

Article

Stability and Elasticity of Topologically Expanded Schwarzite P-Surface Nets

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Abstract

Schwarzites are negatively curved sp^2 -carbon frameworks that can be described as realizations of triply periodic minimal surface (TPMS) nets. This work examines topologically expanded Schwarzite networks derived from P-surface tilings by isolated heptagons, in which neighboring cages are connected via inserted carbon nanotubes rather than through direct links present in the parent Schwarzite. The study focuses on how such topological modifications influence network stability, density, and mechanical response. Density functional theory calculations show that nanotube-mediated expansion systematically reduces framework density while redistributing curvature within the network. A key topological distinction arises between structures formed by separating large cages and those formed by separating small cages. Separation of large cages is equivalent to inserting nanotube segments into adjacent small cages, increasing their effective size and relieving curvature-induced strain, thereby enhancing energetic stability. In contrast, separation of small cages preserves their topology and provides only limited strain relief. Cohesive energy trends correlate with the hexagon-to-heptagon ratio, approaching the graphene limit as topological expansion increases. Mechanical properties follow the same hierarchy, with strain-relieved networks displaying reduced stiffness and greater compliance. These findings indicate that the properties of Schwarzites are governed primarily by topological connectivity and curvature distribution rather than geometric scaling alone, establishing general principles for tuning stability and elasticity in negatively curved carbon networks through controlled topological expansion.

Keywords: Schwarzites; P-surface; triply periodic minimal surfaces; elastic properties; cohesive energy; carbon nanotubes



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1. Introduction

Although still hypothetical, Schwarzites are a promising class of carbon allotropes predicted to combine high mechanical strength with low density, intrinsic porosity, and tunable electronic conductivity [1–4]. From a topological perspective, Schwarzites can be viewed as periodic sp^2 -bonded nets embedded on triply periodic minimal surfaces (TPMS), where negative Gaussian curvature is accommodated through the incorporation of non-hexagonal rings. Among the TPMS families, the P-surface has been the most extensively studied framework for Schwarzite construction and was initially explored using octagonal tilings [1]. More recently, P-surface-based Schwarzite nets incorporating heptagons have been proposed, expanding the range of accessible topologies and curvature distributions [5,6].

According to Euler's theorem, Equation (25) in Ref. [7], 24 heptagons are required per P-surface chamber. In the simplest case, there is one chamber per unit cell, yielding the parent P-Schwarzite topology. The isolated heptagon rule implies the presence of hexagons in the net, with at least a 2:1 ratio of hexagons to heptagons, or a higher ratio in structures where heptagons are more diluted (Table 1).

The possibility of "diluting" the required number of heptagons by increasing the number of hexagons, while preserving the global topological constraint imposed by Euler's theorem, has been recognized in prior work and employed, without systematic analysis, in the construction of several P-surface Schwarzite models (e.g., Ref. [8]). In these studies, additional hexagons are introduced to spatially separate heptagons, thereby reducing local curvature concentration and modifying the geometric distribution of negative Gaussian curvature without violating the overall topological requirement. Despite this recognition, the treatment of heptagon dilution has remained largely ad hoc and case-specific.

In particular, there is no systematic framework that enumerates all admissible dilution patterns for a given P-surface topology or establishes structure–property relationships linking the degree of dilution to key physical properties such as thermodynamic stability and elastic response. This lack of classification obscures fundamental design principles and limits the rational exploration of the Schwarzite structural space. A corresponding topology-guided description of how directional cage separation governs the evolution of structural stability and elastic properties is also absent.

The present work addresses these gaps by providing a systematic classification of heptagon dilution schemes and by quantifying their consequences for stability and mechanical response.

One approach to diluting P-Schwarzites is the insertion of hexagonal fragments between chambers in the form of nanotube connectors that link neighboring P-chambers, as demonstrated by Elias et al. [8] From a graph-theoretical viewpoint, this operation constitutes a topological expansion of a periodic net, in which vertices and edges are added in a highly constrained, symmetry-related manner while preserving global three-dimensional connectivity. Such expansions significantly increase the number of realizable P-Schwarzite nets, albeit often at the cost of reduced symmetry and increased translational periodicity length. At the same time, this structural flexibility provides a route for systematic tuning of density, curvature localization, and physical properties.

In this DFT study, we investigate the stability, density, and elastic properties of P-Schwarzites as a function of the length of nanotube connectors between chambers in two representative systems, P207-C168 and P221-C216. Both structures are topologically unbalanced, meaning that the two sides of the surface are not equivalent, as reflected by the alternation of small and large chambers (Figures 1 and 2). Consequently, nanotube connectors may be inserted between small chambers, large chambers, or both, leading to distinct topological and mechanical outcomes.

As in our previous work [6], we keep heptagons organized in trimers, consistent with Euler's requirement that 24 heptagons be arranged at the eight corners of the cubic P-surface unit cell. An additional mode of dilution, not attempted here, can be achieved by inserting hexagonal rings that separate the heptagons within these trimers, thereby redistributing curvature without altering chamber connectivity.

Table 1. Topological descriptors and DFT-calculated density and energy of Schwarzite TPMS networks incorporating nanotube connectors.

