

Unlocking Emergent Resilience in Amorphous Metamaterials via a Physics-Constrained Energy-Based Framework

Lingyu Jia,^{1,2} Changliang Zhu^{7,8,*}, Qiaozhi Lei,³ Hua Tong,² Jinkui Meng,⁴
Chengyan Xu^{4,†}, Xiangying Shen,^{5,‡} and Lei Xu^{1,6,§}

¹Department of Physics, *The Chinese University of Hong Kong*, Hong Kong, China

²Department of Physics and Anhui Center for Fundamental Sciences in Theoretical Physics,
University of Science and Technology of China, Hefei 230026, China

³Education Center of Experiments and Innovations, *Harbin Institute of Technology (Shenzhen)*,
Shenzhen 518055, China

⁴Savage Laboratory for Smart Materials, School of Materials Science and Engineering,
Harbin Institute of Technology (Shenzhen), Shenzhen 518055, China

⁵School of Science, *Shenzhen Campus of Sun Yat-sen University*,
Shenzhen 518107, People's Republic of China

⁶Shenzhen Research Institute The Chinese University of Hong Kong, Shenzhen 518057, China

⁷College of Mechatronics and Control Engineering, *Shenzhen University*,
3688 Nanhai Avenue, Nanshan District, Shenzhen 518060, China

⁸Institute of Semiconductor Manufacturing Research, *Shenzhen University*,
3688 Nanhai Avenue, Nanshan District, Shenzhen 518060, China



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Mechanical metamaterials achieve their extraordinary properties through their intricate architectures. While amorphous designs can minimize directional bias relative to their regular counterparts, their vast configuration space poses a significant challenge for conventional design strategies. Here, we introduce a physics-constrained, energy-based model framework to navigate this complexity with machine learning. We formulate a multiobjective energy function that encodes desired macroscopic properties—specifically, a target negative Poisson ratio and approximate isotropy—into the network's topology. The design problem is then recasted as finding the ground state of this energy landscape, while operating within a mechanically stable or physics-constrained configuration space. We employ Boltzmann annealing as a physically consistent inference algorithm to identify the optimal low-energy configurations. The structures discovered and fabricated via 3D printing exhibit a highly negative Poisson ratio together with near-equal responses along principal axes (i.e., isotropy along both x and y axes). Remarkably, these optimized structures also reveal highly desirable emergent properties, including exceptional performance in specific energy absorption, impact resistance, and fracture toughness, significantly outperforming regular lattice counterparts. This work establishes a robust and interpretable machine-learning framework for the design of high-performance amorphous metamaterials.

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I. INTRODUCTION

The design of functional materials has historically been dominated by order and crystallinity [1–4], where the presence of a unit cell and spatial symmetry provides a clear path [5,6] from local structure to global properties. [7] Amorphous systems [8,9], from metallic glasses [10] to disordered biological networks [11], present a far greater challenge. Lacking periodic order, their properties are governed by a complex, high-dimensional, and “vast configuration space,” which has largely precluded rational, *ab initio* design [12–14]. Yet, this disorder also offers unique advantages, such as reduced directional bias arising

*Contact author: zhucl@szu.edu.cn

†Contact author: cy_xu@hit.edu.cn

‡Contact author: shenxy66@sysu.edu.cn

§Contact author: xuleixu@cuhk.edu.hk

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from large-scale statistical homogeneity [15,16] and the potential for novel failure mechanisms [17,18] not found in crystals. A central and unresolved problem is, therefore, how we can navigate this vast topological space to find a unique, optimal amorphous structure that is not only functional but also physically stable?

Here, we introduce a conceptual framework that recasts this grand challenge in materials design as an interpretable machine-learning problem rooted in statistical physics. We propose a physics-constrained, energy-based model (EBM) framework that reframes the search for an optimal amorphous topology as the search for the ground state of a carefully constructed, multiobjective energy landscape. This energy function is defined within the constrained space of mechanically stable configurations (requiring an average coordination number $Z \geq 4.0$ in 2D) and encodes the desired macroscopic mechanical response—specifically, a target negative Poisson ratio (ν^*) and approximate mechanical isotropy. The optimal structure is then identified not by a generic algorithm, but through Boltzmann annealing [19], a physically consistent inference process that mimics a physical system cooling to its near-global optimum.

Crucially, this EBM framework is not a “black box.” By locally approximating the complex energy function as a classical Ising Hamiltonian [20,21], our model provides profound physical interpretability. The topological features governing the target behavior are revealed through emergent “local fields” (h_e), which quantify the importance of individual bonds, and “coupling constants” (J_{ef}), which describe the synergistic or antagonistic interactions between them. This establishes an interpretable, physics-based paradigm for navigating the amorphous design space.

Applying this framework, we first address the explicit design target: creating amorphous auxetic metamaterials [22,23] that possess both a highly negative Poisson ratio [24–26] (as low as -0.6 at 5% strain) and approximate isotropy along the principal axes [27]. This goal has remained elusive for traditional periodic designs [28–30], such as reentrant [31], rotating-rigid [32], or chiral structures [33,34], which are fundamentally plagued by mechanical anisotropy [34] or low stiffness [35] and instability [36,37].

More significantly, this physics-based approach leads to the discovery of highly desirable emergent properties not explicitly included in the optimization. The resulting amorphous topologies demonstrate extraordinary mechanical resilience [38,39]. While the EBM was optimized purely for an elastic property (Poisson’s ratio and approximate isotropy), we find this property is profoundly linked to energy absorption [40]. For disordered structures at a similar density, the specific energy absorption (SEA) remains stable for positive ν but increases dramatically as ν becomes more negative, revealing a powerful emergent coupling between elasticity and resilience.

The most striking emergent discovery, however, is an unprecedented enhancement in specific fracture energy,

which characterizes a substantial increase in the overall fracture toughness of the structure [41]. In direct experimental comparisons, our optimal amorphous auxetic structure (N-1-Conv) achieves a specific fracture energy of 2.98 J/g representing an increase to 452% of the 0.66 J/g measured for an ordered, topology-optimized auxetic lattice of braced cross-petal structure (BCPS) [42].

This work establishes a robust and interpretable machine-learning paradigm for creating high-performance amorphous materials. By grounding the design process in the language of statistical physics, we solve not only a decades-old challenge in mechanical metamaterials but also uncover an emergent, topology-driven mechanism [43] for extreme fracture toughness. These findings open a new pathway for the design of multifunctional amorphous systems with significant potential for applications ranging from advanced protective equipment to fundamental studies of disordered matter.

II. METHODS: ENERGY-BASED MODEL FRAMEWORK AND MANUFACTURING

A. EBM framework

Our design approach is based on a physics-constrained, energy-based learning framework. The initial disordered configurations are generated by distorting an ordered triangular lattice, as detailed in Supplemental Material [44]. These initial configurations are then optimized by deleting appropriate bonds between nodes. The search for optimal structures s (where $\{s = s_e\}$ is the binary vector of bonds) is performed within a constrained space of mechanically stable configurations $\mathbb{S}_{\text{stable}}$. This constraint enforces that the average coordination number $Z(s)$ is maintained above the Maxwell stability threshold [$Z(s) \geq Z_{\min} = 4.0$ in 2D]. Details regarding the role of the average coordination number in optimization algorithms are provided in Supplemental Material [44].

Within this stable space, we define a multiobjective energy function $E(s)$ to simultaneously optimize for a target negative Poisson ratio (ν^*) and for approximate isotropy. Approximate isotropy is defined by minimizing the difference between the Poisson ratio measured along the x direction [$\nu_x(s)$] and the y direction [$\nu_y(s)$]. The function is

$$E(s) = \lambda_1 \left(\frac{\nu_x(s) + \nu_y(s)}{2} - \nu^* \right)^2 + \lambda_2 (\nu_x(s) - \nu_y(s))^2, \quad (1)$$

where $E_{\text{Poisson}}(s) = \{[\nu_x(s) + \nu_y(s)]/2 - \nu^*\}^2$ represents the Poisson ratio target term, which drives the average Poisson ratio as the structure approaches ν^* ; $E_{\text{iso}}(s) = [\nu_x(s) - \nu_y(s)]^2$ denotes the approximate isotropy target term serving as a penalty that drives ν_x and ν_y to become

closer to each other. It should be noted that the constraint $\nu_x = \nu_y$ employed in our optimization strictly enforces orthogonal equivalence. While this guarantees symmetric mechanical responses along the two principal axes, it does not represent true rotational isotropy, as off-axis properties are not explicitly constrained. Nevertheless, because disordered networks are statistically homogeneous at sufficiently large scales, enforcing $\nu_x \approx \nu_y$ substantially suppresses directional bias in the effective response and can, in practice, closely approximate isotropic behavior. Therefore, our systems exhibit approximate isotropy. The hyperparameters λ_1 and λ_2 balance these two objectives. The terms $\nu_x(s)$ and $\nu_y(s)$ are computed via discrete network mechanics calculations under orthogonal small-strain displacement conditions (see Supplemental Material [44] section “Boundary Conditions for the Calculation of Poisson’s Ratio.”).

