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Islands in the Gap: Intertwined Transport and Localization in Structurally Complex Materials

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Localized waves in disordered one-dimensional materials have been studied for decades, including white-noise and correlated disorder, as well as quasi-periodic disorder. How these wave phenomena relate to those in crystalline (periodic ordered) materials—arguably the better understood setting—has been a mystery ever since Anderson discovered disorder-induced localization. Nonetheless, together these revolutionized materials science and technology and led to new physics far beyond the solid state. We introduce a broad family of structurally complex materials—chaotic crystals—that interpolate between these organizational extremes—systematically spanning periodic structures and random disorder. Within the family one can tune the degree of disorder to sweep through an intermediate structurally disordered region between two periodic lattices. This reveals new transport and localization phenomena reflected in a rich array of energy-dependent localization degree and density of states. In particular, strong localization is observed even with a very low degree of disorder. Moreover, markedly enhanced localization and delocalization coexist in a very narrow range of energies. Most notably, beyond the simply smoothed bands found in previous disorder studies, islands of transport emerge in band gaps and sharp band boundaries persist in the presence of substantial disorder. Finally, the family of materials comes with rather direct specifications of how to assemble the requisite material organizations.

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The quantum mechanics of wave phenomena in crystals led to unprecedented successes in understanding materials, from conductors to semiconductors and insulators. Technologically harnessing the scientific advances, in turn, led to a scale of social impacts that cannot be understated. However, the vast majority of materials are not so ordered. Understanding the properties of disordered materials was greatly advanced when it was discovered how structural disorder breaks crystalline wave-transport phenomena.

To date, analyzing the material properties arising at these two structural extremes requires distinct concepts and methods. Indeed, regular lattices lead to wavefunction states that extend over the whole system, whereas random lattices produce localized states at all energies. Is there an overarching theory? And, what about the existence of materials that are intermediate, neither perfectly ordered nor utterly random? What is the character of their quantum states?

These challenges have been appreciated for quite some time. Thouless once claimed that it would be impossible to understand the transition from extended states to localized states since there are uncharacterizable states lying between them [1, pg. 96]. We call this *Thouless' challenge*. If we can build “structured disorder” materials as intermediates between total randomness and exact crystalline periodicity, though, then we can begin to study

phenomena between extended and localized states and understand their proper characterization. Here, we address Thouless' challenge by analyzing a class of materials that span these structural extremes—the *chaotic crystals* discovered via X-ray diffraction studies [2]—and identifying a number of novel and counterintuitive material properties.

On the one hand, transport and localization of waves in disordered media has been heavily studied for 60 years, starting with Anderson's pioneering results [3]. He pointed out that disorder can stop wave propagation and diffusion depending on the degree of disorder. He analyzed the tight binding model for a one-dimensional chain of random atoms, in which electrons hop between neighboring sites. There, if the site energies are random, all eigenstates localized [4].

On the other hand, in a periodic chain of atoms, Bloch's theorem says that electrons can transit the lattice without backward scattering. Hence, in exactly periodic lattices all wave states are extended states. Moreover, conduction band structures emerge that are determined by lattice periodicity.

The last two decades witnessed several attempts to probe intermediate states via *correlated disorder*, in which random site energies are pairwise correlated. The first consequence was that correlation renders localization very

sensitive to wave energy. The second was that long-range power-law correlation suppresses localization; this was predicted theoretically [5] and numerically verified [6]. Moreover, with weak disorder, the relation between the Fourier transform of disorder correlation and the localization versus energy dispersion was established [7]. By this, both localization suppression [8] and enhancement [9] can be realized by designing correlation with certain desired, if unphysical, features.