Name	Point Symbol	Hexagons to Heptagons Ratio	Density, g/cm ³	Number of Atoms in the Unit Cell	Number of Atoms in Nanotubes	Electronic Energy, eV	Cohesive Energy per Atom Relative to Graphene, kcal/mol
P207S							
P89-C200-(2222)[1-1-0]	$(6^2.7)_7(6^3)_4$	2.6	0.971	200	32	−30,839.45	4.27
P89-C184-(2222)[1-0-0]	$(6^2.7)_7(6^3)_2$	2.3	1.044	184	16	−28,370.54	4.49
P207-C168	$(6^2.7)$	2.0	1.116	168	0	−25,901.55	4.77
P207-C552-(2222)[8-8-8]	$(6^2.7)_7(6^3)_{16}$	4.3	0.275	552	384	−85,137.04	3.43
P207-C216-(2222)[1-1-1]	$(6^2.7)_7(6^3)_2$	2.3	0.896	216	48	−33,308.48	4.07
P207-C264-(2222)[2-2-2]	$(6^2.7)_7(6^3)_4$	2.6	0.724	264	96	−40,713.93	3.76
P207-C312-(2222)[3-3-3]	$(6^2.7)_7(6^3)_6$	2.9	0.594	312	144	−48,117.65	3.67
P89-C248-(2222)[2-2-1]	$(6^2.7)_{21}(6^3)_{10}$	2.5	0.778	248	80	−38,245.36	3.86
P89-C248-(2222)[3-1-1]	$(6^2.7)_{21}(6^3)_{10}$	2.5	0.793	248	80	−38,244.73	3.92
P16-C264-(2222)[3-2-1]	$(6^2.7)_7(6^3)_4$	2.6	0.737	264	96	−40,713.53	3.80
P89-C296-(2222)[3-3-2]	$(6^2.7)_{21}(6^3)_{16}$	2.8	0.636	296	128	−45,650.5	3.64
P89-C280-(2222)[3-2-2]	$(6^2.7)_3(6^3)_2$	2.7	0.680	280	112	−43,182.17	3.70
P89-C280-(2222)[3-3-1]	$(6^2.7)_3(6^3)_2$	2.7	0.691	280	112	−43,181.77	3.73
P207L							
P89-C216-(31313131)[1-0-0]	$(6^2.7)_7(6^3)_2$	2.3	1.097	216	48	−33,315.2	3.36
P89-C264-(31313131)[1-1-0]	$(6^2.7)_7(6^3)_4$	2.6	1.030	264	96	−40,729.15	2.43
P207-C168	$(6^2.7)$	2.0	1.116	168	0	−25,901.55	4.77
P207-C312-(31313131)[1-1-1]	$(6^2.7)_7(6^3)_6$	2.9	0.928	312	144	−48,140.98	1.95
P207-C456-(31313131)[2-2-2]	$(6^2.7)_7(6^3)_{12}$	3.7	0.734	456	288	−70,376.61	1.10
P207-C600-(31313131)[3-3-3]	$(6^2.7)_7(6^3)_{18}$	4.6	0.579	600	432	−92,612.66	0.65
P89-C504-(31313131)[3-3-1]	$(6^2.7)(6^3)_2$	4.0	0.710	504	336	−77,789.54	0.88
P89-C408-(31313131)[3-1-1]	$(6^2.7)_7(6^3)_{10}$	3.4	0.837	408	240	−62,965.37	1.28
P89-C504-(31313131)[5-1-1]	$(6^2.7)(6^3)_2$	4.0	0.786	504	336	−77,789.58	0.88
P16-C600-(31313131)[5-3-1]	$(6^2.7)_7(6^3)_{18}$	4.6	0.644	600	432	−92,613.46	0.62
P89-C696-(31313131)[5-3-3]	$(6^2.7)_7(6^3)_{22}$	5.1	0.512	696	528	−107,437	0.44
P89-C696-(31313131)[5-5-1]	$(6^2.7)_7(6^3)_{22}$	5.1	0.570	696	528	−107,437.3	0.43
P21-C792-(31313131)[5-5-3]	$(6^2.7)_7(6^3)_{26}$	5.7	0.445	792	624	−122,260.8	0.30

Table 1. Cont.