We employ Boltzmann annealing to find the ground state of this constrained energy landscape. This method interprets the search as a physical process governed by the Boltzmann distribution $\mathbb{P}(s) \propto \exp\{-E(s)/T\}$. The inference process starts from an initial amorphous network at a high temperature T_0 . At each temperature, a series of L_k Markov chain Monte Carlo steps (bond removals or readditions) are proposed. A proposed move to a new state s' is

- (1) Immediately rejected if $s' \notin \mathbb{S}_{\text{stable}}$ [i.e., if $Z(s') < Z_{\min}$]
- (2) Accepted based on the Metropolis criterion if $s' \in \mathbb{S}_{\text{stable}}$, with probability $\alpha(s \rightarrow s') = \min[1, \exp(-\Delta E/T_k)]$, where $\Delta E = E(s') - E(s)$

The temperature is then slowly decreased via a cooling schedule $T_{k+1} = \alpha T_k$ (where $\alpha = 0.95$), allowing the system to settle into a low-energy ground state. (Regarding the selection of the cooling rate α , please refer to Supplemental Material [44] section “Selection of the Cooling Rate α ” for further details.)

A key advantage of this EBM framework is its interpretability. The complex energy function $E(s)$, while globally nonlinear, can be locally approximated around any reference structure s_0 by a class-Ising Hamiltonian via a second-order Taylor expansion:

$$E(s) \approx E(s_0) + \sum_e h_e \delta s_e + \frac{1}{2} \sum_{e,f} J_{ef} \delta s_e \delta s_f, \quad (2)$$

where $\delta s_e = (s_e - s_{0,e})$ is the change in a bond’s state. The first-order term h_e acts as a local field quantifying the importance of an individual bond e to the total energy. The second-order term J_{ef} acts as a coupling constant describing the synergistic or antagonistic interaction between bonds e and f . This Ising-like approximation allows us to move beyond a black-box approach and physically interpret why the network behaves the way it does by quantifying the importance of individual bonds (h_e) and the

cooperative interactions between them (J_{ef}). (See Supplemental Material [44] Theoretical Note I for the full derivation.)

B. System construction and manufacturing by 3d printing

After obtaining the optimal two-dimensional auxetic lattices via the physics-constrained EBM framework, we use the Computer-Aided 3D Interactive Application software to construct our system, as shown in Figs. 1(d)–1(f), and use 3D printing manufacturing technologies to fabricate samples with highly elastic thermoplastic polyurethane material (TPU 95A), as shown in Figs. 1(g)–1(i). Detailed material properties and printing conditions are summarized in Supplemental Material [44].

All samples are controlled to the same dimensions of $60.0 \times 55.0 \times 10.0 \text{ mm}^3$. To ensure general validity, two bond widths, 0.42 and 0.55 mm, are used (the descriptions of the criteria adopted for selecting these widths are presented in Supplemental Material [44]). The 3D printing method is fused deposition modeling, which is suitable for various filling rates to meet lightweight requirements in practical applications.

The designed systems are divided into two types of Poisson ratios: negative Poisson ratio (NPR) and positive Poisson ratio (PPR) [the calculation method is described by Eq. (S22) in Supplemental Material [44], where structures are in the linear elastic state within 5% of strain]. Moreover, the structure of the NPR can be further divided into two types: one is composed by convex polygons only and the other by both convex and concave polygons, as shown in Figs. 1(d) and 1(e), respectively. Note that the concave polygon belongs to the reentrant structure previously studied [31,35]. The structure of the PPR is comprised of a regular rhombus, as shown in Fig. 1(f). We choose the regular rhombus structure for comparison because its coordination number of 4 is the closest integer for a regular structure to match the coordination number of our amorphous structure, which ranges between 4.1 and 4.3.

When compressed, the deformations exhibit distinct behaviors: NPR structures contract in the horizontal direction, as shown in Figs. 1(g) and 1(h), while the PPR structure (rhombus) expands in the horizontal direction, as shown in Fig. 1(i). The naming rules and configurations of the disordered samples are provided in Supplemental Material [44] Fig. S10.

III. RESULTS AND DISCUSSION

A. Poisson’s ratio

In Fig. 2, we demonstrate the deformation response of the NPR and PPR samples under different strains in experiments. The snapshot images are taken by high-speed photography at specific strains: 10%, 20%, 40%, and 80%.

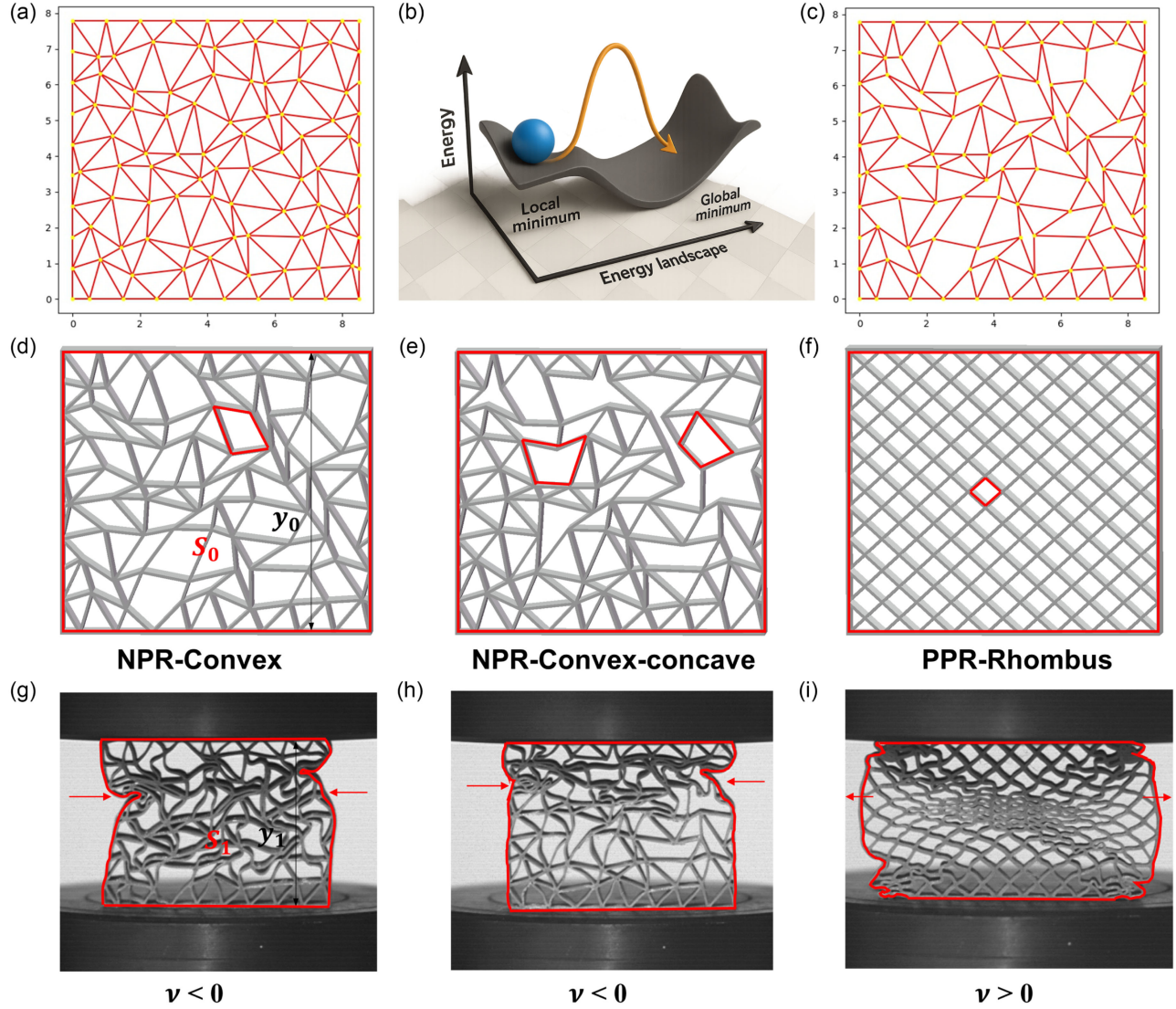


FIG. 1. Designing structure with physics-constrained EBM framework: (a) initial state derived from a perturbed triangular lattice configuration, (b) illustration of the physics-constrained EBM framework, (c) final optimized state, (d) NPR system composed by convex polygons only, (e) NPR system composed by both convex and concave (i.e., reentrant) polygons, (f) regular lattice with positive Poisson ratio (i.e., conventional rhombus network), (g)–(i) negative or positive Poisson ratio appears after compression of the structures above.

The two vertical lines in each image indicate the original system boundary before deformation.

Clearly, under compression the NPR samples in the top two rows [Figs. 2(a) and 2(b)] shrink, while the PPR sample in the bottom row [Fig. 2(c)] expands in the transverse direction, confirming their negative and positive Poisson ratio unambiguously. Also note that the deformation in the regular PPR sample concentrates around the middle (see the bottom row), while the deformation in the amorphous NPR samples is more evenly distributed in the entire sample (see the top two rows). Such a more uniform distribution of deformation is another advantage of our amorphous system, which

reduces the possibility of failure due to large deformations concentrated at specific locations.