Correlated disorder definitely falls in between complete randomness and pure periodicity. However, as implemented, it does not allow one to systematically sweep between the structural extremes. The following puts forward the approach of *structured disorder* to build materials that allow this—their lattices being an amalgam of periodic structure and disorder generated by ϵ -machines, a class of hidden Markov model [10, 11]. Lattices are formed from their realizations which determine site energies across the lattice randomly, but also in a way that gives a systematic dependence on the lattice “history” of preceding energies. This dependence directly controls the degree and character of material correlation. Tuning ϵ -machine parameters, then, one can sweep from a periodic lattice to maximum-disorder structure and on to another periodic lattice. The chaotic crystals so formed are generic in the sense that all possible material lattices can be generated; specifically, stochastic lattices of all different admixtures of periodicity and randomness can be exhaustively enumerated [12]. Constructively, the ϵ -machines give a direct specification, one that is local and so implementable, of how to assemble chaotic crystals.

The following first introduces structured-disorder materials by showing how to generate 1D atomic lattices from an ϵ -machine. It then studies the wavefunction states that arise when sweeping through states intermediate between pure periodicity and maximum disorder. Their nature is analyzed via the energy spectrum of localization. We find materials in which highly enhanced localized states and highly delocalized states coexist, even within very narrow energy ranges. Moreover, at certain energies, a counterintuitive relation emerges between degrees of disorder and localization. In addition, the density of states for these chaotic crystals becomes richly structured, when sweeping from complete randomness to correlated disorder. Previous studies had shown that, with disorder, sharp band-boundaries do not persist and they bleed into band gaps of the unperturbed system. In contrast, we find sharp band-boundaries persisting in the presence of disorder and an abrupt emergence of positive density of states in band gaps, rather than the density of states smoothly stretching across band edges.

Tight Binding Model Following Anderson, we consider the tight-binding model of a one-dimensional material [3]: an electron at energy E moves through a chain of atomic pseudopotentials (energies ϵ_n) with one orbital per atomic site $|n\rangle$. Physical properties of such a lattice are given by the wavefunction $\Psi = \sum_n \psi_n |n\rangle$ determined by Schrödinger’s equation, which we solve iteratively:

$$\psi_{n-1} + \psi_{n+1} = (E - \epsilon_n)\psi_n . \quad (1)$$

(See Supplementary Materials for a review.)

If the chain is a perfectly regular crystal, all site energies ϵ_n are uniform, forming a trivially periodic pattern of pseudopotentials on the lattice. The solution to Eq. (1) is the Bloch wave $\psi_n = e^{ikn}u_n$, with the periodic function u_n indicating the wavefunction is extensive over the whole lattice with a phase prefactor e^{ikn} . If material disorder exists, in contrast, energies ϵ_n are randomly distributed, say according to a Gaussian. Then, all eigenstates of Eq. (1) are spatially localized. In other words, the probabilities $|\psi_n|^2$ in some region dominate over those at other sites outside the region. And so, the wavefunction is trapped there and there can be no electron transport.

Disorder also changes the material’s energy spectrum—eigenvalues of Eq. (1). However, if the chain is a perfect crystal with l atoms per cell, the energy spectrum forms a *band structure* with l conduction bands that support transport. Each band has sharp edges associated with an abrupt change in the density of states (DoS). In the single-band structure that appears for $l = 1$, the allowed energy values are distributed in an ordered pattern in the region $E \in (-2, 2)$. For the familiar Gaussian disordered chain, in contrast, there is no periodicity so that only a single band emerges, with the energy amplitudes scattered randomly within. Moreover, the sharp band edge with crystalline order becomes spread out by the disorder, forming a rounded edge [13]. The correlated disorder case also produces a single band, no matter how the correlation statistics are parametrized [5–7]. The band is squeezed, though, forming very low DoS margins [6]. In short, in these materials disorder smooths band edges.