Name	Point Symbol	Hexagons to Heptagons Ratio	Density, g/cm ³	Number of Atoms in the Unit Cell	Number of Atoms in Nanotubes	Electronic Energy, eV	Cohesive Energy per Atom Relative to Graphene, kcal/mol
P221S							
P123-C280-(1 ⁸)[1-1-0]	$(6^2.7)3(6^3)_2$	2.7	0.823	280	64	−43,201.55	2.10
P123-C248(1 ⁸)[1-0-0]	$(6^2.7)_{21}(6^3)_{10}$	2.5	0.922	248	32	−38,264.76	2.06
P221-C216	$(6^2.7)_7(6^3)_2$	2.3	1.016	216	0	−33,327.63	2.03
P221-C216-(1 ⁸)[2_2_2]	$(6^2.7)_7(6^3)_{10}$	3.4	0.535	408	192	−62,950.83	2.10
P166-C312-(1 ⁸)[1-1-1]	$(6^2.7)_7(6^3)_6$	2.9	0.725	312	96	−48,138.44	2.14
P221-C504-(1 ⁸)[3-3-3]	$(6^2.7)(6^3)_2$	4.0	0.411	504	288	−77,763.37	2.08
P123-C376-(1 ⁸)[1-2-2]	$(6^2.7)_{21}(6^3)_{26}$	3.2	0.597	376	160	−58,013.66	2.10
P47-C408-(1 ⁸)[1-2-3]	$(6^2.7)_7(6^3)_{10}$	3.4	0.551	408	192	−62,951.41	2.07
P123-C440-(1 ⁸)[2-2-3]	$(6^2.7)_{21}(6^3)_{34}$	3.6	0.491	440	224	−67,888.86	2.07
P123C-472-(1 ⁸)[2-3-3]	$(6^2.7)_{21}(6^3)_{38}$	3.8	0.449	472	256	−72,826.55	2.05
P123-C376-(1 ⁸)[3-1-1]	$(6^2.7)_{21}(6^3)_{26}$	3.2	0.614	376	160	−58,013.23	2.12
P123-C440-(1 ⁸)[3-3-1]	$(6^2.7)_{21}(6^3)_{34}$	3.6	0.506	440	224	−67,888.33	2.10
P123-C344-(1 ⁸)[1-1-2]	$(6^2.7)_{21}(6^3)_{22}$	3.0	0.658	344	128	−53,076.04	2.11
P221L							
P123-C280-(2 ⁸)[1-1-0]	$(6^2.7)3(6^3)_2$	2.7	0.978	280	64	−43,211.07	1.32
P123-C248-(2 ⁸)[1-0-0]	$(6^2.7)_{21}(6^3)_{10}$	2.5	1.005	248	32	−38,269.02	1.66
P221-C216	$(6^2.7)_7(6^3)_2$	2.3	1.016	216	0	−33,327.63	2.03
P221-C312-(2 ⁸)[1-1-1]	$(6^2.7)_7(6^3)_6$	2.9	0.939	312	96	−48,151.51	1.17
P221-C408-(2 ⁸)[2-2-2]	$(6^2.7)_7(6^3)_{10}$	3.4	0.850	408	192	−62,976.16	0.67
P221-C600-(2 ⁸)[4-4-4]	$(6^2.7)_7(6^3)_{18}$	4.6	0.669	600	384	−92,628.85	0.03
P221-C792-(2 ⁸)[6-6-6]	$(6^2.7)_7(6^3)_{26}$	5.7	0.527	792	576	−122,278.7	−0.22
P221-C376-(2 ⁸)[2-2-1]	$(6^2.7)_{21}(6^3)_{26}$	3.2	0.886	376	160	−58,034.33	0.83
P123-C408-(2 ⁸)[4-1-1]	$(6^2.7)_7(6^3)_{10}$	3.4	0.883	408	192	−62,977.4	0.60
P47-C440-(2 ⁸)[4-2-1]	$(6^2.7)_{21}(6^3)_{34}$	3.6	0.843	440	224	−67,918.15	0.53
P123-C472-(2 ⁸)[4-2-2]	$(6^2.7)_{21}(6^3)_{38}$	3.8	0.800	472	256	−72,859.5	0.44
P123-C504-(2 ⁸)[4-4-1]	$(6^2.7)(6^3)_2$	4.0	0.780	504	288	−77,801.64	0.33
P123-C536-(2 ⁸)[4-4-2]	$(6^2.7)_{21}(6^3)_{46}$	4.2	0.737	536	320	−82,743.62	0.23
P123-C344-(2 ⁸)[2-1-1]	$(6^2.7)_{21}(6^3)_{22}$	3.0	0.916	344	128	−53,093.69	0.93

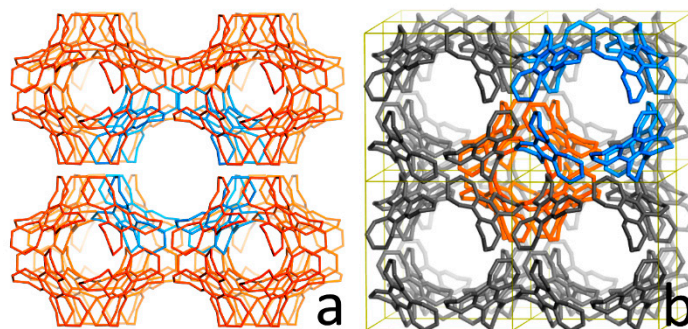


Figure 1. Illustration of two sides of the surface through local chamber environments in P207-C168: (a) each large chamber is surrounded by eight small chambers; (b) each small chamber is surrounded by eight large chambers. Different colors are used to highlight small and large chambers as parts of the whole structure.

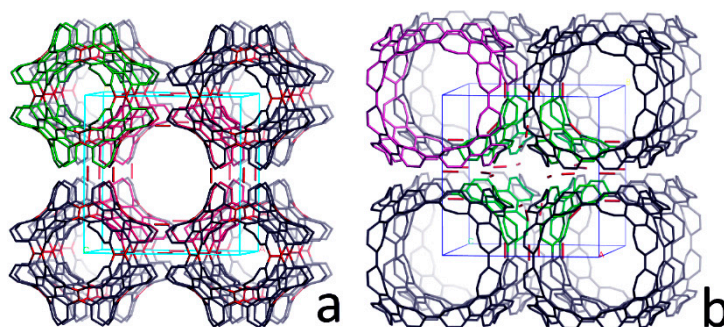


Figure 2. Illustration of two sides of the surface through local chamber environments in P221-C216: (a) each large chamber is surrounded by eight small chambers; (b) each small chamber is surrounded by eight large chambers. Different colors are used to highlight small and large chambers as parts of the whole structure.