Note that the instantaneous Poisson ratio is not a constant but dependent on deformation. We can obtain their instantaneous values under different strains by calculating them within a small range of strain, 10%, to obtain ν for every 10% of deformation (see the detailed calculation method in Supplemental Material [44] section “Materials and Experiments”). The instantaneous ν values under different strains are shown in Fig. 2(d). The general trend is clear: ν typically increases with strain in the NPR samples but decreases with strain in the PPR samples, and all curves tend to converge to small magnitudes due to the really

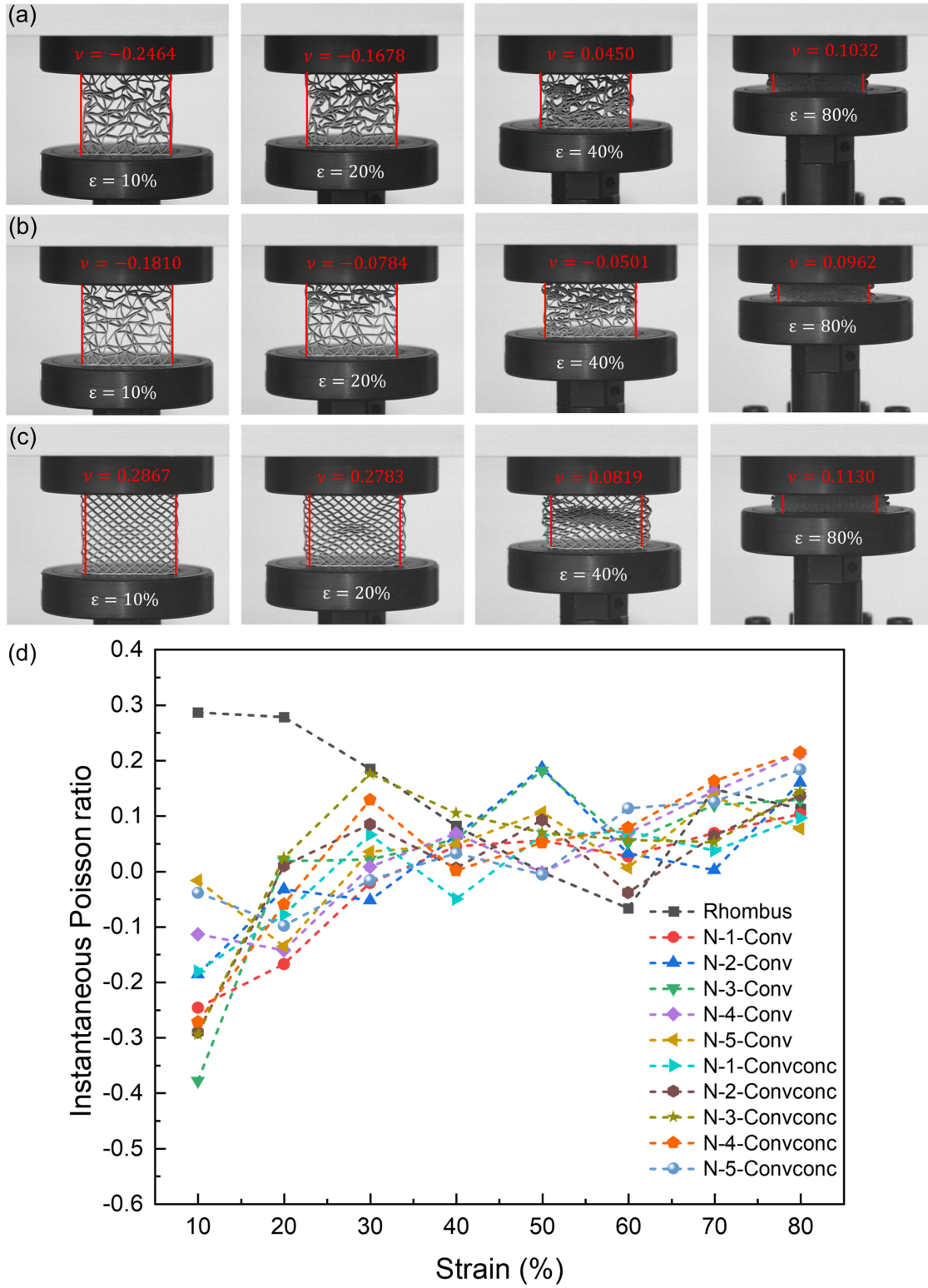


FIG. 2. (a)–(c) Images of NPR (rows 1, 2) and PPR (row 3) structures with different deformations: 10% (column 1), 20% (column 2), 40% (column 3), 80% (column 4). (d) The variation of instantaneous Poisson ratio versus strain.

dense configurations at very large strains that prevent significant transverse deformations.

More specifically, the trend of decreased magnitude in the NPR samples can be attributed to the growing perturbation to our specially designed NPR structures by increasing deformations, whereas in regular PPR samples, it is due to the destruction of local inversion symmetry by increasing deformations [59,60].

Notably, even within the elastic-plastic transition regime at large strains (approximately 10% strain)—a range where the Poisson ratio has rarely been measured in previous studies—our NPR samples [colored symbols in Fig. 2(d)] achieve a broad range of $-0.4 < \nu < 0$. This highlights the versatility and effectiveness of the designs enabled by the physics-constrained EBM framework in achieving a wide spectrum of Poisson ratios.

B. Mechanical resistance and energy-absorption performance

To illustrate the mechanical resistance and energy absorption of our samples under a slow quasistatic compression, we conduct compression tests on samples with different structures and bond widths.

The experimental results are summarized in Fig. 3. Figures 3(a) and 3(b) show the complete stress-strain curves with the strain ϵ up to 80%. To ensure robust results, two bond widths $t = 0.42$ mm and $t = 0.55$ mm, are tested in Figs. 3(a) and 3(b). To obtain a general result, we measure ten NPR amorphous samples and one regular PPR lattice (rhombus) sample at each bond width. The ten NPR samples exhibit Poisson ratios ranging from highly negative to nearly zero under a small strain of 2.5%. The ones containing convex structures are labeled “Conv,” and the ones containing both convex and concave structures are labeled “Convconc.” All curves exhibit a similar trend: a slow increase below the densification strain (near 70% of strain) and a sharp increase after it.

To give a better illustration, we first focus on the strain range $\epsilon > 70\%$, as shown in Figs. 3(c) and 3(d): These enlarged curves clearly show that the PPR-rhombus curve is consistently below the NPR curves, demonstrating that NPR structures can absorb significantly more energy than the PPR counterpart at the large strain range (energy absorbed is the area below the curve). We also show the enlarged curves in the strain range of $\epsilon < 70\%$ in Figs. 3(e) and 3(f): Under the strains below 50%, the PPR-rhombus curve behaves very close to the NPR curves, and the two begin to deviate from each other above 50% of strain, indicating that better energy absorption of the NPR samples appears at large strains. To summarize, the NPR samples exhibit a much better energy-absorption ability than the PPR-rhombus sample under large strains.

We also find a difference caused by the bond width. At the width of 0.42 mm, the NPR samples exhibit stress over

2 times greater than that of the PPR-rhombus sample at 80% of strain, while it decreases to less than 2 times at the width of 0.55 mm. This can be attributed to the fact that at a reduced width, the structural characteristics of the sample become more pronounced, leading to a marked distinction between the NPR and PPR-rhombus samples. Conversely, at a greater width, the intrinsic material properties become more important due to the increased amount of material, which reduces the structural difference and results in a smaller difference between the NPR and PPR-rhombus samples.

We summarize all the energy-absorption data in Figs. 3(g) and 3(h) to reveal a general trend. To ensure a fair comparison among different samples, which may vary in material use due to differences in configurations and bond numbers, we calculate the average density of each sample and compare them at the same density. The average density is determined by dividing the total mass of the sample by its total volume (including the empty spaces within the structure). Consequently, samples with more empty space have a lower density.

For both bond widths of 0.42 and 0.55 mm, a clear negative correlation is observed: As the average Poisson ratio [see Supplemental Material [44] Eq. (23)] decreases, the energy absorbed during 80% strain increases significantly. This indicates superior energy-absorption performance for the NPR samples (see data for samples with densities of $\rho = 0.22$ g/cm³ for 0.42-mm bond width and $\rho = 0.28$ g/cm³ for 0.55-mm bond width). Specific data and structures supporting this conclusion are provided in Supplemental Material [44] (see Tables S3 and S4 for disordered NPR samples and the regular PPR-rhombus sample, and Fig. S10 for additional structural comparisons). Similarly, samples with zero and positive Poisson ratios also exhibit a negative correlation between the average Poisson ratio and the total energy absorption, although they possess relatively high material densities ($\rho = 0.25$ g/cm³ and $\rho = 0.31$ g/cm³ for bond widths of 0.42 and 0.55 mm, respectively). This further confirms that the negative Poisson ratio effect plays a crucial role in enhancing the energy-absorption capability.

It is also important to note that the average Poisson ratios shown in Figs. 3(g) and 3(h) may not appear highly negative because they are averaged over the entire 80% strain range, during which the energy absorption accumulates. However, these samples exhibit a highly negative Poisson ratio at small deformations [see data in Fig. 4(b)], which was typically the range measured in previous studies.