Structured Disorder Our challenge then is to systematically combine periodic lattices (especially those with periodicity $l > 1$) and lattices with different degrees of disorder. We also want the resulting combination—which we call *structured disorder*—to be maximally expressive, so that every possible disordered material can be described. To implement this, we regard the chain as a stochastic process that evolves from left to right. Then we take the class of ϵ -machines as the stochastic process generator. ϵ -Machines form a class of hidden Markov

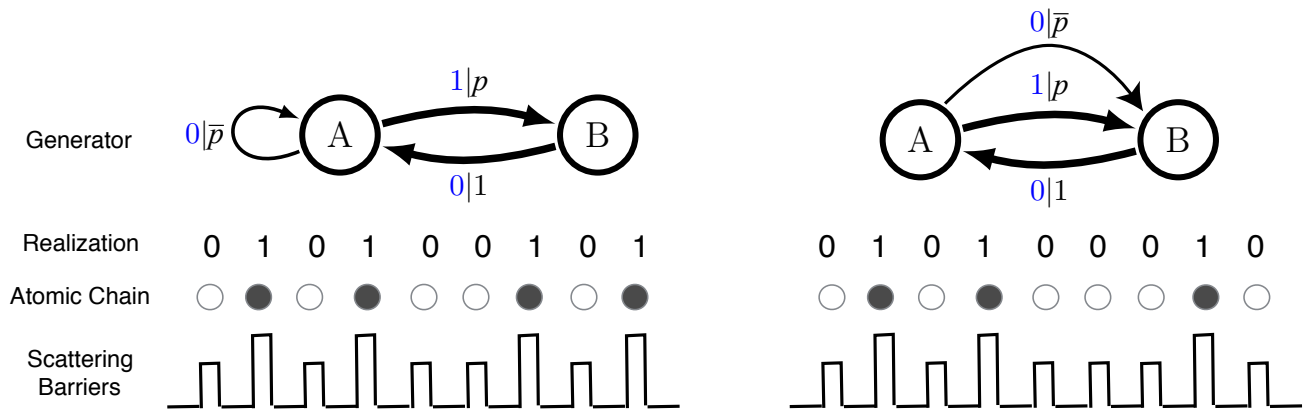


FIG. 1. Constructing structurally complex materials: (left) Golden Mean chaotic crystal—(top) Golden Mean Process ϵ -machine with two states A and B and three transitions labeled $x|p$ for taking the transition with probability p (or, $\bar{p} = 1 - p$) and emitting symbol $x \in \{0, 1\}$, (bottom) Resulting lattice of scattering barriers (or pseudopotentials). (right) Noisy Period-2 chaotic crystal—(top) Noisy Period-2 Process ϵ -machine, (bottom) Resulting lattice of scattering barriers. White atom site energies $\epsilon_0 = 0.0$ and black atom $\epsilon_1 = 0.5$.

model (HMM) [14] whose statistical properties can be completely analyzed in closed form [15] and which can express every stochastic process. In fact, as a representation ϵ -machines allow for an exhaustive enumeration of stochastic processes in terms of the latter’s structure (memory) and disorder (randomness) [12]. Said simply, a given ϵ -machine specifies how to construct a chaotic crystal and the enumeration provides a systematic way to explore this large class of materials.

Figure 1 shows how the construction works. The state transition diagram at the top depicts the ϵ -machine that generates the *Golden Mean Process*—all binary strings are produced, except those with consecutive 1s. At each time step t , the generator is in one of two states $S_t \in \{A, B\}$. A transition (labeled $x|p$) from current state to the next S_{t+1} is taken with the probability p and the observable symbol $x_t \in \{0, 1\}$ is emitted. For example, if $S_0 = A$ and the ϵ -machine emits symbol $x_0 = 1$, then system transitions to $S_1 = B$. At that point, a single transition emitting $x_1 = 0$ and moving to state $S_2 = A$ is allowed. Thus, in the realizations $x_0x_1x_2 \dots x_{N-1}$ generated by this ϵ -machine consecutive 1s are forbidden.

We then construct a structured-disorder lattice from a given realization by successively translating the observed symbols to atom types or, more literally, to distinct local pseudopotentials. Let’s map $x = 0$ to a “white” atom and $x = 1$ to a “black” atom. Alternatively, if we were to work with the Kronig-Penny model, we would map 0, say, to a weaker scattering barrier and a 1 to a stronger scattering barrier. (This mapping is depicted in the bottom two rows in Fig. 1.)