To facilitate systematic classification of the resulting structures, we employ a previously introduced topological descriptor, the neck configuration, which characterizes the ring sequence around the chamber openings [6]. This descriptor allows one to distinguish between expansions involving small or large chambers and to track how local topology propagates into extended motifs. In the example shown in Figure 3, the nanotube segment represents a translational continuation of the original neck topology of the P207-C168 large chamber, with the 31313131 descriptor transcriptionally copied from the chamber boundary to the nanotube perimeter. The neck configuration dictates the type of nanotube formed, either zigzag or armchair, without invoking chirality in the conventional nanotube sense. This descriptor also distinguishes small and large chambers, reflecting differences in chamber diameter and volume through the neck size, defined by the number of atoms (2222 vs. 31313131 in P207-C168, respectively).

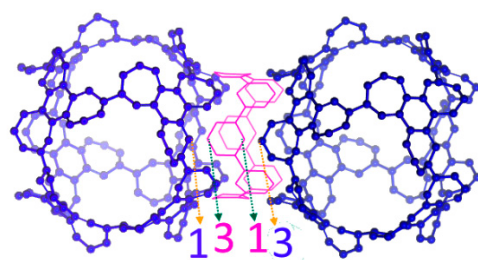


Figure 3. Shortest possible nanotube connector inserted between two large chambers of P207-C168, illustrating transcription of the 31313131 neck-configuration descriptor from the chamber opening to the nanotube.

The nomenclature for Schwarzites introduced earlier [6] has been extended here to accommodate the newly constructed topologies. In its original form, the designation consisted of the TPMS type, the space-group symmetry, the atom type (C for carbon), and the number of carbon atoms in the unit cell. In the present work, the notation is augmented to indicate the resulting space-group symmetry after topological expansion, the neck-configuration descriptor (given in round brackets and specific to either small or large chambers), and the lengths of the nanotube connectors along the crystallographic x, y, and z directions (given in square brackets). Connector lengths are expressed in integer units of the shortest possible nanotube fragment, which is case-specific and dictated by the neck topology. For example, P89-C184-(2222)[1-0-0] denotes a P-surface-based Schwarzite in which small chambers, identifiable by the neck configuration 2222 inherited from the parent net P207-C168, are separated by insertion of the shortest nanotube connector along the x axis, with no connectors inserted along the y and z axes.

2. Computational Method

The Materials Studio, version 2024, DFT computational package, supplied by Dassault Systèmes Biovia Corporation, San Diego, CA, USA, was employed to construct unit cells of the previously reported [5,6,9] P-surface Schwarzites P207-C168 and P221-C216 by inserting nanotube connectors of varying lengths, with diameters determined by the size of the chamber openings. Geometry and unit cell optimization for each periodic structure and elastic constants for selected structures were completed by CASTEP [10] within the generalized gradient approximation (GGA) for the electron exchange and correlation based on the work of Perdew et al. using PBE [11] functional. As a trade-off between accuracy and computational cost, particularly for the large, low-symmetry structures in our set, the same Tkatchenko-Scheffler (TS) exchange correlation [12] was applied uniformly to all unit cells, regardless of size to address dispersive interactions. All calculations were performed spin restricted. Koelling-Harmon scalar treatment [13] was used to incorporate relativistic effects into pseudopotentials generated on the fly.

The plane-wave energy cutoff was set to 600 eV. The Brillouin zone was sampled according to the Monkhorst-Pack [14] scheme with the grid $2 \times 2 \times 2$. Structural relaxation was performed until the change in total energy was less than 0.00002 a.u. SCF density convergence and gradient convergence were set to 0.00001, and 0.004 a.u., respectively.

The topology analysis was performed, and standard Point Symbol nomenclature was generated using ToposPro software 2024 [15] in accordance with the guidelines outlined in Ref. [16].

3. Results and Discussion

3.1. Density, Ring Statistics, and Energetic Stability of Topologically Expanded Schwarzite Nets

The present series of Schwarzite structures is generated by topological expansion of two parent nets, P207-C168 and P221-C216, through insertion of tubular graphitic connectors between symmetry-equivalent cage openings (Figures 4 and 5). This construction preserves the global net topology while systematically increasing the repeat unit size and modifying the local ring statistics. As a result, density, curvature distribution, and energetic stability can be tuned independently of the parent TPMS class.

For all families considered, the calculated mass density decreases monotonically with increasing connector length, reflecting the growing fraction of quasi-graphitic segments relative to curved cage walls. This trend is independent of whether large or small cages are separated and is therefore a direct geometric consequence of topological expansion. Densities decrease from values exceeding $1.0 \text{ g}\cdot\text{cm}^{-3}$ for parent nets to below $0.5 \text{ g}\cdot\text{cm}^{-3}$

for the largest expanded structures, placing these Schwarzites among the lowest-density fully sp^2 -bonded carbon nets reported to date.

