatile photonic platform. Originally assumed to be less robust than the ‘strong’ 3D TIs, weak 3D TIs have been recently shown to possess rich physics and unexpectedly strong protection against disorder42, when combined with their straightforward practical realization, the latter feature becomes of significant interest in photonics.

Results

Design of the topological metacrystal. Corroborated by rigorous numerical simulations, we demonstrate that SPT nontrivial states can be engineered in metacrystals that preserve electromagnetic duality—an internal symmetry of the electromagnetic fields responsible for the SPT phase9,21,22,38. To this end, the duality of the electromagnetic eigenmodes, otherwise broken by the material’s response9, is restored by careful design of the building
blocks of the 3D photonic lattice, referred to as meta-atoms. This ensures the presence of a proper pseudo-spin degree of freedom, which is odd under TR operation, and enables emulation of a weak 3D topological phase of light. Introduction of bianisotropy into such a dual system is achieved by proper reduction of the weak 3D topological phase of light. The BZ of the 3D hexagonal lattice is shown as an inset between a and b. Insets in c, d. 2D projection of the 3D Dirac cone in the vicinity of the K point and emergence of the topological bandgap induced by the bianisotropy. The structure parameters are \( a_0 = 6.5 \text{ cm}, a_1 = 0.69a_0, d = 4.76 \text{ cm}, h = 2.11 \text{ cm}, \epsilon_{d} = 81, \epsilon_{p} = 3 \).

The topological photonic metacrystal introduced here is schematically shown in Fig. 1a. It features a 3D hexagonal lattice of dielectric disks with permittivity \( \epsilon_d \) embedded into a matrix with permittivity \( \epsilon_p \). The dielectric disks (meta-atoms) and their 3D periodic arrangement are designed so that the photonic band structure exhibits two overlaid 3D Dirac points near the K and K’ points in the Brillouin zone (BZ), as shown in Fig. 1. The structure parameters were optimized such that there is a frequency range where only the two 3D Dirac cones exist, that is, there are not any other modes for any Bloch vector within the 3D BZ that would belong to this frequency range. Each of the four observed Dirac bands originates from the electric and magnetic dipolar modes of the disks with their dipole moments aligned in the \( x-y \) plane and perpendicular to the axes of the disks (Fig. 2a). It is important that the very possibility to emulate a true 3D Dirac dispersion with the four linear bands overlaid in a pairwise manner—the characteristic of relativistic massless spin-\( \frac{1}{2} \) fermions described by the Dirac equation—is enabled by the duality symmetry of the system. Electromagnetic duality is a natural property of the electromagnetic field in free space, which reflects the symmetry of Maxwell’s equations with respect to the electric and magnetic components of electromagnetic waves. This symmetry, which is typically broken by an uneven material’s response to electric and magnetic fields, is restored in our structure for the in-plane \( (xy) \) components thanks to its careful design. Therefore, this...
The same happens for the system studied here if the duality is violated. However, it is important to mention that the duality is provided by the design of the meta-atoms, and stems largely from the local response. As a result, the SPT phase reported here can be quite robust against lattice perturbations, which are one of the most common classes of disorder. Moreover, our previous 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) is tolerated to some degree, that is, as long as the perturbation to the band structure due to a mismatch between magnetic and electric dipolar modes does not exceed that produced by the bianisotropy.

The metacrystal with broken $\sigma_z$ symmetry, achieved by removing part of the dielectric disks, is shown in Fig. 1b. Its band structure, given in Fig. 1d, clearly reveals a full omnidirectional 3D bandgap. The modes of this gapped structure do not resemble those of the former Dirac points. This magneto-electric coupling, referred to as bianisotropy, has an effect equivalent to the spin–orbit interaction in condensed-matter systems (Supplementary Sections A and B).