To facilitate the comparison of the energy-absorption capabilities between our disordered auxetic structures and other structures, we calculate the value of the specific energy absorption (SEA), which is an important quantity commonly used to evaluate the energy-absorption capacity. It is defined as the following [69,70]:

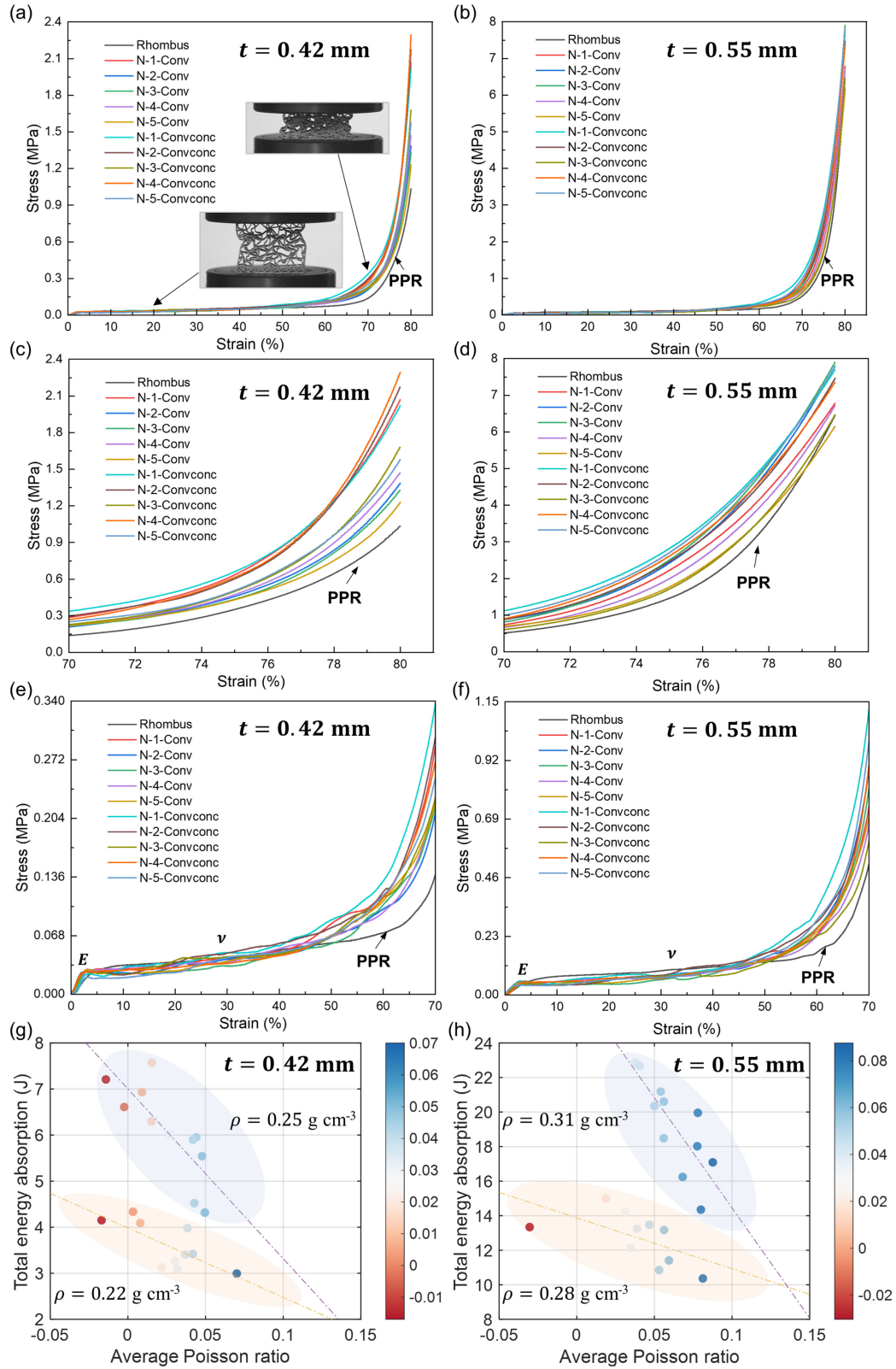


FIG. 3. (a),(b) Stress-strain curves for thickness 0.42 and 0.55 mm, respectively. (c),(d) Stress-strain curves at 70%–80% strain range. (e),(f) Stress-strain curves below 70% of strain. (g),(h) Energy-absorption ability increases with decreased Poisson ratio for all our samples.

$$\sigma_p = \frac{\int_0^{\varepsilon_d} \sigma(\varepsilon) d\varepsilon}{\varepsilon_d}, \quad (3)$$

$$\text{SEA} = \frac{\int_0^{\delta} F d\delta}{M} = \frac{\int_0^{\varepsilon_d} \sigma(\varepsilon) d\varepsilon}{\rho^*} = \frac{\sigma_p \varepsilon_d}{\rho^*}, \quad (4)$$

$$\frac{d}{d\varepsilon} \left[\frac{\int_0^{\varepsilon_d} \sigma(\varepsilon) d\varepsilon}{\sigma(\varepsilon)} \right] \bigg|_{\varepsilon=\varepsilon_d} = 0, \quad (5)$$

where F is the compressive force, δ is the vertical compression displacement or strain, and M and ρ^* are the mass and average density of the sample. ε_d represents the densification strain at which the stress-strain curve rises sharply [see Figs. 3(a) and 3(b)]. ε_d values [71] can be determined according to the expression (5). σ_p can be obtained from the area under the stress-strain curves in Figs. 3(a) and 3(b). Thus, we can obtain the SEA values of our NPR samples. Similarly, the SEA values of other structures can also be calculated with the same method.

To comprehensively analyze the relationship between energy absorption [SEA (J/g)] and various parameters, such as Poisson's ratio, order and disorder, and density, we present the experimental results in Fig. 4. The mechanical curves of all samples are shown in Supplemental Material [44] Fig. S12.

Figure 4(a) compares the SEA between disordered (solid symbols) structures and ordered structures (open symbols). For disordered structures (i.e., solid symbols), higher densities in general can increase structural moduli and lead

to a larger SEA, as we naturally expect. Because lighter density and higher SEA are preferred, regions more toward the upper left indicate a better performance. Thus, the disordered structures represented by solid symbols exhibit better energy-absorption performance, as demonstrated by their more upper left positions. Note that the ordered structures exhibit either positive Poisson ratios, such as the rhombus structure, or negative Poisson ratios, as identified in prior topology optimization studies [42], including BCPS (braced cross-petal structure), CPS (cross-petal structure), and HGS (hourglass structure). Thus, Fig. 4(a) indicates that regardless of the Poisson ratio, disorder itself can enhance energy-absorption performance, consistent with previous studies [72]. (The detailed influence of boundary conditions is provided in Supplemental Material [44]).

When comparing structures with the same density, the SEA values of disordered lattices (marked by the solid hexagon) from our work is much better than that of topology-optimized periodic structures (marked by the hollow triangle) reported by Bohara *et al.* [42]. Considering the auxetic metamaterials, the best-performing disordered structure [the highest point encircled by the blue line in Fig. 4(a)] exhibits a 22% higher-energy SEA compared to the best periodic sample (CPS) obtained through topological optimization, despite the disordered sample being only 90% as dense as the ordered one.

Next and more importantly, we illustrate our key point: the sole effect of a negative Poisson ratio on energy-absorption enhancement. To avoid disturbances arising from density

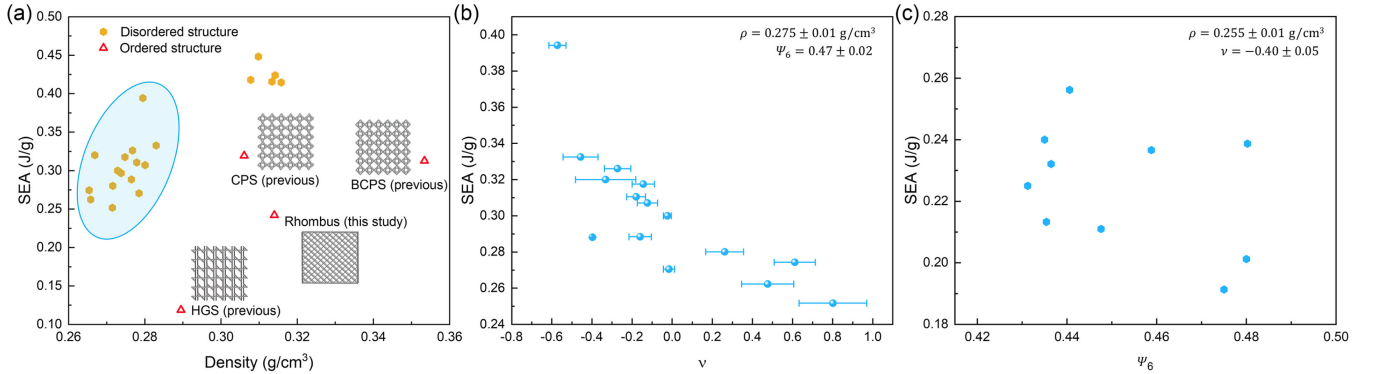


FIG. 4. (a) SEA versus density for disordered structures are plotted by solid symbols. As expected, higher density generally leads to higher SEA due to their larger moduli. Ordered structures are also plotted as open symbols. Because lighter density and higher SEA are preferred, regions more toward the upper left exhibit better performance. Clearly, the disordered structures perform better than the ordered structures, as demonstrated by their more upper left positions. (b) Disordered structures with similar densities around $0.275 \pm 0.01 \text{ g/cm}^3$ encircled by the blue solid line in (a) are plotted with respect to Poisson ratio ν . These samples have both similar densities and similar degrees of disorder. SEA rises sharply for negative ν , indicating a better energy absorption for negative Poisson ratio unambiguously. (c) For disordered structures, SEA versus the bond-orientational order parameter (Ψ_6) at similar densities around $0.255 \pm 0.01 \text{ g/cm}^3$ and similar Poisson ratio (ν) around -0.40 . Clearly, the SEA shows no systematic trend with respect to Ψ_6 , indicating that it remains largely insensitive to structural disorder within our Ψ_6 range of 0.4 to 0.5. All structures are fabricated with the bond width of 0.55 mm (selected to facilitate comparison with existing literature [61–68]), including the topologically optimized structures used for comparison. Additionally, the external dimensions of the comparison structures are controlled to match those of our structures ($60.0 \times 55.0 \times 10.0 \text{ mm}^3$) as much as possible (not matching perfectly due to different aspect ratio). The stress-strain curves of more configurations are provided in Supplemental Material [44] Figs. S11 and S12. Note that the errors of the SEA values in (c) are all within the range covered by the symbols.

