Topologically Localized Insulators

Bastien Lapierre, Titus Neupert, and Luka Trifunovic
Department of Physics, University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland

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We show that fully localized, three-dimensional, time-reversal-symmetry-broken insulators do not belong to a single phase of matter but can realize topologically distinct phases that are labeled by integers. The phase transition occurs only when the system becomes conducting at some filling. We find that these novel topological phases are fundamentally distinct from insulators without disorder: they are guaranteed to host delocalized boundary states giving rise to the quantized boundary Hall conductance, whose value is equal to the bulk topological invariant.

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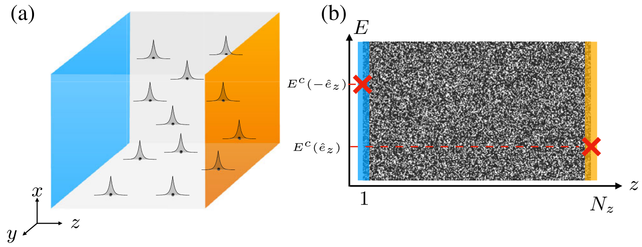
Introduction.—The discovery of the quantum Hall effect revealed that topology, a branch of mathematics, plays an important role for understanding properties of quantum materials. Topological quantum materials are typically bulk insulators with boundaries that are perfect metals [1,2]. Further developments [2,3] showed that superconductors can be topological, too. These developments led to the complete classification of (noninteracting) topological phases, the result known as tenfold way or "periodic table of topological phases of matter" [4,5]. The modes that appear on the boundary of topological quantum materials are called topological and anomalous—they typically give rise to either quantized electrical or thermal responses and promise many applications in the areas of quantum computing [3], backscattering-free quantum transport, and even catalysis [6].

More recently [7–15], it was shown that crystalline symmetry adds a new twist to the topological classification: a three-dimensional topological crystalline insulator or superconductor can have topological modes (states) appearing on its hinges (corners) while its faces (and hinges) are insulating. Interestingly [10,16,17], crystalline symmetry can turn an atomic insulator topological, in which case they may or may not have fractionally quantized boundary charges. Moreover, the crystalline symmetry facilitates the discovery of topological materials [18–22], with many thousand candidates being predicted [18,23] and some experimentally confirmed [24–28].

Not only the boundary of a topological material but also its bulk electronic states have intriguing properties: all topological insulators, in the absence of crystalline and sublattice symmetries, have an obstruction to full localization of its occupied bulk electronic states [29]. This property is best studied in the case of quantum Hall insulators [31], where in the presence of disorder topology guarantees the existence of a single energy per Landau level where delocalized states appear. Similarly, the obstruction to full localization was established for the case of quantum spin Hall [32] and three-dimensional topological insulators [33]. Hence, within the tenfold-way paradigm, a fully localized insulator (i.e., an Anderson insulator at all fillings) is guaranteed to be topologically trivial.

In this Letter, we introduce a new notion of topology that applies to fully localized insulators, i.e., Anderson insulator at *all* fillings, in contrast to tenfold-way topological phases which are required to be insulating only at one particular filling [34]. In particular, we consider three-dimensional systems without time-reversal symmetry and find topologically distinct fully localized insulators that can be labeled by integers. The phase transition can occur only if the system becomes conducting at some filling. We refer to these topologically nontrivial phases as "topologically localized insulators" (TLIs). We show that, although all the bulk states of a TLI are exponentially localized, there is an obstruction to localizing them all the way down to an atomic limit. Importantly, electronic states with support close to the boundary carry quantized Hall conductance which can be measured in the Corbino geometry via flux insertion. Note that, for the slab geometry in Fig. 1(a), the boundary consists of two disjoint planes with normals $\pm\hat{e}_z$, and the Hall conductances of these two planes are quantized to the opposite value due to their opposite orientation. Furthermore, at each of these planes, topologically protected delocalized states [31] emerge and remain so under an arbitrarily strong disorder at the boundary, see Figs. 1(b) and 1(c). We conclude that the boundary of a TLI is anomalous since it cannot be realized as a two-dimensional system: a disordered two-dimensional Chern insulator can host delocalized bulk states only up to disorder strengths that do not close its mobility gap [36]. (A Chern insulator is a finite-dimensional Hilbert-space version of a quantum Hall insulator.)

