Molecular Space Frames: An Atomically Precise Aerogel

Abstract.

The ultimate limit in one approach to the design of very light and very strong structures is to combine (1) the concept of a space frame (common in architecture) with (2) fractal repetition of a shape on smaller and smaller scales, (3) the inherent crystallographic nature of repeating structures, and (4) the limits of our manufacturing capabilities imposed by the atoms from which we build products.

The result is a class of very light, very strong structures composed of struts and nodes which are self-similar at multiple scales, are particularly easy to describe when a material is described in terms of a unit cell which is repeated to fill three dimensional space, and have a simple molecular structure.

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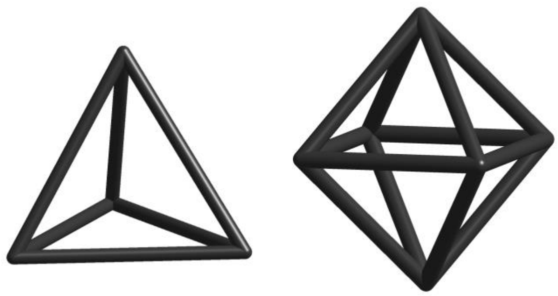
Introduction

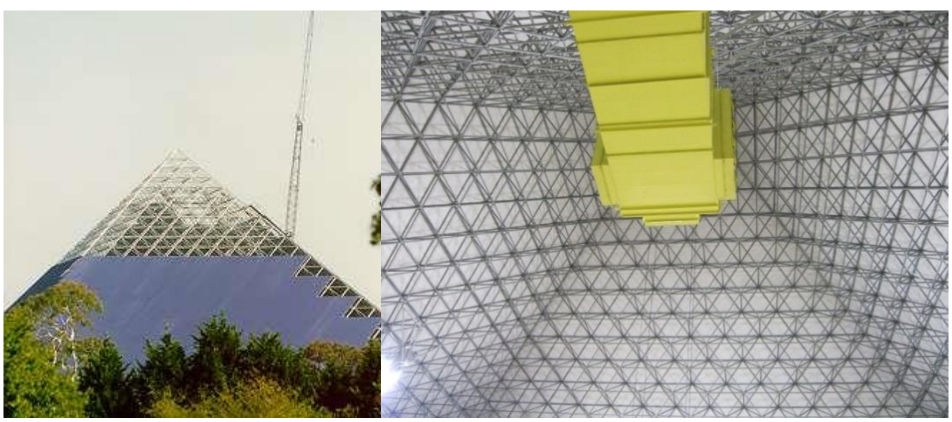
In *Ultralight Fractal Structures from Hollow Tubes*[1] it was shown that a substantially larger compressive load could be supported by a space frame in the shape of a rod than a simple rod of similar mass. Here, we extend this concept to a Molecular Space Frame (MSP): an extremely light weight, strong, rigid, three dimensional structure that can have an arbitrary shape. To accomplish this, we rely heavily on the use of triangles, a structural element which offers great stiffness at low weight. The simplest three dimensional structures that can be made of triangles are the tetrahedron and octahedron (**Fig. 1**).

Figure 1. Tetrahedron (left) and octahedron (right).



If we combine these two geometrical forms in a uniform fashion, we get a space frame, common in architecture and construction (**Fig. 2**).[2]

Figure 2. The Pyramid, at California State University (Long Beach), is the largest space frame in North America.



[1] Daniel Rayneau-Kirkhope, Yong Mao, Robert Farr, "Ultralight Fractal Structures from Hollow Tubes", Phys. Rev. Lett. 109(2012):204301, http://prl.aps.org/abstract/PRL/v109/i20/e204301.
[2] See https://en.wikipedia.org/wiki/Space_frame. Space frames were independently invented by Alexander Graham Bell, Buckminster Fuller, and others interested in high strength, light weight, and simplicity.