For the Golden Mean ϵ -machine with small \bar{p} , the cell

$x_nx_{n+1} = 10$ dominates and only occasionally 0s appear between them. We see that, in this case, the lattice is a modification of a common dislocation type of disorder. However, dislocated atoms are only of type 0.

In addition to generating dislocation-disordered lattices, there are multiple ways to combine periodic structures of 01s with disorder 0s. For example, we can place disorder at every other site. The result is the chaotic crystal generated by *Noisy Period-2 Process’* ϵ -machine shown in Fig. 1(b). In the cell 01, only the first atom has a chance to be a type-0 atom; the second is fixed to be a type-1 atom. Notably, this type of structured disorder is realized in metamaterials with alternating stacks of two layers [16]. Though apparently closely related—at first blush the ϵ -machines seem nearly identical, only the $0|\bar{p}$ transition has been redirected—the Golden Mean and Noisy Period-2 chaotic crystals exhibit dramatically distinct localization phenomena, as we now show.

Results To compare their material properties, we adapt transfer matrix products [17] to quantify the localization degree Λ , which is the inverse Lyapunov exponent for the corresponding 2D map of wave vectors $(\psi_n, \psi_{n-1}) \in \mathbb{R}^2$; see Supplementary Materials. As a main diagnostic, the following focuses on the *localization energy spectrum* $\Lambda(E)$: Λ versus electron energy E .

For Golden Mean chaotic crystals, p operates as a control for tuning from a period-2 lattice to white-noise disorder. When $p \approx 1$, the period-2 pattern dominates the structured disorder. When $p \approx 0$, the lattice is the simplest periodic structure of all type-0 atoms. The lattice inherits no structure from the period-2 tuning and the behavior appears as it does with very weak white-noise

disorder. (See Fig. 2(Top).) For $p = 0.9$, even though the lattice has very little disorder, the localization can be very strong around energy range $E \in [0.0, 0.5]$ —the energy band gap for the unperturbed period-2 lattice. Inside the two unperturbed bands, localization is very weak. So, the Golden Mean chaotic crystal inherits the band structure from the period-2 lattice. Decreasing p , this inheritance weakens. And, for $p = 0.3$, the localization length versus energy curve is basically flat as seen with Gaussian disorder.

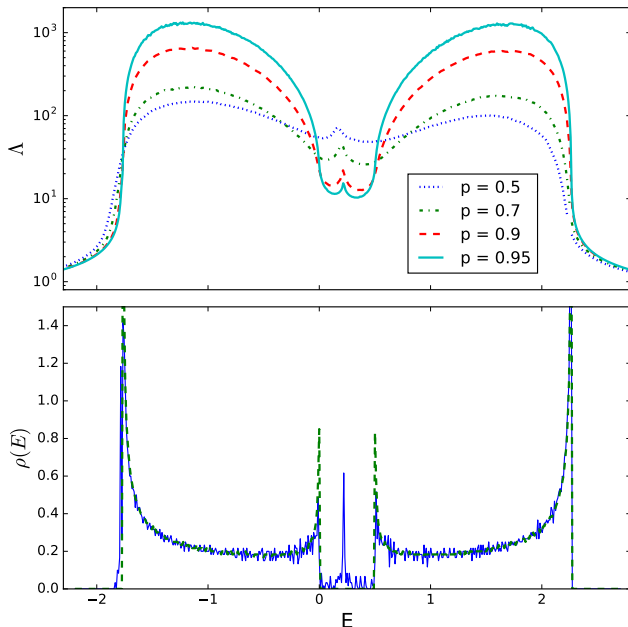


FIG. 2. Golden Mean chaotic crystal: (Top) Localization length Λ versus energy E for various disorder control settings p . $p = 0.9$ indicates little degree of disorder, but the localization is very strong around the band gap at $E = 0$. (Bottom) Corresponding density of states $\rho(E)$. The green dashed line delineates the band boundaries for the unperturbed period-2 lattice. While the blue curve is for the Golden Mean chaotic crystal. Note the very sharp peak in $\rho(E)$ for new states in the gap. $\Lambda(E)$ is also positively correlated with this DoS feature.