Model.—We construct a TLI by stacking two-dimensional layers in the z direction. We divide the Hilbert space spanned by electronic orbitals of a single layer into the blue and the orange subspaces, see Fig. 2(a). We require that for the blue



(c)

	Strong TI	TLI
Bulk	Obstruction to full localization	Fully localized
Boundary	Delocalized	Obstruction to full localization

FIG. 1. (a) TLI with $N_{\rm TLI} = 1$ for open boundary conditions along z direction only: all the bulk states are localized by disorder, while the two boundary surfaces (orange and blue) host delocalized states and have opposite quantized Hall conductance. (b) The energies $E^c(\pm\hat{e}_z)$ of delocalized states are not constrained by the bulk. (c) Comparison between TLIs and strong topological insulators (TIs). (A TI is called strong if its existence does not rely on translational symmetry.).

(orange) subspace filled with electrons, the layer has Hall conductance $\sigma_{xy} = e^2/h$ ($\sigma_{xy} = -e^2/h$). Hence, not all blue (orange) orbitals in Fig. 2(a) can be exponentially localized. On the other hand, if we couple the blue orbitals from the layer z to the orange orbitals from the layer $z+1$, the hybridized orbitals can be all exponentially localized, as in the case of eigenstates of the following tight-binding model of a TLI:

$$H = \sum_{\vec{R}\alpha,\vec{R}'\alpha'} t_{\vec{R}\alpha}^{\vec{R}'\alpha'} |\vec{R}\alpha\rangle\langle\vec{R}'\alpha'|, \tag{1}$$

with the hopping amplitudes and on-site potentials (for $\vec{R} = \vec{R}'$) expressed as

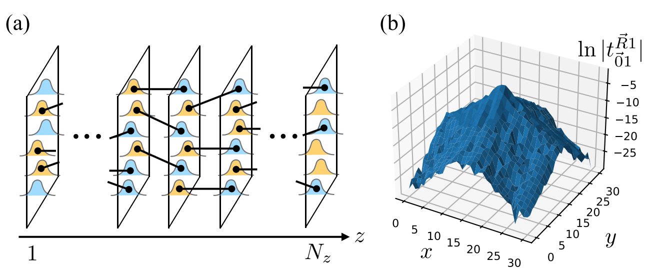


FIG. 2. (a) TLI construction from stack of two-dimensional layers in z direction. The Hilbert space of each layer is divided into two subspaces spanned by blue and orange orbitals: occupying only blue (orange) orbitals with electrons results in quantized Hall conductance of the layer $\sigma_{12} = e^2/h$ ($\sigma_{12} = -e^2/h$). The blue (orange) orbitals cannot all have exponential localization; exponential localization is obtained by hybridizing differently colored orbitals from neighboring layers. (b) Distance dependence of the hopping elements $\ln|t_{\vec{0}1}^{\vec{R}1}|$ of the TLI with $\vec{R} = (x, y, 0)$ for the system size $N_x = N_y = 31$, where $t_{\vec{0}1}^{\vec{R}1}$ is defined below Eq. (1). We observe an exponential decay of the hopping elements $t_{\vec{0}1}^{\vec{R}1}$ in all directions.

$$t_{\vec{R}\alpha}^{\vec{R}'\alpha'} = \sum_{\vec{R}''\alpha''} W_{\vec{R}''\alpha''} C_{\vec{R}\alpha}^{\vec{R}''\alpha''} (C_{\vec{R}'\alpha'}^{\vec{R}''\alpha''})^*. \tag{2}$$

The atomic orbitals of the above stack of layers are denoted by $|\vec{R}\alpha\rangle$, with $\alpha \in \{1,2\}$ an orbital degree of freedom and $\vec{R}$ a three-dimensional cubic lattice vector. $W_{\vec{R}\alpha}$ are independent, uniformly distributed in $[-W, W]$, random real numbers. The coefficients $C_{\vec{R}'\alpha'}^{\vec{R}\alpha}$ are defined through the lattice vector basis expansion of the wave functions

$$|w_{\vec{R}\alpha}\rangle \equiv \mathcal{P}_z^-|\vec{R}\alpha\rangle + \mathcal{P}_{z+1}^+|(\vec{R}+\hat{e}_z)\alpha\rangle, \tag{3}$$