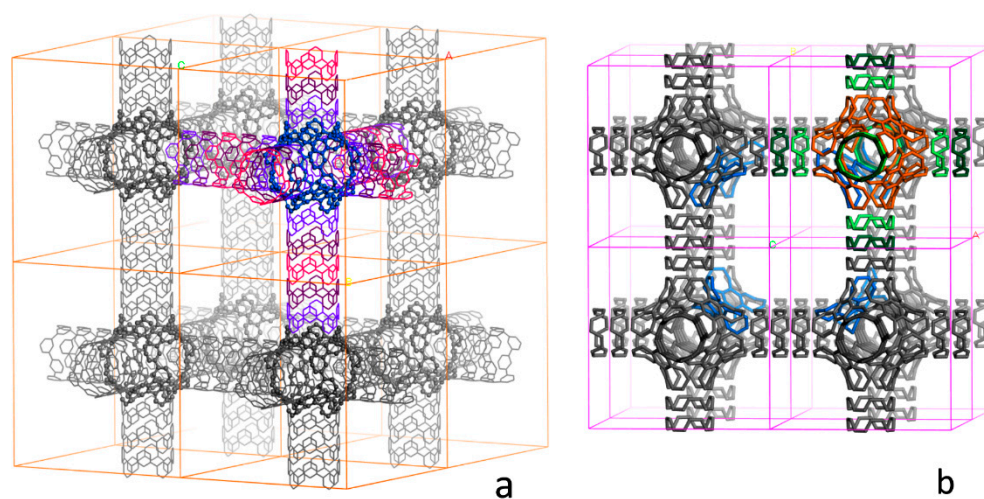


Figure 4. Examples of topologically expanded P207-C168 Schwarzite nets. (a) Insertion of the same length-5 zig-zag nanotube connectors between large chambers along all the x, y, and z crystallographic axes enlarges the neighboring small chambers, yielding the expanded net P207-C888-(31313131)[5_5_5]. (b) Insertion of the same length-3 armchair nanotube connectors between small chambers along all the x, y, and z axes enlarges the large chambers, producing the net P207-C312-(2222)[3_3_3]. Coloring is used to help visualize the different elements, chambers, and individual segments of the nanotube connectors.

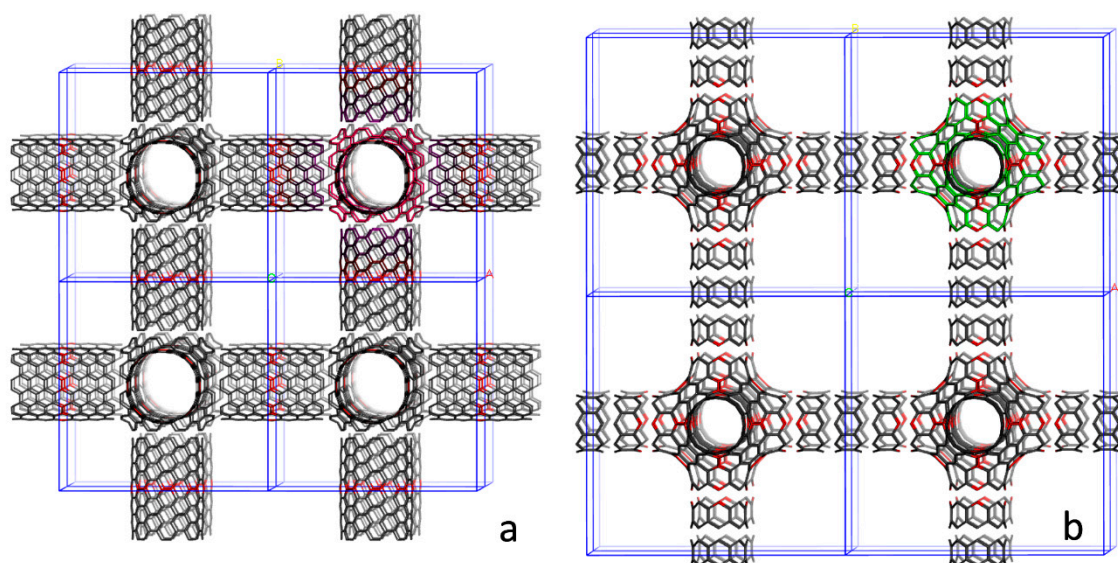


Figure 5. Examples of topologically expanded P221-C216 Schwarzite nets. (a) Insertion of the same length-6 armchair nanotube connectors between large chambers along all the x, y, and z crystallographic axes enlarges the neighboring small chambers, yielding the expanded net P221-C216-(2^8)[6-6-6] (b) Insertion of the same length-3 zig-zag nanotube connectors between small chambers along all the x, y, and z axes enlarges the large chambers, producing the net P221-C216-(1^8)[3-3-3]. Coloring is used to help visualize chambers and connections between nanotube segments.

In contrast, the behavior of the cohesive energy relative to graphene exhibits a pronounced dependence on which type of cage is separated (Figure 6, Table 1). When tubular connectors are inserted between large cages (P207L and P221L families), a steep reduction in the cohesive energy penalty is observed. For example, the parent P207-C168 net exhibits a cohesive energy difference of 4.77 eV per atom relative to graphene, whereas expanded

derivatives approach values close to zero and even slightly negative for large P221-based nets. This strong energetic stabilization indicates efficient relaxation of topological strain.