and degree of disorder, we ensure that all our samples have similar densities and similar degrees of disorder, adjusting only their Poisson ratio. These samples are represented by the encircled symbols in Fig. 4(a). Because we adjust the Poisson ratio by eliminating bonds, these structures have smaller densities ($0.275 \pm 0.01 \text{ g/cm}^3$) than the original structures ($0.31 \pm 0.01 \text{ g/cm}^3$), which inevitably causes smaller SEA due to reduced moduli, as we naturally expect.

Clearly, the SEA values of these encircled symbols vary significantly and distribute randomly in Fig. 4(a). However, when we plot them with respect to the Poisson ratio ν in Fig. 4(b), a clear trend shows up: SEA remains relatively stable for positive ν while increasing dramatically for negative ν . Therefore, we can conclude that within the category of disordered structures, which already have better energy absorption than ordered structures, a negative Poisson ratio enhances SEA even further.

Furthermore, Fig. 4(c) investigates the influence of disorder—quantified by the bond-orientational order parameter Ψ_6 (as detailed in Supplemental Material [44])—on the SEA for structures with similar densities and Poisson ratios. Notably, no systematic correlation is observed between the SEA and Ψ_6 , likely because all structures fall within the disordered regime ($0.4 < \Psi_6 < 0.5$).

As a result, the best option should be disordered structure combined with the negative Poisson ratio. This is clearly demonstrated by the data point with the most negative ν , which exhibits an SEA close to 0.4 J/g and approaches its high-density counterparts while at a much lower density. Moreover, in Fig. 4(b), we designed a series of disordered structures whose Poisson ratio can vary continuously and broadly from -0.6 to 0.8 with very similar densities. In contrast, the ordered lattices [42] generated from topology optimization have only a few distinct Poisson ratio values at very different densities. Thus, our design demonstrates a wide coverage range of Poisson ratios and a consistency of densities, indicating a much better tunability and controllability than ordered lattices from topology optimization.

Therefore, by separately investigating the two factors, order and disorder and Poisson ratio, we illustrate that (1) disordered structures perform better than ordered structures, and (2) a negative Poisson ratio improves energy absorption even further.

To further illustrate the stress distribution under various deformations across different samples, we performed numerical simulations using Abaqus Explicit finite element software, as shown in Fig. 5. The simulations were conducted for three types of samples: (1) the regular auxetic structure (CPS) obtained from a topology optimization design [42], (2) the regular rhombus structure with a positive Poisson ratio, and (3) the amorphous auxetic structure (N-1-Conv) created using our physics-constrained EBM framework.

Clearly, there are much more high-stress regions (labeled in red) in the two regular lattices, Figs. 5(a) and 5(b), than

in the amorphous auxetic structure of Fig. 5(c). Moreover, these high-stress regions tend to accumulate and align in specific directions for regular structures, forming weak bands as indicated by the red arrows in the last column. By contrast, the disordered auxetic structure exhibits much less high-stress red regions at small strains ($\epsilon \leq 40\%$), and they also distribute much more randomly and uniformly at high strains ($\epsilon > 40\%$). Such a random distribution prevents the formation of weak bands that appear in the regular structures, which may induce system failure due to the accumulation of high-stress regions along specific directions. Therefore, the stress distribution clearly shows that our disordered auxetic structure exhibits superior performance of deforming uniformly and randomly, which can effectively prevent system failure triggered by stress concentration at specific locations and/or along specific directions.

C. Impact resistance and antifracture performance

The impact resistance and antifracture capabilities can be tested through the drop-hammer impact test (see Supplemental Material [44] Fig. S13) to detect the rapid mechanical response under a situation similar to a real impact scenario. To develop low-density materials for impact resistance, we manufacture truss-dominated prototypes based on the previous NPR structures, which have a relative density only around 0.30 (i.e., sample density divided by parent material density). The dimensions of the impact samples are $x \times y \times z = 208.0 \times 28.0 \times 100.0 \text{ mm}^3$ and the bond width is 0.42 mm .

As shown in Figs. 6(a)–6(f), structures designed using our physics-constrained EBM framework, along with their regular counterparts, are arranged in the x - y plane with seven identical unit cells combined via mirror symmetry. These structures extend uniformly in the z dimension.

The impact tests are performed across all sample categories. For the NPR samples, we select three structures: the disordered 1-Conv and 1-Convconc, and the regular CPS, as they demonstrate excellent energy-absorption performance under quasistatic compression tests [Fig. 3 and Supplemental Material [44] Fig. S11]. Similarly, for the PPR group, we select the disordered 4-Conv and 3-Convconc, along with the regular rhombus samples, based on the same criteria.

The manufactured prototype samples for the drop-hammer tests are exceptionally long in the x direction, with dimensions of $208.0 \times 28.0 \times 100.0 \text{ mm}^3$. This extended geometry allows us to conduct three independent impact tests at distinct, spatially separated locations on the same structural prototype without boundary interference. This ensures good statistical reliability ($N = 3$) for the tests conducted at each impact energy level.

The impact resistance of the samples is evaluated by the load-displacement curve recorded during the drop-hammer impact [73]. We select three impact energy values, 10 , 50 ,

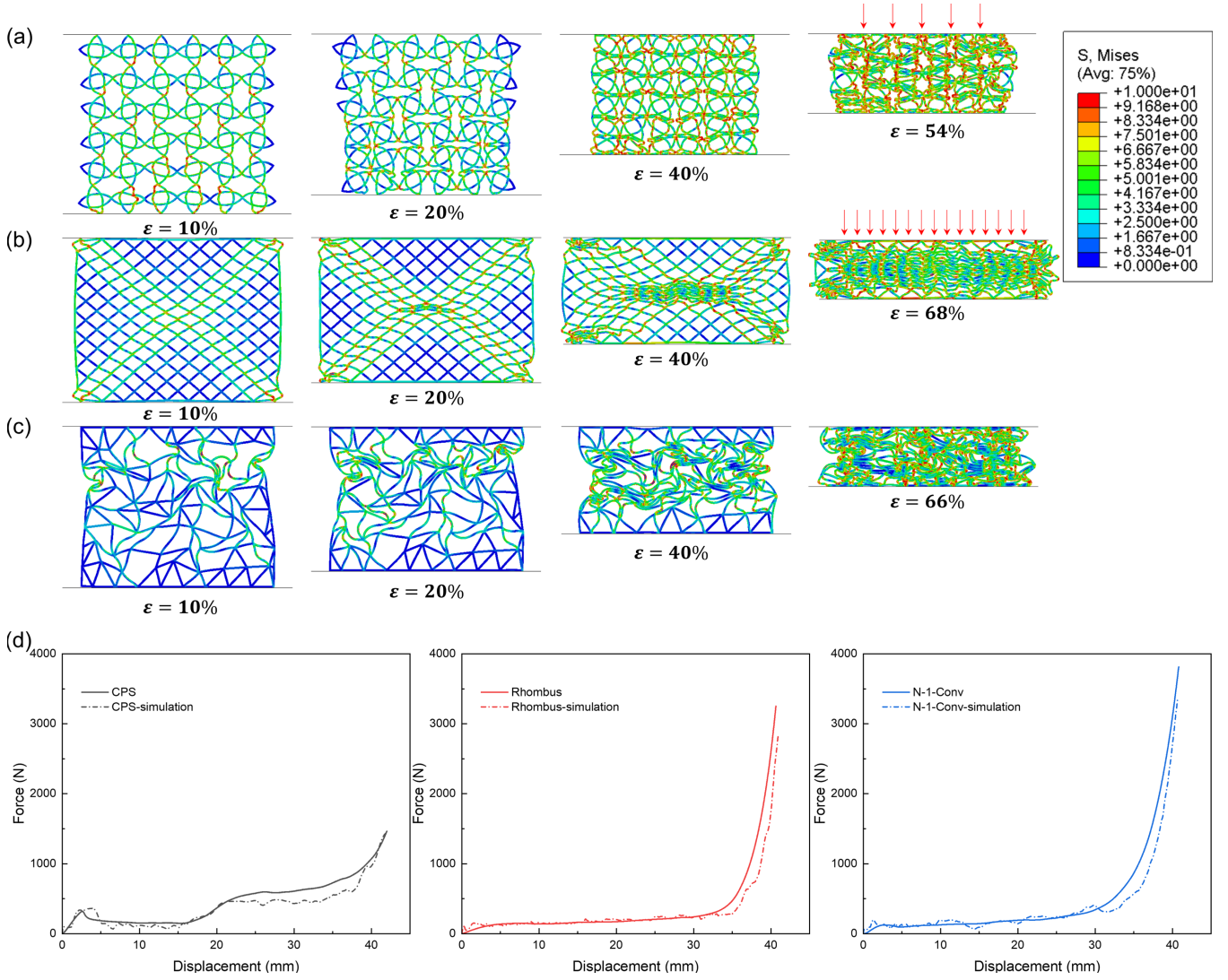


FIG. 5. (a)–(c) Stress distribution in regular auxetic structure (a), regular rhombus structure with positive ν (b), and disordered auxetic structure (c). (d) Force-displacement curves from experiment (solid) and simulation (dashed) agrees well. (Sample size: $60 \times 55 \times 10$ mm).

and 150 J that correspond to low-, intermediate-, and high-impact loads to evaluate the mechanical response and deformation behaviors of the samples.