i.e., $|w_{\vec{R}\alpha}\rangle = \sum_{\vec{R}'\alpha'} C_{\vec{R}'\alpha'}^{\vec{R}\alpha}|\vec{R}'\alpha'\rangle$, where $\mathcal{P}_z^+$ ($\mathcal{P}_z^-$) is the projector onto the blue (orange) subspace of the layer z. Such $\mathcal{P}_z^+$ and $\mathcal{P}_z^-$ can be obtained as the projectors on the occupied and empty bands of a two-band (disorder-free) Chern insulator defined on layer z (see Supplemental Material [37] for a concrete model). It is crucial to note that $|w_{\vec{R}\alpha}\rangle$ are exponentially localized, and orthonormal $\langle w_{\vec{R}'\alpha'}|w_{\vec{R}\alpha}\rangle = \delta_{\vec{R}\vec{R}'}\delta_{\alpha\alpha'}$, leading to exponentially decaying matrix elements $t_{\vec{R}\alpha}^{\vec{R}'\alpha'}$, see Fig. 2(b). The exponential localization of $|w_{\vec{R}\alpha}\rangle$ follows from that of $\mathcal{P}_z^{\pm}|\vec{R}\alpha\rangle$ [42], whereas orthonormality can be satisfied only for the Hilbert space onto which $(\mathcal{P}_z^- + \mathcal{P}_{z+1}^+)$ projects, see Supplemental Material [37]. The states $|w_{\vec{R}\alpha}\rangle$ form a complete set of localized eigenstates of H under periodic boundary conditions.

From the above construction it is evident that for a z-terminated crystal, there are unpaired blue (orange) orbitals on the layer $z = 1$ ($z = N_z$) which, when filled with electrons, give quantized Hall conductance $\sigma_{xy} = e^2/h$ ($\sigma_{xy} = -e^2/h$), see Fig. 1. Additionally, if a magnetic flux quantum $\Phi_0 = h/e$ is threaded through the layers, the blue subspace of each layer expands to accommodate one more electron, while the orange subspace shrinks by the same amount—this statement is know as Streda's theorem [43]. Hence, if the bulk is fully filled with electrons, the applied flux Φ_0 transfers one electron from layer z to layer $z+1$ resulting in the bulk polarization $P_z \sim 1$. Accordingly, the corresponding component of the bulk magnetoelectric (ME) polarizability tensor is quantized, $(\alpha_{\rm ME})_{zz} = 1$.

The construction presented above resembles pictorially the construction of both the one-dimensional dimerized Su-Schrieffer-Heeger model [44] and the Kitaev chain [3]. Despite this similarity, we find the obtained phase to be truly three-dimensional: the quantized surface Hall conductance takes the same value for every orientation of the boundary, as we demonstrate numerically further below. Furthermore, the bulk magnetoelectric polarizability tensor is found to be isotropic $\alpha_{\rm ME} \equiv (\alpha_{\rm ME})_{ii} = 1$. This statement is further corroborated by the existence of a truly three-dimensional bulk topological invariant.

Bulk topological invariant $N_{\rm TLI}$.—For a bulk Hamiltonian H, with all eigenstates localized, the unitary U that diagonalizes H can be chosen such that its matrix elements are exponentially localized in the basis $|\vec{R}\alpha\rangle$

$$\langle\vec{R}'\alpha'|U|\vec{R}\alpha\rangle \sim e^{-\gamma|\vec{R}-\vec{R}'|}, \qquad (4)$$

for some positive constant γ. More concretely, we define U as mapping localized eigenstates $|\psi_n\rangle$ of H onto atomic orbitals $|\vec{R}\alpha\rangle$, i.e., $U|\vec{R}\alpha\rangle = |\psi_{n(\vec{R},\alpha)}\rangle$, such that condition (4) is satisfied. The assignment defined by $n(\vec{R},\alpha)$ is not unique [45]. The bulk integer invariant can be expressed as $N_{\rm TLI} = \nu[U]$,

$$\nu[U] = \frac{i\pi\epsilon^{ijk}}{3V}\mathrm{Tr}(U^\dagger[\hat{X}_i,U]U^\dagger[\hat{X}_j,U]U^\dagger[\hat{X}_k,U]), \quad (5)$$

with $V = N_x N_y N_z$ being the volume of the system and $\hat{X}_i = \sum_{\vec{R}\alpha} R_i|\vec{R}\alpha\rangle\langle\vec{R}\alpha|$ the ith component of the position operator, $i = 1, 2, 3$, $\vec{R} = (x, y, z)$, and the summation over repeated indices is assumed (We note that similar invariant appears in the anomalous Floquet-Anderson insulator and its multi-drive generalization [46,47]). The above expression is guaranteed to take integer values as long as (4) is satisfied [48]. Note that, for a finite system size, the commutators $[\hat{X}_i, U]$ need to be approximated, see Supplemental Material [37]. It can be analytically shown that $N_{\rm TLI} = 1$ for the model (1), see Ref. [37].