Curiously, inherited band structure does not always disappear with increasing disorder. For Noisy Period-2 chaotic crystals, periodicity 2 persists for any p value, except $p = 0$. In other words, only even or odd sites (depending on the realization’s beginning) can have black atoms, no matter how different the realization is from the underlying period-2 lattice. With its different underlying structure, the Noisy Period-2 crystal has a completely different localization versus energy curve; see $\Lambda(E)$ in Fig. 3(Top). Localization is still strong inside the band gap. However, at the right boundary of the left band, the localization length increases and forms a singularity.

Delocalization here is due to the persistent periodicity in the Noisy Period-2 Process. A typical delocalized wave is shown at the upper left corner in Fig. 3(Top). A significant feature is the strong periodic modulation of the wave amplitude. One sees that these “bumps” are amplified and localized. With energy E closer to the critical value $E_c = 0$, the bump width increases and localization weakens. At E_c , the wave reduces to a single bump with linear expanding envelope; see the upper right corner in Fig. 3(Top). Hence, the Lyapunov coefficient γ vanishes and localization is completely suppressed. Across the singularity boundary, though, inside the unperturbed band gap, localization is greatly enhanced. So, an abrupt transition from extensive state (conductor) to strongly localized state (insulator) is achieved within an exceedingly narrow energy range. Such abrupt transition features can be harnessed to design new 1D layered structures for capturing and transporting electrons in desired regions. In addition to novel localization properties, nontrivial features arise in a chaotic crystal’s density of states around band boundaries and band gaps. With normal disorder added to the period-2 lattice, the band structure only smooths out at band boundaries. In the Golden Mean chaotic crystal, however, new states emerge in the *middle of the unperturbed gap*. Specifically, at $p = 0.95$ the DoS shows a sharp peak at energy $E = 0.25$ with low density nearby; see Fig. 2(Bottom). In other words, rather than shrinking the band gap, an island of highly localized states emerges within the gap. Corresponding to the DoS, the $\Lambda(E)$ also shows a peak at the same energy. This is explained by Jones and Thouless’s theorem on the relation between localization level and DoS [18, 19]. Specifically, in exponentially localized states, the localization level at energy E is positively related to the number of states existing around E . For energy inside the band gap, except the island, nearby states are fewer so that localization is stronger. At the island energy, though, there are more nearby states, so a peak in $\Lambda(E)$ is observed; though still highly localized compared to the inside-band wavefunctions.

The emergence of localization islands suggests a novel way to manipulate a material’s conductivity. By tuning the Golden Mean’s disorder, we can turn-on a new “band” in the band gap that absorbs eigenstates previously at conducting bands’ edges. Thus, if the Fermi surface is at the gap’s middle, even small Golden Mean disorder will strongly suppress conductance.

The Noisy Period-2 chaotic crystal, see Fig. 3(Bottom), exhibits the same positive relation between localization length $\Lambda(E)$ and the DoS. This time, though, the smoothing of the right band is the same as that seen with normal