As for any other SPT phase, breaking the underlying symmetry eventually results in the removal of vital degeneracies in the band structure and in the collapse of the topological phase. In topological crystalline insulators, for example, disorder destroys the topological state and improper surface cuts produce a gap in the surface states.
bands at the K point, the K′ point can be described by an effective Hamiltonian (see Methods).

\[ H = \omega_0 + \gamma_1 \hat{\sigma}_x (\delta k_x \hat{\sigma}_z + \delta k_y \hat{\sigma}_y) + \gamma_2 \hat{\sigma}_z (\delta k_z + m \hat{\sigma}_z) \]  

(1)

where \( \hat{\sigma}_x \) and \( \hat{\sigma}_z \) are Pauli matrices operating in the subspaces of polarization (pseudo-spin) and orbital momentum (dipole/p-orbital orientation), respectively, \( m \) is the effective mass term induced by the bianisotropy, \( \omega_0 \) is the frequency of the Dirac bands at the K point, \( \gamma_1 \) is the in-plane (out-of-plane) Dirac velocity and \( \delta k \) is the deviation of the wavevector from the K point. The Hamiltonian in equation (1) describes the 3D Dirac conical dispersion with the mass term inducing a bandgap opening and leading to the appearance of the surface state at the domain walls (Supplementary Section D). Note that the Hamiltonian in equation (1) also provides a local description near the K point with the sign of the mass term reversed, \( m \rightarrow -m \).

Interestingly, the structure of the Hamiltonian can also be understood in terms of the field profiles of the modes shown in Fig. 2a. Specifically, we consider here two mechanisms of bianisotropy induced by breaking the \( \varepsilon_z \) symmetry, which can be due to (i) the change in the disks geometry or (ii) the out-of-plane propagation \( k_z \neq 0 \). Thus, the first mechanism of symmetry reduction leads to the mass term in equation (1). It represents a conventional (geometrical) bianisotropy, that is, coupling between electric (even) and magnetic (odd) modes and, as it follows from equation (1), can be understood as the result of mixing of the same components of the electric fields of the two sub-bands in Fig. 2a.

The perturbative approach also makes it possible to consider the second mechanism of bianisotropy due to the finite values of \( \delta k_z = k_z \) (the third term in equation (1)), which is essential for 3D Dirac dispersion in our system. In this case, as follows from equation (2) (see Methods), the gap opening is the result of hybridization between even and odd modes via mixing of electric and magnetic field components phase-shifted with respect to each other by \( \pi/2 \), as illustrated in Fig. 2b. Equation (2) also yields the second term in the Hamiltonian (equation (1)), describing the gap opening for a finite in-plane propagation \( \delta k_{||} \neq 0 \) (for symmetric disks and \( \delta k_z = 0 \)). In this case, the mixing of odd and even modes does not occur and the gap opens solely due to the mixing of the electric and magnetic field components of the same mode, leading to the well-known in-plane Dirac-like spatial dispersion.

The effective photonic Hamiltonian in equation (1) is equivalent to a family of condensed-matter Hamiltonians locally describing 3D...
topological phase is the emergence of gapless surface states, which is one of the most important consequences of stacking 2D topological systems. Therefore, the system under study represents a photonic analogue with these 2D structures, and it exhibits a weak topological phase emerging from stacking 2D topological systems.

Gapless surface states. One of the most important consequences of topological phase is the emergence of gapless surface states, which may occur either on the external interfaces with a topologically trivial system or at the domain walls separating two topological systems of distinct classification. A 2D topological domain wall separating 3D structures with opposite signs of the effective mass \( m \), that is, opposite bianisotropy, fulfills the requirements imposed by the SPT phase of the proposed design (see Methods): (i) it preserves the duality and the pseudo-spin degree of freedom and (ii) it prevents leakage of the surface states due to the presence of a complete 3D bandgap in both topological half-spaces. Such 2D domain walls should host topological surface states exhibiting linear 2D Dirac-like dispersion, with the Dirac cones that always appear in pairs at the \( K \) and \( K' \) points projected onto the 2D surface of the corresponding cut of the crystal.

The analytical calculations within the effective Hamiltonian approach (Supplementary Section D) indeed predict the presence of gapless surface states confined to the domain walls. Unlike 2D systems such as graphene, quantum spin Hall states and their photonic analogues, which are described by two-component wavefunctions and host edge states with linear 1D bands, the 3D system under study is locally (near the \( K \) and \( K' \) points) described by the four-component wavefunction. Therefore, it emulates even more closely the relativistic Dirac equation, exhibiting 2D surface states with conical bands. In this context, the surface modes can be viewed as the well-known Jackiw–Rebbi states, which exist at the boundary between two half-spaces hosting relativistic quantum particles of opposite mass. Thus, the system studied here can also be viewed as a classical emulator of 3D relativistic Dirac fermions.