Expression for the boundary Hall conductance σ^∂_{12}.—We consider a slab geometry with the width much larger than the localization length. Let us denote the eigenstates of H that are localized on one of the two surfaces by $\{|\psi_n^{\rm surf}\rangle\}$, irrespective of their energy. Since all the bulk states are localized, some of these states can be safely included in the set $\{|\psi_n^{\rm surf}\rangle\}$ without affecting the resulting surface Hall conductance. The Hall conductance of the system when the states $\{|\psi_n^{\rm surf}\rangle\}$ are filled with electrons is given by the Chern number [36] $\sigma^\partial_{12} = (e^2/h)\mathrm{Ch}[\mathcal{P}^{\rm surf}]$,

$$\mathrm{Ch}[\mathcal{P}] = \frac{2\pi i}{N_1 N_2}\mathrm{Tr}(\mathcal{P}[[\hat{X}_1,\mathcal{P}],[\hat{X}_2,\mathcal{P}]]), \qquad (6)$$

where $\mathcal{P}^{\rm surf} = \sum_n |\psi_n^{\rm surf}\rangle\langle\psi_n^{\rm surf}|$ and $\hat{X}_{1,2}$ are the two components of the position operator along the slab. When the matrix elements of $\mathcal{P}^{\rm surf}$ are exponentially localized, analogous to condition (4) with $\mathcal{P}^{\rm surf}$ in place of U, $\mathrm{Ch}[\mathcal{P}^{\rm surf}]$ is guaranteed to take integer values [36].

The bulk-boundary correspondence of TLIs takes the following form:

$$\sigma^\partial_{12} = N_{\rm TLI}\frac{e^2}{h}. \qquad (7)$$

We demonstrated that the above relation holds for the model above Eq. (1), for the z-terminated crystal. Below we demonstrate numerically that it also holds for the x- and y-terminated crystals (hard-wall boundary), as well as for a perturbed version of the model (1). The general proof of relation (7) for an arbitrary model of a TLI in the same phase as (1) directly follows, as the surface Hall conductance can change only if delocalized states move to the surface, which is forbidden for TLIs in the same phase, as all the states in the bulk are localized.

The quantized Hall conductance of a TLI's boundary comes together with the quantized (isotropic) magnetoelectric polarizability coefficient $\alpha_{\rm ME}$ of its bulk. This follows directly from the arguments presented in Ref. [49]: when the slab is fully filled with electrons, the electrons are "inert" and do not respond to an external magnetic field. Since the boundary has nonzero quantized Hall conductance, it follows from the Streda theorem [43] that the filling of the boundary changes by an integer amount $(\sigma^\partial_{12}h/e^2)$ when the flux $\Phi_0 = h/e$ threads the slab. This charge needs to be compensated by the bulk; from this compensation, it follows that the bulk, fully filled with electrons, has an isotropic and quantized magnetoelectric polarizability tensor $\alpha_{\rm ME} = N_{\rm TLI}$.

Numerical results.—We perturb the model in Eq. (1) by including nearest-neighbor hopping that eventually pushes the TLI into a metallic phase. We define $H(\lambda) = H + \lambda H'$ with

$$H' = \sum_{\langle\vec{R}\vec{R}'\rangle\alpha}(t_1|\vec{R}'\alpha\rangle\langle\vec{R}\alpha| + t_2|\vec{R}'\alpha\rangle\langle\vec{R}\,\bar{\alpha}\,|) + \mathrm{H.c.}, \quad (8)$$

where $\bar{1} = 2$, $\bar{2} = 1$, and $\langle\vec{R},\vec{R}'\rangle$ denotes summation over all nearest-neighbor pairs of lattice vectors. Below, we set $t_1 = 10t_2 = 1$, $W = 1$, and consider a one-parameter family of the Hamiltonians $H(\lambda)$, $0 \le \lambda \le 1$.