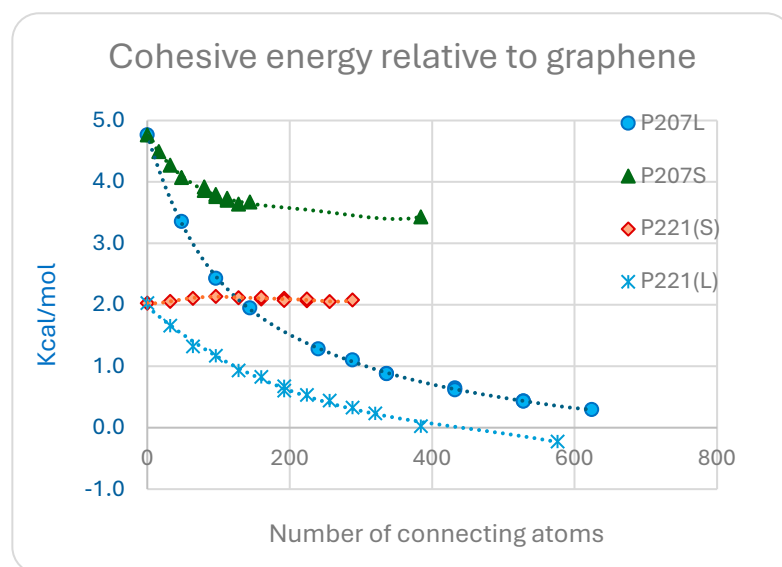


Figure 6. DFT calculated cohesive energy per carbon atom in expanded Schwarzite nets relative to that in graphene as a function of the total number of atoms used in nanotube connectors.

By comparison, insertion of connectors between small cages (P207S and P221S families on Figure 6) leads to only modest or negligible stabilization. In the P207S series, the cohesive energy decreases gradually to values around 3.6–3.9 eV per atom, while in the P221S series it remains nearly constant at approximately 2.0–2.1 eV per atom despite substantial reductions in density. These results demonstrate that preservation of small cages maintains a high degree of local curvature and limits strain relaxation.

This dichotomy can be rationalized in terms of local ring statistics and curvature localization. Separation of large cages induces a topological reorganization of neighboring small cages, effectively separating heptagon trimers and redistributing negative Gaussian curvature over extended graphitic segments. As a consequence, the original small cages expand and lose their highly constrained character (Figure 6, graphs for P207L and P221L families). In contrast, when small cages are separated, their local ring environment remains intact, while curvature redistribution occurs primarily through enlargement of large cages, which is energetically less effective.

The same conclusion emerges from analysis of the hexagon-to-heptagon ratio, which provides a quantitative topological measure of curvature dilution (Table 1). For all expanded nets this ratio increases with connector length, approaching the graphene limit of infinity corresponding to zero Gaussian curvature. However, the increase is much more rapid for nets in which large cages are separated, consistent with their markedly enhanced energetic stabilization. These observations indicate that topological strain in Schwarzites is localized primarily within small cages characterized by high heptagon density, rather than being uniformly distributed over the minimal surface.

3.2. Elastic Response and Its Relation to Topological Strain Relaxation

The four Schwarzite structures for which full elastic tensors were calculated, P207-C168, P89-C184-(2222)[1-0-0], P221-C216, and P221-C312-(2⁸)[1-1-1], establish a direct connection between the energetic/topological trends discussed above and the elastic response of the nets.

The parent nets P207-C168 and P221-C216 exhibit the highest densities and the largest cohesive energy penalties relative to graphene. Consistent with their compact connectivity and short load-bearing paths, both structures display comparatively high bulk and Young's moduli (Table 2). At the same time, their elastic response reflects significant curvature-induced strain localized within the cages, as evidenced by moderate hardness values and non-negligible elastic anisotropy.

Table 2. Elastic and mechanical properties of Schwarzites and reference materials.

Structure/Material	B (GPa)	G (GPa)	E (GPa)	E/ ρ (GPa·cm ³ /g)	ν	H (GPa)	K _{IC} (MPa·m ^{1/2})	A _U
P221-C216	96.24	41.17	108.10	106.4	0.313	4.87	—	0.38
P221-C312-(2̂8)[1-1-1]	79.93	41.34	105.78	112.7	0.279	6.06	0.96	0.80
P207-C168	113.7	44.37	117.78	105.5	0.327	4.63	—	0.33
P89-C184-(2222)[1-0-0]	95.91	40.16	107.73	103.2	0.313	4.86	1.03	0.24
Graphene (2D)	—	—	~1000	442.5	~0.16	—	~4–5	—
Graphite	33–36	4–5	10–15	5.53	~0.20	~0.5	~0.8–1.0	high
Aluminum (fcc)	~76	~26	~70	25.9	0.34	~1.0	~25–35	~0
Titanium (hcp)	~110	~44	~116	25.7	0.32	~3.0	~55–115	moderate

Notes. Hill-averaged elastic constants are reported for Schwarzite structures. B: bulk modulus; G: shear modulus; E: Young's modulus; E/ ρ : specific stiffness; ν : Poisson's ratio; H: hardness estimated using the Tian model; K_{IC}: fracture toughness; A_U: universal elastic anisotropy index. Reference data for graphene, graphite, aluminum, and titanium were taken from Refs. [17–20] Graphene values correspond to in-plane response; bulk elastic constants are not defined.