To corroborate our analytical results, we performed a set of large-scale full-vector numerical simulations with the finite-element method solver COMSOL Multiphysics. First, we considered the vertical topological domain wall in the middle of a supercell of 24 meta-atoms with the periodic boundary conditions imposed in all three directions. The domain wall represents an interface between two topological crystals whose meta-atoms have their narrow section facing opposite directions along the \( z \) axis, which results in the reversal of bianisotropy across the wall. The schematic view of the structure with such a vertical domain wall and the 3D BZ projected onto the corresponding rectangular 2D cut are shown in Fig. 3a,b, respectively. The band structure for this case is presented in Fig. 3c,d, where the two panels in Fig. 3c show two different cuts of the 2D band structure \( \omega(k_x, k_y) \) along high-symmetry directions in the projected rectangular 2D BZ and reveal two pairs of surface states. The surface states appear within the bandgap region and cross it such that they interconnect lower and upper bulk bands. The 3D band diagram shown in Fig. 3d exposes one of the Dirac cones corresponding to the surface states near the projected K point of the 3D BZ (an identical cone at \( K' \) is not shown). The confinement of the surface states to the domain wall is confirmed by their field profiles for all directions within the plane of the domain wall. As an illustration, the corresponding electric-field densities are plotted in Fig. 4b, for several points on one of the isofrequency contours shown in Fig. 4a.

At this point, it is important to emphasize the difference between the discovered surface states and conventional surface waves of photonic crystals, which may also exhibit a Dirac-like dispersion. The latter typically happens for any 3D crystal when the interface possesses a hexagonal symmetry. In this case, the surface states with Dirac-like dispersion emerge at the \( K \) and \( K' \) points as a direct consequence of the lattice symmetry. However, the surface states reported here appear on the vertical cut, and its ‘rectangular symmetry’ alone cannot result in the emergence of surface states with conical dispersion. Indeed, in our case, the Dirac cones emerge at the projected K and K’ points of the 3D lattice that do not represent high-symmetry points of the projected 2D rectangular BZ. This is another confirmation that the surface states on the vertical domain walls are ensured by duality and bianisotropy and, therefore, are topological in their nature.

Spin-locking of the surface states. As in the case of 3D electronic TIs, the surface states in our system also exhibit a property of spin-locking that endows the system with topological robustness. Both analytical results (Supplementary Section D) and numerically

![Figure 4](https://example.com/figure4.png)

**Figure 4 | Spin-locking of the topological surface states.** **a.** The isofrequency (0.99 GHz) contour on the Dirac cone illustrating the property of spin-locking. The polarization configurations of electric and magnetic field components are illustrated by red and blue arrows both schematically and from numerical results given by the fields inside the cross-sections of the dielectric disks for eight points on the contour indicated by blue dots and numbers. The phase shift between electric and magnetic dipolar components \( \Delta \) varies from 0 to 2\( \pi \) along the contour. **b.** The field profiles illustrating the localization of the surface states to the domain wall for the values of the wavevector on the contour shown in **a.**
calculated field profiles show that the pseudo-spin configuration is uniquely defined by the direction of the surface mode wavevector \( \mathbf{k} \). This property of spin-locking of the pseudo-spin degree of freedom to the propagation direction of the surface states is the key property responsible for the robustness of the surface states. Spin-locking can be directly seen by calculating the expectation value of the spin onto the coordinate plane \((y-z)\) of the domain wall for the effective Hamiltonian in equation (1). This leads to the expression

\[
\langle \psi_{\pm}^{(1)} | \hat{S}_z | \psi_{\pm}^{(1)} \rangle = \frac{v_x k_z}{\Omega_x} \hat{y} + \frac{v_y k_z}{\Omega_y} \hat{z}
\]

where \( \Omega_x \) is the eigenfrequency of the surface state, which shows that for all values of \( k_z \) the eigenstates are characterized by a spin rotated with respect to their propagation direction, as schematically depicted by the coloured arrows in Fig. 4a.