We first study the metal-insulator transition using level spacing statistics. To this end, we compute the average level spacing ratio [50,51] $r = \langle\langle r_n\rangle_n\rangle_W$ around the middle of the spectrum, where $r_n = \min\{s_n, s_{n+1}\}/\max\{s_n, s_{n+1}\}$ with $s_n = E_{n+1} - E_n \ge 0$ being the level spacing and E_n, $n = 1, \ldots, 2V$, the ordered eigenvalues of $H(\lambda)$. For $\lambda < \lambda_c$, r decreases with increasing system size, approaching the value $r_{\rm PE} \approx 0.38$ of the Poisson ensemble (PE). All eigenstates are localized in this regime. For $\lambda > \lambda_c$, r increases with increasing system size, approaching the value $r_{\rm GUE} \approx 0.60$ of the Gaussian unitary ensemble (GUE). The system is in a metallic phase at half-filling (a mobility edge appears). From this one-parameter scaling, we find the metal-insulator transition at half filling occurs at $\lambda_c \approx 0.088 \pm 0.002$, see Fig. 3(a).

As long as $H(\lambda)$ is in the localized phase, the condition (4) is satisfied and $N_{\rm TLI}$ and σ^∂_{12} are guaranteed to take integer values for large enough system size [36,48]. In practice, for the system sizes we consider in Fig. 3, we find that the quantization of $N_{\rm TLI}$ and $\sigma^\partial_{12}h/e^2$ breaks before the value of λ_c is reached. In Fig. 3, we show that the range of λ

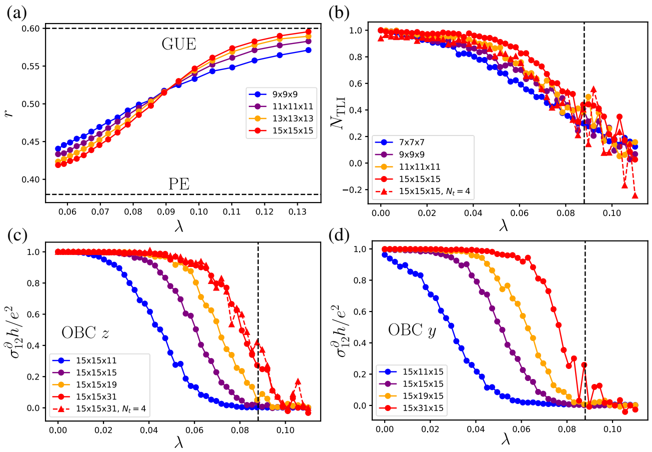


FIG. 3. (a) Estimate of λ_c from mean level spacing ratio r as function of λ.r is computed over 500 eigenstates in the middle of the spectrum, considering 10^3 disorder realizations. (b) The winding number N_{TLI} is computed for different system sizes with increasing hopping strength λ, where the quantized plateau increases with system size for $\lambda < \lambda_c$. (c) Surface Chern number for the hard-wall open boundary conditions (OBC) in z direction as function of λ. (d) Same as (c), for OBC in y direction. No disorder averaging was performed for the winding and Chern numbers, apart from the blue curves where average was performed over five disorder realizations, as well as the red curves in (b) and (c) for $\lambda < \lambda_c$. The dashed curves in (c) and (d) are for the finite-range hopping version of the model (1) with $N_t = 4$, see the main text.

for which N_{TLI} and $\sigma_{12}^{\partial} h/e^2$ are quantized extends as the system size is increased, showing the tendency toward the value λ_c.

We note that, although the tight-binding model (1) has exponentially decaying hopping amplitudes (Fig. 2), the system remains in the same phase for a finite-range hopping version of this model. We have checked this explicitly by truncating the exponential tail of the wave functions $|w_{\vec{R}\alpha}\rangle$, i.e., setting $C_{\vec{R}'\alpha'}^{\vec{R}\alpha} = 0$ for $|\vec{R} - \vec{R}'| > N_t$. The results for $N_t = 4$ are given by dashed curves in Figs. 3(c) and 3(d), from which one can conclude that the phase is stable under such truncation, although the truncation increases the localization length as indicated by less good quantization.

Quantized Hall response.—The quantized response of a TLI can be probed in the Corbino geometry by adiabatic flux insertion. Since the TLI's bulk is fully localized, the boundary can be doped with electrons independent of the bulk. The boundary of a TLI, fully filled with electrons, gives the same response to flux insertion as a torus-shaped, half filled, two-dimensional Chern insulator (extrinsic second-order TI [52]), see Supplemental Material [37]. The main difference between these two setups is that the response of a TLI remains quantized under an arbitrarily strong boundary disorder, whereas a half filled Chern insulator gets trivialized above certain critical disorder strength [36].