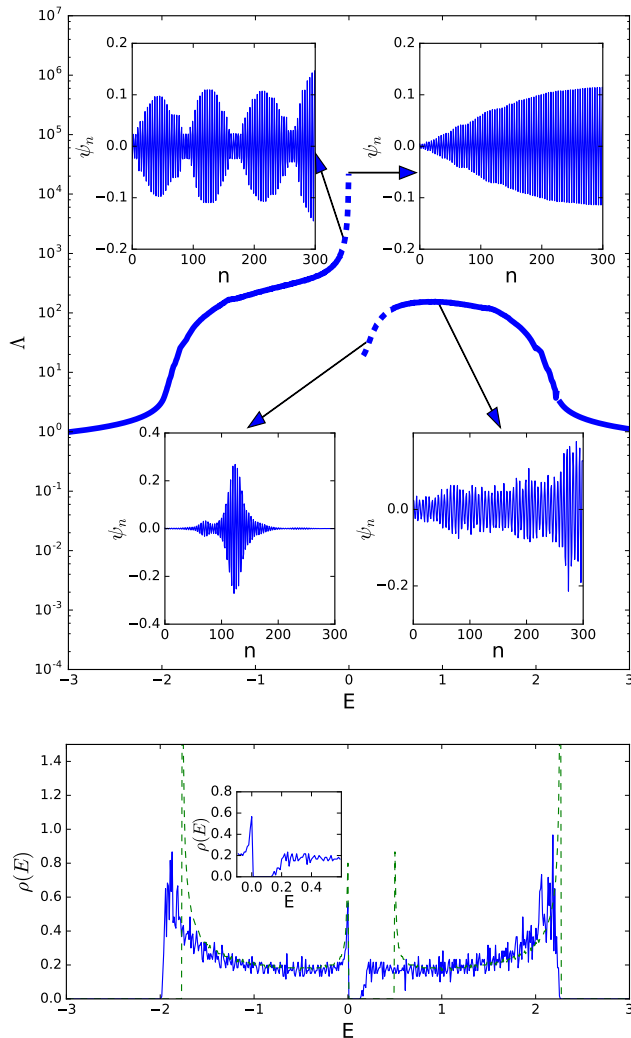


FIG. 3. Noisy Period-2 chaotic crystal with $p = 0.5$: (Top) Localization length Λ versus energy E and typical wavefunctions at four different E . Left upper: Connected bump-like delocalized state at $E = -0.03$. Right upper: Linear expanding wave in a single bump at $E = -0.0004$. Left lower: Enhanced localized state at $E = 0.23$. And, right lower: Typical localized state at $E = 1.00$. (Bottom) Corresponding density of states $\rho(E)$. The green dashed line delimits the band boundaries that would be exhibited for the unperturbed period-2 lattice. While the blue curve is for the structured disorder in the Noisy Period-2 chaotic crystal. Notably, the gap’s left boundary persists without broadening. As a consequence, the DoS remains high in the unperturbed left band. We do observe delocalization at this energy, showing positive relation with the DoS. In the inset figure, a zoom-in display of DoS near the band gap highlights this relation.

disorder. However, the left band’s boundary persists exactly as if it was an unperturbed band boundary. The high DoS inside the boundary also remains. Correspondingly, we observe delocalization around this boundary. Notably, the Jones and Thouless’s theorem does not apply here

since it is valid only for exponentially localized states and not for the new “modulated-bumps” wavefunction.

Conclusion Our strategy in the preceding is simple to state: We revisited Anderson localization theory and band-gap theory from the perspective of computational mechanics. The latter gave a systematic and quantitative view of the spectrum of structural complexity as one looks across processes with different mixtures of structure and disorder. Its lesson is that the most structurally complex processes occur in the intermediate regime of disorder—not exactly periodic, not utterly random. The result of this synthesis was several fold. First, we introduced a new family of chaotic crystal materials and gave a constructive specification (the ϵ -machine) for how to assemble them. Second, our explorations found that this family exhibits a range of novel, perhaps surprising properties. Strong localization emerges from weak disorder. Enhanced localization and transport coexist within narrow energy ranges. Islands of localized states arise within band gaps. And, sharp band-gap boundaries persist in the presence of substantial disorder. Practical consequences immediately suggest themselves.

Localization enhancement is a prospect for insulator material design. For a period-2 lattice with a single valence electron, the Fermi-surface is in the band gap, resulting in an insulator. Adding Golden Mean disorder leads to a DoS island just around the Fermi-surface. Since states in the island are strongly localized, a superinsulator is constructed with very little disorder. Also, for Noisy Period-2 disorder, the gap between extensive states and strongly localized states can be very small. There, an external electric field will cause electronics to drift, via the transition through the narrow band gap. Once transmitted, though, the electrons are localized again. The induced electron drift and sudden-stop phenomena provides yet another kind of material property control.