As demonstrated in Fig. 6(g), under low-energy impact conditions, all curves exhibit similar behavior without showing a systematic trend. However, as the impact energy increases to intermediate and high levels, the responses change significantly. As shown in Figs. 6(h) and 6(i), the impact responses distinctly separate into two groups: One group exhibits small maximum loads but large displacements, while the other shows significantly larger maximum loads with small displacements. Both of our disordered NPR structures fall into the first group, indicating a soft-landing response to abrupt impacts. This behavior is particularly desirable, as these structures can absorb a large amount of energy due to their large displacements, while experiencing a relatively small impact force. Besides the

two disordered NPR samples, the PPR rhombus sample also appears in the small-load group; however, it does not absorb as much energy as the two NPR structures, as demonstrated in Fig. 6(j). By contrast, all other categories, including the regular NPR structure (i.e., CPS) and the two disordered PPR samples, fall into the second group, indicating an undesirable scenario where large impact forces are experienced during impact.

By integrating the load-displacement curves, we calculate the energy absorbed by these structures, as shown in Fig. 6(j). Clearly, the best-performing structure is our disordered NPR sample, NPR 1-Conv, which outperforms all other structures across all tested energy levels. The second-best performer is another disordered NPR sample, NPR 1-Convconc, which ranks second in energy absorption for both low- (10 J) and high- (150 J) impact conditions. These findings clearly demonstrate that our

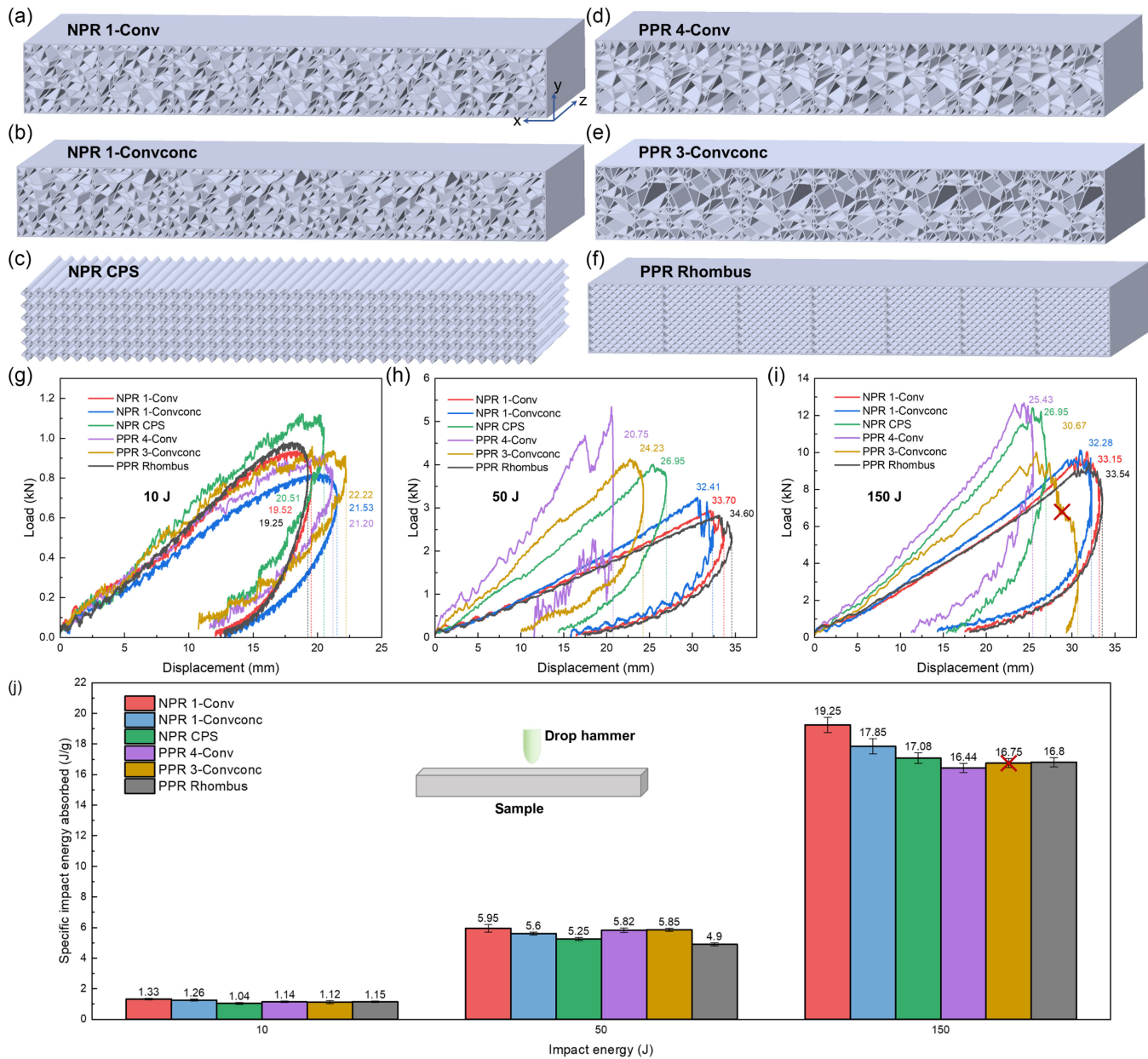


FIG. 6. (a)–(f) The structures of prototype material based on our physics-constrained EBM framework designs, with seven unit cells combined via mirror symmetry. (a) NPR-convex material based on NPR 1-Conv unit cell, (b) NPR-convex-concave material based on NPR 1-Convconc unit cell, (c) NPR-material based on CPS unit cell, (d) PPR-convex material based on PPR 4-Conv unit cell, (e) PPR-convex-concave material based on PPR 3-Convconc unit cell, (f) PPR-material based on Rhombus unit cell. (g)–(i) Impact resistance capacities under 10- (low), 50- (intermediate), and 150-J (high) loads. (j) The specific impact energy absorbed by all samples is evaluated, with our disordered NPR samples, NPR 1-Conv and NPR 1-Convconc, ranking as the top two performers among all tested structures.

disordered NPR samples exhibit superior impact energy absorption compared to all other structures, including the regular NPR structure (CPS), the regular PPR structure (rhombus), and the two disordered PPR structures (PPR 3-Convconc and PPR 4-Conv).

Furthermore, no complete failure is observed in the disordered NPR samples even under very high-impact energies of 150 and 200 J. In contrast, one disordered PPR sample (PPR 3-Convconc) experiences catastrophic

failure at 150 J [indicated by the red X in Figs. 6(i) and 6(j)], and two disordered PPR samples (PPR 3-Convconc and PPR 4-Conv) completely fail at 200 J (see Supplemental Material [44] Fig. S14). The fact that our disordered NPR samples maintained structural integrity highlights yet another facet of the superior impact resistance inherent in our disordered auxetic design.

To investigate fracture resistance, we conducted fracture experiments on a total of 22 different structures, covering

all categories of structures, including both ordered and disordered, as well as NPR and PPR configurations (see Supplemental Material [44] Figs. S16 and S17). The fracture processes of representative structures are demonstrated in Fig. 7(a), including N-1-Conv and N-1-Convconc for disordered NPR structures, P-4-Conv and P-3-Convconc for disordered PPR structures, BCPS for the topologically optimized regular NPR structure, and rhombus for the regular PPR structure. The samples are designed with a prefabricated microcrack in the middle of one side, which is pulled apart during the experiment. The fracture experiment methodology was developed and refined based on prior research focusing on metamaterials with enhanced fracture resistance and energy-absorption capabilities [41,74].

Figure 7(a) demonstrates the fracture curves, i.e., load versus pulling distance as we pull each sample apart until complete fracture. The numbers on each curve indicate obvious fracture events, and the fracture paths are shown as red curves in the corresponding right panel. We have tested both disordered samples from our design and regular samples from previous studies [42] made with the same materials and dimensions. Apparently, disordered structures regardless of their positive or negative Poisson ratio have longer fracture paths and are more difficult to fracture, while regular lattices regardless of their positive or negative Poisson ratio have much shorter fracture paths and are easier to fracture.