Topological expansion produces distinct mechanical responses depending on which type of cage is separated. In P89-C184-(2222)[1-0-0], derived from P207-C168 by inserting a single shortest nanotube along one crystallographic axis and thus separating only small cages, the Young's modulus (107.7 GPa) is only moderately reduced relative to the parent net (117.8 GPa). The bulk and shear moduli show similarly modest reductions, indicating that partial strain relaxation can be achieved without a substantial loss of mechanical rigidity. This behavior reflects the limited nature of the topological modification: expansion along a single direction relieves local curvature without significantly altering the global load-bearing topology.

In contrast, P221-C312-(2̂8)[1-1-1], obtained by separating large cages along all three crystallographic axes, exhibits a more pronounced topological expansion. This modification results in a substantial energetic stabilization relative to the parent P221-C216 net, reflecting effective relief of curvature-induced topological strain. Although the density and bulk modulus are reduced, the Young's modulus remains comparable to that of the parent structure (105.8 vs. 108.1 GPa), demonstrating that extensive topological expansion does not necessarily lead to mechanical softening. Instead, the increased universal anisotropy index and higher hardness (6.06 GPa vs. 4.87 GPa in the parent P221-C216) suggest a redistribution of stiffness associated with the insertion of nanotube connectors and the resulting heterogeneity in load transfer. Given the limited dataset (four structures), this interpretation should be considered tentative and reflects two competing effects: the reduction in density and bulk modulus, which typically lowers hardness, and the emergence of a heterogeneous load-bearing network in which stiff nanotube struts are embedded within a more compliant porous matrix. This heterogeneity generates local strain gradients that resist indentation-induced deformation. The sharp rise in the universal anisotropy index (A_U from 0.38 to 0.80) is consistent with this picture, indicating that directional stiffness variations can enhance resistance to plastic flow under indentation. Consequently, reduction in topological strain does not necessarily imply a proportional loss of stiffness, nor does lower density guarantee lower hardness.

On a mass-normalized basis, P221-C312-(2̂8)[1-1-1] exhibits the highest specific stiffness (112.7 GPa·cm³/g) among the four structures, exceeding that of the denser parent P221-C216

(106.4 GPa·cm³/g). This confirms that extensive topological expansion improves mechanical efficiency per unit mass, a desirable feature for lightweight structural applications.

Notably, the stiffest structure among the four, P207-C168, is also the least energetically stable, whereas P221-C312-(2⁸)[1-1-1] represents a more balanced compromise between rigidity and stability. This decoupling highlights an important distinction: mechanical rigidity is governed primarily by global connectivity and load-bearing topology of the net, whereas energetic stability is controlled by local ring statistics and curvature localization.

4. Conclusions

Analysis of the energetic, density, and elastic properties of Schwarzite nets constructed via tubular connector insertion establishes a topology-driven framework for controlling density, curvature distribution, and mechanical response. Topological expansion through nanotube connectors modifies the spatial separation of negatively curved units, enabling independent tuning of global density and local strain without changing the genus of the underlying TPMS.

Density decreases predictably with increasing connector length, largely independent of cage type, confirming tubular insertion as a robust route to ultralight, fully sp²-bonded periodic networks. At the same time, curvature is redistributed: connector insertion between large cages is topologically equivalent to expansion of the small cages, which relieves strain in highly curved regions.

Energetic stabilization is governed primarily by curvature dilution, i.e., increasing the hexagon-to-heptagon ratio. This reduces local strain without eliminating negative Gaussian curvature, indicating that stability is controlled by curvature distribution rather than curvature magnitude. In contrast, mechanical response reflects a balance between connectivity and heterogeneity: compact topologies maximize elastic moduli, whereas expanded networks can retain competitive stiffness through anisotropic, strut-mediated load transfer.

Given the limited dataset, the observed increase in hardness in selected expanded structures is interpreted as arising from competing effects: reduced density and bulk modulus versus enhanced anisotropic load transfer due to heterogeneous architecture. This suggests a partial decoupling between stiffness, density, and resistance to indentation.

Intermediate expansion regimes (e.g., P221-C312-(2⁸)[1-1-1]) provide a favorable balance of low density, reduced topological strain, and robust elastic response, identifying them as promising design targets.

Topology-Guided Design Rules

- Density control: Density decreases predictably with increasing connector length, largely independent of cage topology.
- Curvature management: Stabilization is achieved through heptagon dilution, which reduces local curvature concentration without altering global negative curvature.
- Strain localization: Strain is concentrated in small, heptagon-rich cages; their expansion is the primary route to energetic stabilization.
- Topological equivalence: Connector insertion between large cages is equivalent to expansion of small cages, which governs strain redistribution.
- Mechanical response: Elastic moduli scale with connectivity, while stiffness can be partially preserved via anisotropic, strut-mediated load transfer.
- Optimal regime: Intermediate expansion provides the best balance of density reduction, strain relief, and mechanical robustness.