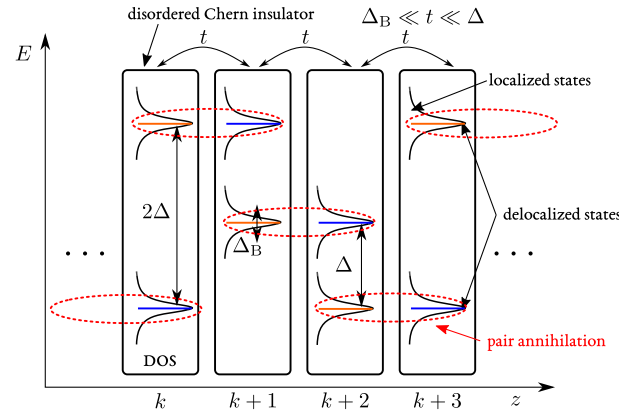


FIG. 4. Sketch of the layer construction for the three-dimensional TLI. A stack along z direction of two-band disordered Chern insulators, with the bandwidth Δ_B and the gap Δ or 2Δ, becomes fully localized due to interlayer coupling t such that $\Delta_B \ll t \ll \Delta$. For each layer, density of states (DOS) is shown, and the delocalized states depicted in orange (blue) carry a positive (negative) quantized Hall conductance.

Resonant energy model for a TLI.—In the model defined in Eq. (1), disorder is introduced in a highly nontrivial way that is not natural to occur in experimental systems. Here we suggest an alternative model realization of a TLI can be obtained by stacking two-dimensional Chern insulators with generic disorder. We assume that each Chern insulator has two bands and a band gap Δ or 2Δ (depending on the layer) that is much larger than the bandwidth. Disorder will broaden the "bands" to a band with Δ_B, but should be weak enough to maintain $\Delta_B \ll \Delta$. There is a single energy per band [36], where delocalized states appear. We mark these energies in blue or orange in Fig. 4, depending on the sign of their quantized Hall conductance. The parameters of the layers repeat with the period three, and the system is tuned such that differently colored delocalized states from neighboring layers are on resonance. When only resonant interlayer coupling is considered, the model is dimerized, with each dimer being a fully localized phase since it belongs to a two-dimensional unitary class and has zero Hall conductance. Hence, the delocalized states from neighboring layers "pair annihilate," leaving only unpaired delocalized states on the boundary of the resulting three-dimensional system. We anticipate the localization length (in the xy plane) of each dimer to be rather large in this model due to exponential sensitivity of the localization length in two-dimensional unitary class [53]. The off resonant interlayer coupling tends to delocalize some bulk states, but we expect for strong enough disorder and for large enough flatness ratio Δ/Δ_B (see Fig. 4) that the system is in the same phase as the above-mentioned dimerized limit. The detailed study of the model is left for future works.

Conclusions.—Topology of tenfold-way (strong) TIs [2,4,5] poses an obstruction to localization by disorder of its occupied bulk states [31–33]. Correspondingly, topological Anderson insulators [35] are Anderson insulators only at certain but not all fillings and the topological charge is carried by their delocalized bulk states only. Our main result is finding that fully localized insulators can be topologically nontrivial, too. In particular, we construct a three-dimensional model with broken time-reversal symmetry, where topology poses an obstruction to localization of its fully localized bulk states all the way down to the atomic limit. We find that the three-dimensional fully localized insulator, with broken time-reversal symmetry, does not represent a single phase of matter, but rather contains infinitely many phases that are labeled by integers. Here, the Anderson model of localization, in the absence of mobility edge, corresponds to a topologically trivial insulator and is labeled by $N_{\mathrm{TLI}} = 0$, whereas topologically nontrivial localized insulators are guaranteed to host states delocalized along the crystal's insulating boundary that give rise to the quantized Hall conductance (7) in Corbino geometry. Crucially, these delocalized boundary states remain topologically protected in the presence of an arbitrarily strong boundary disorder. We introduced the method to construct these novel insulators, which is readily generalizable to include additional symmetries (e.g., time reversal). We hope that this Letter will motivate experiments where quantized responses are observed in out-of-equilibrium settings.

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