More specifically, in disordered samples, crack propagation does not follow a single pathway. Instead,

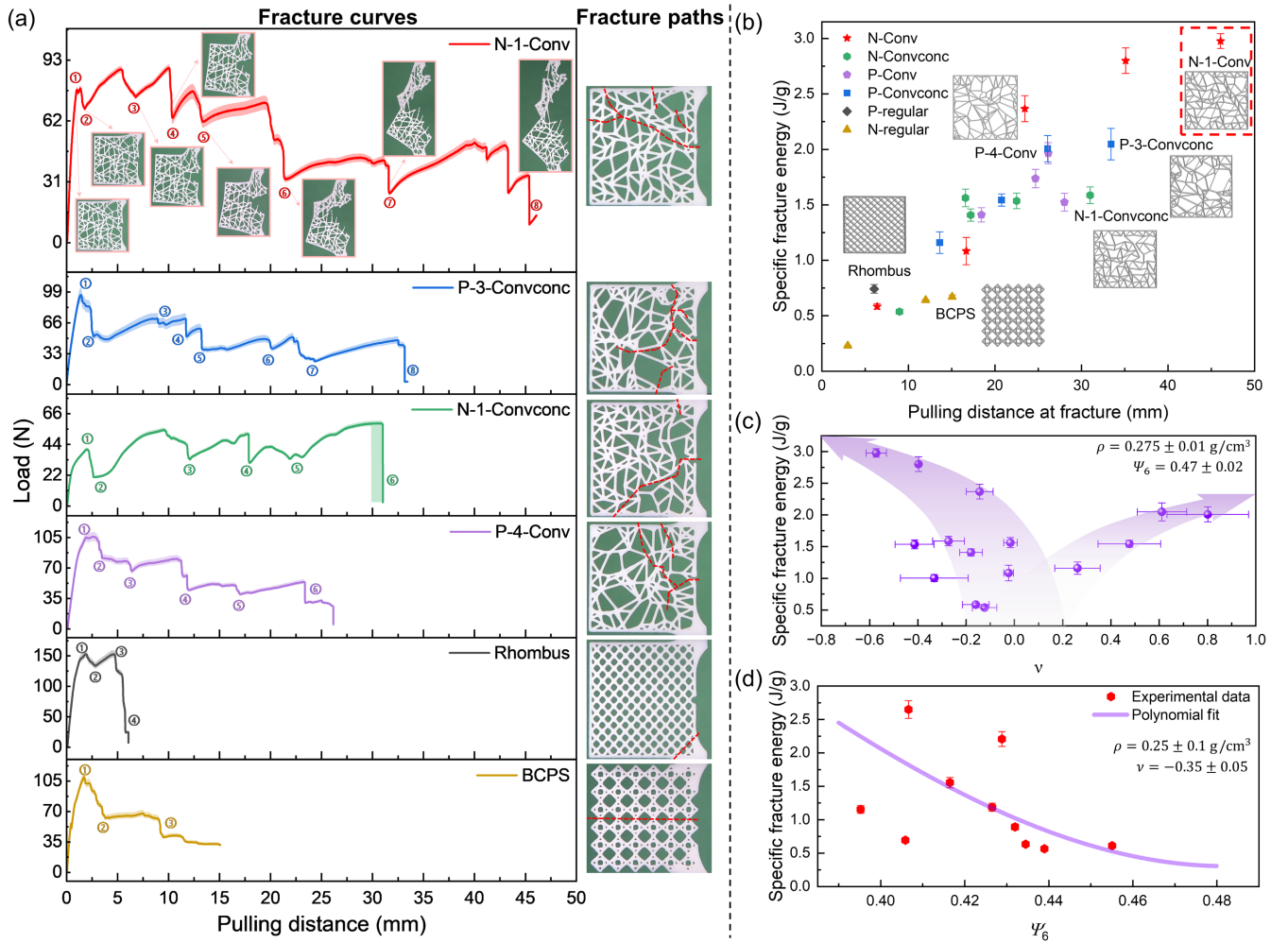


FIG. 7. (a) Fracture curves and the corresponding fracture paths indicated by red dashed curves during the fracture experiment. (b) Consumed energy deduced from areas under the fracture curves and corresponding pulling distances at the instant of complete fracture for representative samples. The dashed box indicates the sample with the best performance in both the specific fracture energy and the compressive SEA in Fig. 4(b). (c) V-shaped dependence of specific fracture energy on the Poisson ratio (ν) at similar densities (ρ) and disorder (Ψ_6). Arrows indicate the direction of increasing specific fracture energy with varying Poisson ratios. (d) Specific fracture energy decreases with the order parameter Ψ_6 , indicating that more disordered samples exhibit better fracture resistance. Note that all samples are controlled at similar densities (ρ) and Poisson ratio (ν). The fracture curves corresponding to the experimental data points are provided in Supplemental Material [44] Fig. S19.

small cracks continuously formed in new locations where structural integrity was compromised or where stress concentrations arose as the load increased. These cracks gradually coalesced into a single fracture line that extended through the entire sample, ultimately leading to complete failure. Thus, the point of collapse depends on when discrete cracks merge into a major, continuous fracture.

Such a delayed collapse indicates a greater generation of minor cracks prior to the formation of major cracks that cause significant damage. This behavior is demonstrated in Fig. 7(a) by disordered samples N-1-Conv, N-1-Convconc, P-4-Conv, and P-3-Convconc, which benefited from improved ductility stemming from disordered configurations. Conversely, rapid collapse typically occurs when a major crack forms and propagates rapidly, either originating from a single point or from very few nearby discrete points, as demonstrated by the two regular BCPS and rhombus samples. This behavior leads to material brittleness originating from mechanical anisotropy. Therefore, when collapse begins at multiple points in disordered samples, it tends to delay failure compared to those cases where major rupture starts from a single location in regular samples. More experimental details can be found in Supplemental Material [44] Fig. S18 and Table S5.

The area under the fracture curve is the energy consumed in resisting fracture, referred to as the work of fracture, which serves as a measure of fracture toughness [41,72,75]. The work of fracture per unit mass or specific fracture energy plotted against the pulling distance at the instant of complete fracture is shown in Fig. 7(b). Representative structures in Fig. 7(a) are specifically included in Fig. 7(b) for a clear demonstration. In general, a longer pulling distance corresponds to higher energy consumption, indicating a better fracture resistance. It is evident that the regular lattices, such as BCPS and rhombus, exhibit much shorter pulling distances compared to the disordered structures. Consequently, the disordered samples demonstrate significantly better fracture toughness [41,76].

Figure 7(b) provides a comprehensive mapping of the fracture performance across all categories of our disordered and ordered samples. To ensure statistical reliability and reproducibility, we 3D print three identical samples for each data point and average their fracture measurements. Samples within the same structural category (i.e., NPR and PPR, ordered and disordered, convex and convex-concave) are represented by identical symbols, with their fracture energy varying due to our progressive optimization.

As expected, a higher specific fracture energy generally corresponds to a larger pulling distance. Notably, all regular samples, including both rhombus and BCPS lattices, perform below almost all disordered samples, highlighting the inherent advantage of structural disorder in enhancing fracture resistance. In particular, the best-performing disordered auxetic sample, N-1-Conv (enclosed by the red dashed box), demonstrates a significant 452%

enhancement in fracture energy compared to its regular NPR counterpart (the BCPS lattice). This result clearly shows that disordered auxetic structures generated by our EBM framework are superior to previous regular structures in enhancing fracture resistance and delaying fracture.

As we can optimize structures by tuning both disorder and Poisson ratio, their independent impacts on fracture resistance are analyzed using a controlled-variable approach. We first examine the influence of the Poisson ratio (ν) on fracture resistance by systematically varying ν while holding other parameters, such as density (ρ) and disorder (Ψ_6), constant, as shown in Fig. 7(c). Our experimental results demonstrate that the specific fracture energy increases with the magnitude of the Poisson ratio ($|\nu|$) in both the positive and negative ν regimes, forming a V-shaped profile centered at $\nu = 0$. This toughening effect at elevated $|\nu|$ aligns with observations in noncrystalline solids, such as metallic glasses [77,78] and disordered cellular foams [79]. This parallel finding suggests that the Poisson ratio can serve as a universal factor for fracture resistance, spanning from atomic-scale amorphous alloys to the macroscopic disordered networks studied here.

The exceptional fracture resistance at both extremes of the Poisson ratio (ν) spectrum—highly positive and highly negative—can be attributed to the delocalization of strain fields [80,81]. In both regimes, enhanced strain redistribution and delocalization at high $|\nu|$ effectively reduces stress singularities at the crack tip, delaying the onset of premature failure. Additionally, for highly negative ν (auxeticity), an extra resistance mechanism occurs at the crack tip, beyond the effects of strain delocalization. Under tensile loading, auxetic structures undergo transverse expansion, which points opposite to the direction of crack propagation, effectively counteracting the crack-opening force. Consequently, structures with a negative Poisson ratio can exhibit an even greater fracture resistance compared to those with a conventional positive Poisson ratio, as demonstrated in Fig. 7(c) [81].