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Abbreviations

The following abbreviations are used in this manuscript:

DFT	Density Functional Theory
TPMS	Triply Periodic Minimal Surface
GGA	Generalized Gradient Approximation

References

1. Mackay, A.L.; Terrones, H. Diamond from Graphite. *Nature* **1991**, *352*, 762. [[CrossRef](#)]
2. Felix, L.C.; Ambekar, R.; Tromer, R.M.; Woellner, C.F.; Rodrigues, V.; Ajayan, P.M.; Tiwary, C.S.; Galvao, D.S. Schwarzites and Triply Periodic Minimal Surfaces: From Pure Topology Mathematics to Macroscale Applications. *Small* **2025**, *21*, 2400351. [[CrossRef](#)] [[PubMed](#)]
3. Han, M.Y.; Özyilmaz, B.; Zhang, Y.; Kim, P. Energy Band-Gap Engineering of Graphene Nanoribbons. *Phys. Rev. Lett.* **2007**, *98*, 206805. [[CrossRef](#)] [[PubMed](#)]
4. Chi, S.; Kim, C.; Lee, Y.; Choi, M. Diversity in Atomic Structures of Zeolite-Templated Carbons and the Consequences for Macroscopic Properties. *JACS Au* **2024**, *4*, 1489–1499. [[CrossRef](#)] [[PubMed](#)]
5. Ignatchenko, A.V.; Willower, J.P. Schwarz P-Surface via Isolated Sp² Carbon Heptagons: Design and Properties. *J. Comput. Chem.* **2023**, *44*, 954–961. [[CrossRef](#)] [[PubMed](#)]
6. Ignatchenko, A.V. Launching Graphene into 3D Space: Symmetry, Topology, and Strategies for Bottom-Up Synthesis of Schwarzites. *J. Org. Chem.* **2025**, *90*, 971–983. [[CrossRef](#)] [[PubMed](#)]
7. King, R.B. Negative Curvature Surfaces in Chemical Structures. *J. Chem. Inf. Comput. Sci.* **1998**, *38*, 180–188. [[CrossRef](#)]
8. Elías, A.L.; Perea-López, N.; Rajukumar, L.P.; McCreary, A.; López-Urías, F.; Terrones, H.; Terrones, M. Chapter 17—Three-Dimensional Nanotube Networks and a New Horizon of Applications. In *Nanotube Superfiber Materials*; Schulz, M.J., Shanov, V.N., Yin, Z., Eds.; William Andrew Publishing: Boston, MA, USA, 2014; pp. 457–493. [[CrossRef](#)]
9. Lenosky, T.; Gonze, X.; Teter, M.; Elser, V. Energetics of Negatively Curved Graphitic Carbon. *Nature* **1992**, *355*, 333–335. [[CrossRef](#)]
10. Clark, S.J.; Segall, M.D.; Pickard, C.J.; Hasnip, P.J.; Probert, M.J.; Refson, K.; Payne, M.C. First Principles Methods Using CASTEP. *Z. Krist.* **2005**, *220*, 567–570. [[CrossRef](#)]
11. Perdew, J.P.; Burke, K.; Ernzerhof, M. Generalized Gradient Approximation Made Simple. *Phys. Rev. Lett.* **1996**, *77*, 3865–3868. [[CrossRef](#)] [[PubMed](#)]
12. Tkatchenko, A.; Scheffler, M. Accurate Molecular Van Der Waals Interactions from Ground-State Electron Density and Free-Atom Reference Data. *Phys. Rev. Lett.* **2009**, *102*, 73005. [[CrossRef](#)] [[PubMed](#)]
13. Koelling, D.D.; Harmon, B.N. A Technique for Relativistic Spin-Polarised Calculations. *J. Phys. C Solid State Phys.* **1977**, *10*, 3107–3114. [[CrossRef](#)]
14. Monkhorst, H.J.; Pack, J.D. Special Points for Brillouin-Zone Integrations. *Phys. Rev. B* **1976**, *13*, 5188–5192. [[CrossRef](#)]
15. Blatov, V.A.; Shevchenko, A.P.; Proserpio, D.M. Applied Topological Analysis of Crystal Structures with the Program Package ToposPro. *Cryst. Growth Des.* **2014**, *14*, 3576–3586. [[CrossRef](#)]

16. Blatov, V.A.; O’Keeffe, M.; Proserpio, D.M. Vertex-, Face-, Point-, Schläfli-, and Delaney-Symbols in Nets, Polyhedra and Tilings: Recommended Terminology. *CrystEngComm* **2010**, *12*, 44–48. [[CrossRef](#)]
17. Lee, C.; Wei, X.; Kysar, J.W.; Hone, J. Measurement of the Elastic Properties and Intrinsic Strength of Monolayer Graphene. *Science* **2008**, *321*, 385–388. [[CrossRef](#)] [[PubMed](#)]
18. Blakslee, O.L.; Proctor, D.G.; Seldin, E.J.; Spence, G.B.; Weng, T. Elastic Constants of Compression-Annealed Pyrolytic Graphite. *J. Appl. Phys.* **1970**, *41*, 3373–3382. [[CrossRef](#)]
19. Simmons, G. Single Crystal Elastic Constants and Calculated Aggregate Properties. *J. Grad. Res. Cent.* **1965**, *34*, 1.
20. Lütjering, G.; Williams, J.C. Fundamental Aspects. In *Titanium*; Lütjering, G., Williams, J.C., Eds.; Springer: Berlin/Heidelberg, Germany, 2003; pp. 13–50. [[CrossRef](#)]
21. Ignatchenko, A. Alexey Ignatchenko Research Group Website, Schwarzite Nanotube Architecture Database. Available online: <http://citadel.sjfc.edu/faculty/aignatchenko/nanotubes.html> (accessed on 1 February 2026).

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