In addition to this analytical description, the full-wave numerical results also allow us to explain the property of spin-locking in terms of the electric and magnetic fields of the surface states. To this aim, it is instructive to use the unique correspondence between the spin and the orbital momentum of the surface states that occurs due to the spin–orbit coupling induced by the bianisotropy. It has been previously demonstrated in 2D \(^3\) that the electric and magnetic dipolar components of the edge state appear to be circularly polarized and are in phase and out of phase with respect to each other for opposite spins and propagation directions, thus revealing the spin-locked character of the mode. This property can be generalized to the 3D case, where the phase between the two electric and magnetic dipoles varies continuously along the iso-frequency contour from 0 to \( 2\pi \) and, at the same time, the polarization of the electric dipolar components varies from circular left to linear to circular right, as indicated in Fig. 4a.

Figure 5 | Topological robustness of surface states propagating along a sharply curved 2D domain wall formed in the middle of the all-dielectric 3D topological insulator. a, The shape of the domain wall: blue and orange circles indicate up and down orientations of the meta-atoms, respectively. b–f, The field distribution of the surface modes propagating without reflection across the domain wall with the sequence of sharp bends depicted in a. Each subplot corresponds to a given value of the out-of-plane wavevector component \( k_z \).

The edge and surface states of topological systems are of significant interest due to their unique property of topological robustness, which manifests itself as reflectionless propagation and insensitivity to defects and disorder that do not violate the symmetry underlying a particular SPT state. We show that the surface states of the 3D all-dielectric system considered here exhibit a similar property. To this end, we performed first-principles numerical studies of the surface states propagating along a curved topological domain-wall with two sharp bends, as shown in the top left panel of Fig. 5a. In contrast to the edge modes confined to 1D interfaces of 2D topological systems, the 2D surface states of our 3D metacrystal can propagate in two dimensions. This allows us to test their robustness for multiple values of the out-of-plane wavenumber \( k_z \), which is equivalent to sweeping the wavevector along the circular iso-frequency contour in Fig. 4a. The results of the numerical simulations for the vertical cut of the domain wall are shown in Fig. 5, and demonstrate that the field intensity remains uniform as it propagates along the domain wall regardless of the bends. Hence the wave avoids back-reflection from the sharp bends; in particular, this circumvents formation of standing-wave interference patterns that would necessarily occur in the straight segments of any conventional non-topological waveguide. In 2D photonic systems this robustness of the edge modes has been attributed to the property of pseudo-spin locking, which manifests as the one-to-one correspondence between a polarization configuration of the wave and its propagation direction. The same holds true for the 3D system studied here, with the exception that the pseudo-spin of the mode changes continuously as the wavevector sweeps around the Dirac cone (Fig. 4a and Supplementary Section D). However, it is worth noting that by experiencing a sequence of scattering events the surface state can always make a 180° turn that, due to the spin-locking property, will be accompanied by a spin flip. In this respect, 3D TIs (either photonic or electronic) can be viewed as less robust than their 2D ‘cousins’. Nonetheless, if compared to transport through non-topological states, transport through surface states in 3D TIs will be robust because the likelihood for disorder to produce a 180° turn through a sequence of scattering events is small.
Discussion
We have theoretically demonstrated the first implementation of a weak 3D photonic TI. The all-dielectric metacrystal design proposed here represents a classical toy model emulating relativistic fermions, offering unique opportunities to study fundamental physics in a predictable and highly controllable manner. Such table-top all-dielectric photonic structures could be precisely engineered to exhibit fascinating physical phenomena that have so far evaded observation. In particular, the observation of the surface states predicted here would provide the first experimental evidence for the existence of edge states with coherent and robust wave localisation, i.e. unconventional topological edge states that exhibit reflectionless routing of electromagnetic radiation along arbitrarily shaped pathways in 3D, which makes these modes promising for applications in photonics. The proposed all-dielectric platform could also avoid undesirable effects such as ohmic loss, which is inevitably present in metallic and plasmonic structures. Our design facilitates topological states in photonic-compatible dielectric and semiconductor materials (see the discussion in Supplementary Section G), thus reducing the technical difficulties associated with the use of magnetic materials and external magnets required to induce topological order in systems with broken TR symmetry.