How might one test for these predicted phenomena? Direct experimental probes of Anderson localization in electronic waves is notoriously challenging, owing to electron-electron interactions. However, nanowires provide a possible 1D setting for observing electron localization [20, 21]. There are also other arenas in which the wave phenomena predicted here should arise. For example, disordered photonic materials and waveguides have led to successful experimental observation of localization of light and microwaves. All of our predictions can be verified on such systems with designed materials and waveguide geometries, requiring relatively simple experimental setups.

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Supplementary Materials
*Islands in the Gap:
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TIGHT BINDING MODEL

Consider the tight-binding model of a one-dimensional material [3]. Its Hamiltonian describes an electron at energy E moving through a chain of atomic pseudopotentials with one orbital per atomic site:

$$\hat{H} = \sum_n^{N-1} \epsilon_n |n\rangle \langle n| + \sum_{\langle n,m \rangle} t |n\rangle \langle m|, \quad (\text{S1})$$

where $|n\rangle$ is the orbital at site n with energy ϵ_n and the second term corresponds to the hopping between nearest neighbor sites $\langle n, m \rangle$ with hopping rate t . For simplicity, we investigate *diagonal disorder* focusing on effects arising from disorder in site energies ϵ_n , while regarding hopping rate t as uniform between neighbors. We set the rate $t = 1$ and define it as the unit for site energy disorder.

Physical properties of such a lattice are determined by a Schrödinger wave equation specified by the Hamiltonian in Eq. (S1). For the tight-binding model, we expand the electron's eigenfunction Ψ in terms of $|n\rangle$:

$$\Psi = \sum_n^{N-1} \psi_n |n\rangle. \quad (\text{S2})$$

We solve for the wavefunction via an iterative relation between neighboring sites:

$$\psi_{n-1} + \psi_{n+1} = (E - \epsilon_n)\psi_n,$$

where we must specify the initial condition ψ_0 and ψ_1 at, say, the lattice's left end. The lattice's right end is site $N - 1$.

**NUMERICAL SIMULATION AND
 QUANTIFIERS**

To compare their material properties, we adapt transfer matrix products [17] to quantify the localization degree. Rewriting the tight-binding model of Eq. (1) into a map

T_n of vectors $(\psi_n, \psi_{n-1}) \in \mathbb{R}^2$ gives:

$$\begin{bmatrix} \psi_{n+1} \\ \psi_n \end{bmatrix} = \begin{bmatrix} E - \epsilon_n & -1 \\ 1 & 0 \end{bmatrix} \times \begin{bmatrix} \psi_n \\ \psi_{n-1} \end{bmatrix}. \quad (\text{S3})$$

The product $Q_N = \prod_{n=1}^N T_n$ controls whether the wave amplifies or attenuates going from left to right, from $n = 0$ to $n = N - 1$. The more rapid the divergence, for example, the stronger the localization, assuming the localized packet's peak occurs at the far right.

Interpreting the wavefunction transfer matrix as a dynamical system, we employ the Lyapunov coefficient γ to measure the exponential rate of divergence per site:

$$\gamma = \lim_{N \rightarrow \infty} \log \left(\frac{\|Q_N\|_2}{N} \right). \quad (\text{S4})$$

$\Lambda = \gamma^{-1}$ is a wavefunction's localization characteristic length. Small Λ indicates strong localization and no transport. As a main diagnostic, the following focuses on the *localization energy spectrum* $\Lambda(E)$: Λ versus electron energy E .

Following in the long tradition of numerical simulation of disorder, we study $\Lambda(E)$ on a chain of 10^6 sites. This gives excellent convergence across different structured disorder realizations. For white atoms, we set the site energy to $\epsilon_0 = 0.0$, while $\epsilon_1 = 0.5$ for black atoms. In this case, the period-2 lattice has an energy gap of width 0.5. This allows us to easily observe phenomena arising inside the gap. For the density of states, we calculate the eigenvalue distribution of the Hamiltonian matrix for a system with 6×10^3 sites; which also achieves excellent convergence.