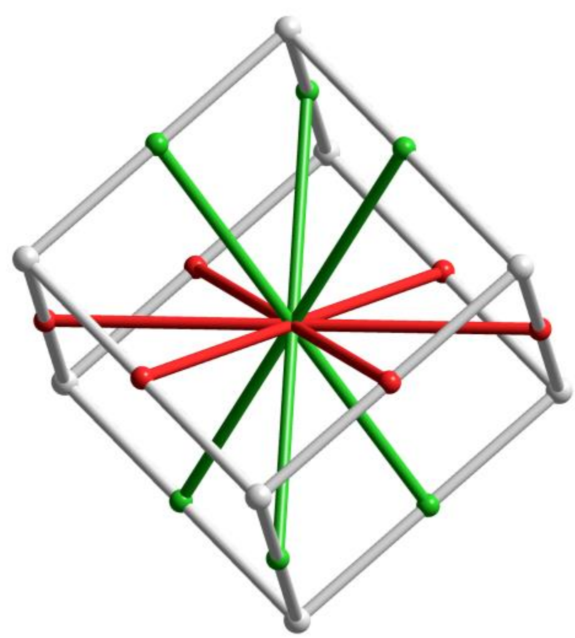
Struts and Nodes

Space frames are built from struts and nodes. Struts are in pure compression or pure tension, and connect nodes. In a uniform space frame, all struts are the same length. Nodes are attached to as many as 12 struts. In a uniform space frame a node is at the center of a rhombic dodecahedron and the struts are orthogonal to its faces[3].

In non-uniform space frames, the length of struts can vary, as can the angles between struts at a node. This results in multiple different types of struts and nodes and can, in the worst case, result in every strut and every node in the finished structure being unique. In a uniform space frame, all struts and all nodes are identical – which greatly simplifies manufacturing, supply chain logistics, and assembly operations.

A node can be thought of as a sphere in the center of a cube with twelve short struts connecting to the centers of the 12 edges of the cube.

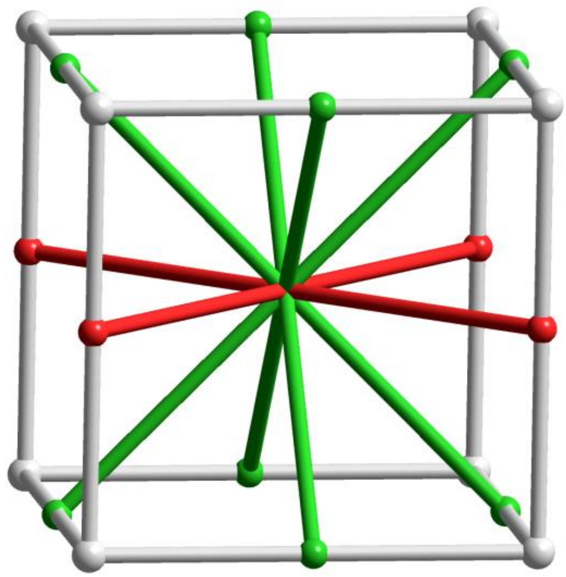
Figure 3. Tripodal view of space frame node.



In **Fig. 3** above, there are 12 connections, with the 6 colored red in a plane, and the 6 colored green forming two tripods, one inverted. In this view, a space frame can be thought of as a stacked set of planes, each plane supported from below by tripods and supporting another plane above on tripods. There are 4 sets of stacked planes, each set stacked in parallel to one of the 4 faces of a tetrahedron, the 4 stacked planes interlocking to form the space frame. By inspection and symmetry, we can see that any two red half-struts in the cube are at 60°, 120° or 180° angles to each other.

[3] One can also think of the 12 struts as exiting each node along the face normals of a rhombic dodecahedron; see **Fig. 10**).

Figure 4. Tetrapodal view of space frame node.



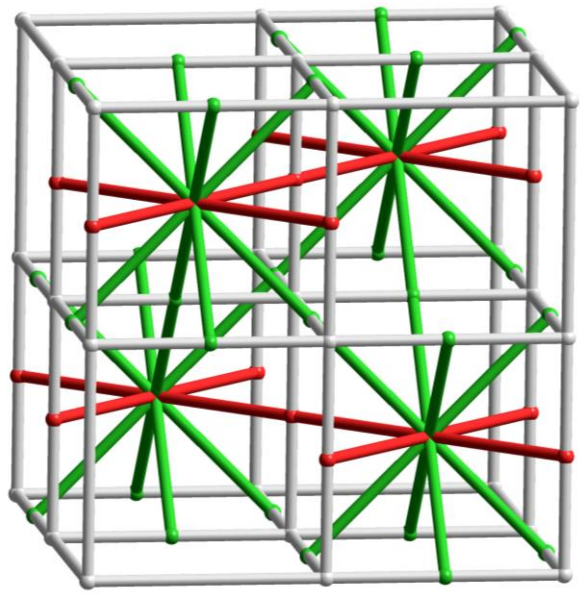
Another perspective on a space frame is illustrated in **Fig. 4**, in which the 12 connections are divided into 4 colored red in a plane, and 8 colored green that form two four-legged tetrapods, one inverted. In this case, the space frame can be thought of as a stacked set of planes, each plane supported from below by tetrapods and supporting another plane above on inverted tetrapods. There are 3 sets of stacked planes, each set of planes stacked in parallel to one of the surfaces of the cube, the 3 sets of stacked planes interlocking to form the space frame. By inspection and symmetry, we can see that any two red half-struts in the cube are at 90° or 180° angles to each other. We conclude that the angle between any two struts or half-struts connected to a node must be 60°, 90°, 120° or 180°.