Methods
Methods and any associated references are available in the online version of the paper.

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Methods

Electromagnetic perturbation theory. In the perturbative approach, we construct the effective Hamiltonian starting with the trivial four-fold degeneracy at the K point and introduce two classes of perturbations: (i) the dielectric perturbation induced by the removal of a circular segment of the disks and (ii) the perturbation induced by the change in the propagation direction (deviation from the K point). The effect of both of these perturbations was determined from numerically calculated unperturbed fields (that is, for the symmetric disk at the K point) by using equations of degenerate perturbation theory (Supplementary Section A). This theory can be summarized by the following two equations, which allow us to calculate matrix elements of the 4 × 4 Hamiltonian (up to a normalization factor):

$$\Delta_{mn} = -\int d^3r \delta E_i a_{E,\alpha} E_n^\alpha$$

$$\{S\}_{mn} = \int d^3r \left\{ E_i \times H_m^\alpha + E_m^\alpha \times H_n \right\}$$

where $\Delta_{mn}$ describes the change in the Hamiltonian due to the perturbation of the dielectric constant by $\delta E_i(r)$, while $\{S\}_{mn}$ reflects the change due to the displacement of the Bloch vector from the K point, $E_i$ and $H_n$ are electric and magnetic fields of the unperturbed n-th eigenmode and the integration is over the unit cell volume $V$. Each of the four unperturbed eigenmodes corresponding to the two overlaid Dirac cones near the K (K') point can be labelled by its symmetry with respect to $\sigma_y$ as electric (even) or magnetic (odd) and lower or upper half of the cone, as shown in Fig. 2. These modes constitute the four-component basis wavefunctions $\psi = [a_1^{(even)}, a_3^{(even)}, a_2^{(odd)}, a_4^{(odd)}]$, where the amplitude $a_{m(\alpha)}$ is the linear dipolar polarization of the electric (magnetic) mode. Then, the matrix obtained with the use of equations (2) and (3) can be transformed (i) in the angular momentum (dipolar) subspace with the use of unitary operator $U_1 = [\exp(-ia/2), i\exp(-ia/2), -\exp(ia/2), i\exp(ia/2)]$, which brings the modes to the basis of circularly polarized states where a parametrizes the cut of the Dirac cone at a constant frequency $38$, and (ii) in the pseudo-spin subspace (constituted by the electric and magnetic degrees of freedom) $U_2 = [1,1; 1, -1]$, which brings it to the basis of spin-up and spin-down modes $9$. These two transformations allow us to construct the effective Dirac-like Hamiltonian of the form given in equation (1).

Choice of the topological interface. While in condensed-matter physics one typically considers a natural boundary of a TI with the topologically trivial vacuum, in electromagnetics such an open boundary would necessarily lead to power leakage of the surface states, at least for a subset of the wavevectors lying above the light cone. However, even for modes lying below the light cone, any encounter of a defect (even a topology-preserving defect) will result in scattering into free space. Another seemingly natural choice as an interface to a topological system is a perfect electric conductor (PEC). While known to work in systems with TR-symmetry broken by magnetization $3,4$, this is not always a suitable choice for SPT systems as it can break the symmetry underlying the topological phase, including the duality. Indeed, since the PEC boundary condition has a different effect on the electric and magnetic components of the fields, it violates the duality, which in turn results in a breakdown of the pseudo-spin degree of freedom and prevents the formation of the topological surface state at the interface.

We note that in addition to the surface states confined to the domain wall, which necessarily hosts two Dirac cones, we were able to obtain a surface state with the dispersion in the form of a single isolated surface at the Γ point (Supplementary Section E) for proper dual boundary condition. However, such dual boundary is hardly feasible in practice.

Data availability. Data that are not already included in the paper and/or in the Supplementary Information are available on request from the authors.