Regarding the role of disorder in the specific fracture energy, we systematically vary the order parameter Ψ_6 while keeping other parameters fixed, as shown in Fig. 7(d). We find that the specific fracture energy systematically increases as the samples become more disordered (i.e., with smaller Ψ_6). Disorder improves specific fracture energy by inducing crack deflection, resulting in a more tortuous cracking trajectory that increases the total fracture energy required for failure.

To summarize, by combining two distinct yet complementary mechanisms—negative Poisson ratio and structural disorder—our structures achieve a synergistic effect, delivering exceptional performance in fracture resistance compared to optimizing either parameter in isolation. Consequently, we conclude that disordered auxetic structures designed using our physics-constrained EBM framework outperform ordered structures developed through

topology optimization in achieving the combined objectives of a freely adjustable Poisson ratio, reduced structural density, superior energy absorption, and enhanced fracture resistance.

D. Enhanced performance and potential applications

In Fig. 8(a), we compare the SEA of our auxetic NPR samples with other structures utilized for energy absorption [61–68] (compression SEA) or fracture resistance [82–85]

(fracture SEA). To ensure a fair comparison, all structures are fabricated from the parent materials with similar densities (i.e., TPU, light metal foam, PU foam, polylactic acid, and photopolymer resin). Compared to all previous structures, our structures either exhibit a much lower density or a much higher energy-absorption capacity (i.e., higher SEA), or both, demonstrating the superior performance of our physics-constrained EBM framework design. Notably, the highest SEA for energy absorption previously achieved involved manufacturing an intricate

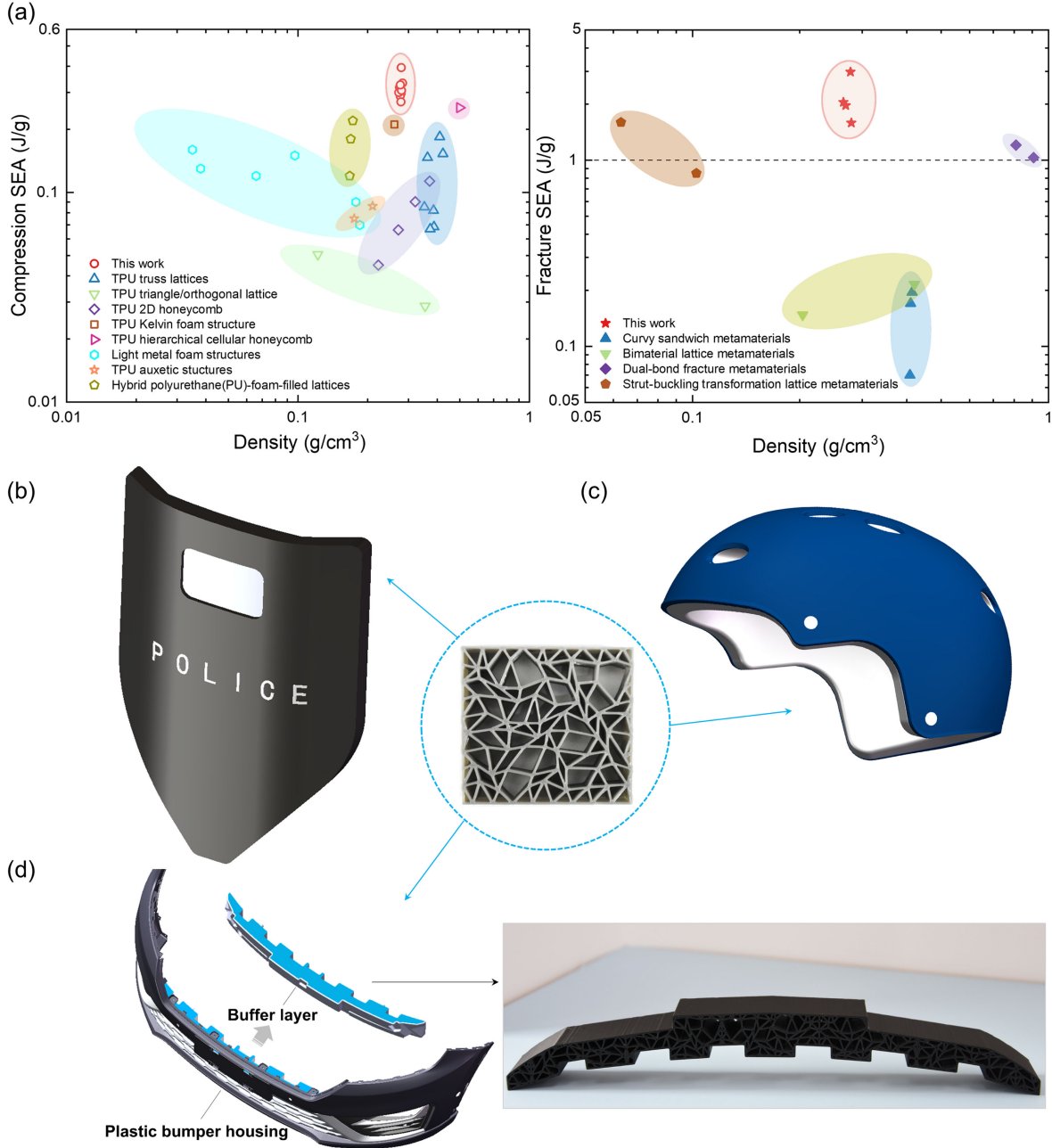


FIG. 8. (a) Comparing energy-absorption capabilities and fracture resistance performance of our systems with previous structures [61–68,82–85]. Our systems demonstrate higher SEA values at lower densities. (b)–(d) Potential applications of our systems in ballistic shields, helmets, and car bumpers. Note that the 3D-printed car bumper prototype is based on our NPR structure which has the best energy-absorption performance.

core-shell microstructure using complex supercritical CO₂-foaming technology [64]. In contrast, our systems achieve similar or even greater SEA through a physics-constrained EBM framework and employing straightforward 3D-printing techniques. Meanwhile, our structures also fall within the high-performance regime in evaluating fracture SEA. Comparable performance in prior studies was typically achieved through ultrafine bonds exploiting natural buckling deformation, fabricated using ultrahigh-precision methods [85]. Obviously, our design simultaneously achieves high energy absorption and superior fracture resistance, performing comparably to or even surpassing previously reported structures optimized for a single objective. In addition, it features a simple and cost-effective fabrication process, offering substantial benefits for industrial applications.

By utilizing a physics-constrained EBM framework, we have engineered NPR materials characterized by highly negative Poisson ratios and mechanical isotropy. Our experiments demonstrate that these structures exhibit significantly enhanced energy absorption at lower densities [as shown in Figs. 3(g), 3(h), 4(a), and 8(a)], improved impact resistance [Figs. 6(g)–6(j)], and superior fracture toughness [Figs. 7(a) and 7(b)]. These exceptional mechanical properties suggest a range of practical applications. For instance, these materials could be utilized in the construction of ballistic shields and helmets, as shown in Figs. 8(b) and 8(c). Additionally, they can be applied in making buffer layers for car bumpers, as shown by a 3D-printed prototype in Fig. 8(d). These potential applications highlight the practical value of our NPR materials designed through a physics-constrained EBM framework, which may lead to significant advancements in safety and protective equipment.

IV. CONCLUSIONS

To conclude, we have introduced a physics-constrained EBM framework for the inverse design of amorphous auxetic metamaterials. By defining a multiobjective energy function that targets both a negative Poisson ratio and approximate isotropy, we recast the design problem as finding the ground state of a complex energy landscape. We employed Boltzmann inference (realized via simulated annealing) to solve this problem within a mechanically stable configuration space.

The resulting designs, validated experimentally, exhibit a highly negative Poisson ratio (as low as -0.6 at 5% strain) and superior isotropy. Crucially, these optimized structures also demonstrate exceptional emergent properties not explicitly included in the optimization, including significantly enhanced energy absorption, impact resistance, and fracture toughness. The energy absorption of our optimal auxetic design achieves a 22% higher SEA compared to the best periodic sample from topological optimization, while being 10% less dense. In terms of specific fracture energy,

our disordered auxetic structures show a 452% improvement over ordered counterparts.

This work demonstrates that the design of high-performance amorphous materials can be successfully framed as an interpretable, energy-based machine-learning problem. This approach not only yields structures with superior, multifunctional mechanical performance, but also, through its connection to statistical physics models, provides a pathway to understanding the underlying structure-property relationships. These materials are highly suitable for practical applications in various industries, such as protective shields, helmets, and car bumpers. In other words, this work bridges the gap between statistical physics concepts and practical materials engineering, demonstrating that the vast, complex configuration space of amorphous structures is not a barrier, but rather a rich landscape for discovering materials with unprecedented, multifunctional performance.

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L. X. and X. S. conceived the research. L. J., C. Z., X. S., and L. X. designed the research. L. J. performed the experiments, simulations, and analysis. C. Z. developed the optimization code and implemented the numerical computations. X. S. derived the EBM model. J. L., H. T., J. M., and C. X. helped with the experiments. L. J., C. Z., X. S., and L. X. prepared the manuscript. L. X., C. X., and X. S. supervised the research, and L. X. oversaw and coordinated the research.

L. J., C. Z., and L. X. are coauthors of a filed China Patent No. 202410824753.8, which describes the method used herein.

DATA AVAILABILITY

The data that support the findings of this study are not publicly available because they contain commercially sensitive information. The data are available from the authors upon reasonable request.

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