Note that the cubes in this space frame occupy 3 dimensions much as the red squares occupy a red-and-black checkerboard in 2 dimensions – if you move left, right, forward, backward, up or down from a cube in the space frame, you find an empty cube-sized hole. There are eight directions in which you can move, which we might designate (1,1,1), (1,1,-1), (1,-1,1), (1,-1,-1), (-1,1,1), (-1,1,-1), (-1,-1,1) and (-1,-1,-1). We arbitrarily designate two members of this set of eight directions as D1 and D2. If we are at any cube we will find that by moving in direction D1 and then moving in direction D2, we will again be at some cube in this space frame, for any directions D1 and D2. If we just move in direction D1, we will be in a cube-sized hole.

Note also that the frame of the cube illustrated in **Figs. 3 & 4**, outlined in gray, is not part of the physical space frame. It is included in the illustration solely to help the mind understand the nature and symmetries of the system. The 12 red and green half-struts shown connecting the node at the center of the white cube to the white edges of the cube constitute the single "monomer" which, when many of them "crystallize," would form a space frame. Each half-strut would bond linearly to another half-strut on another monomer to form a whole strut that would join the two nodes from the two monomers.

A unit cell of a space frame is illustrated below in **Fig. 5**. It is composed of 4 space frame nodes alternately occupying 4 of the 8 cubes into which the unit cell can be divided.

Figure 5. A unit cell of a space frame, composed of 4 space frame nodes, holds a single tetrahedron.



Consistent with the above discussion, **Fig. 6** below illustrates a segment of space frame showing the tripods and inverted tripods between two planes with triangular facets, while **Fig. 7** illustrates a segment of space frame showing the tetrapods and inverted tetrapods between two planes with square facets. Note that the nodes are identical in both illustrations. The difference is solely in the lattice plane we are exposing on the surface. The square two-plane space frame motif is typical in many open roof applications in architecture, for example, the sheltering cover between buildings in a shopping center or in front of a theater.

Figure 6. Tripodal view of space frame with multiple nodes.

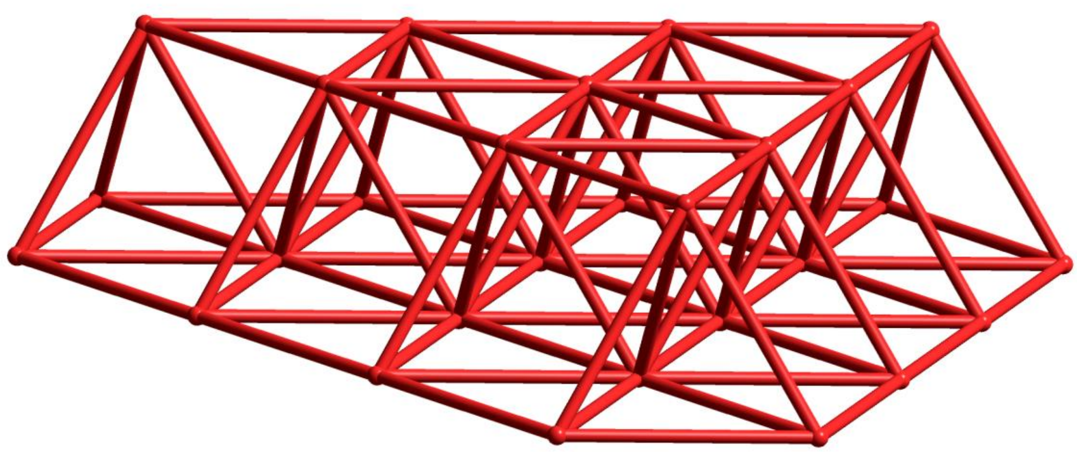
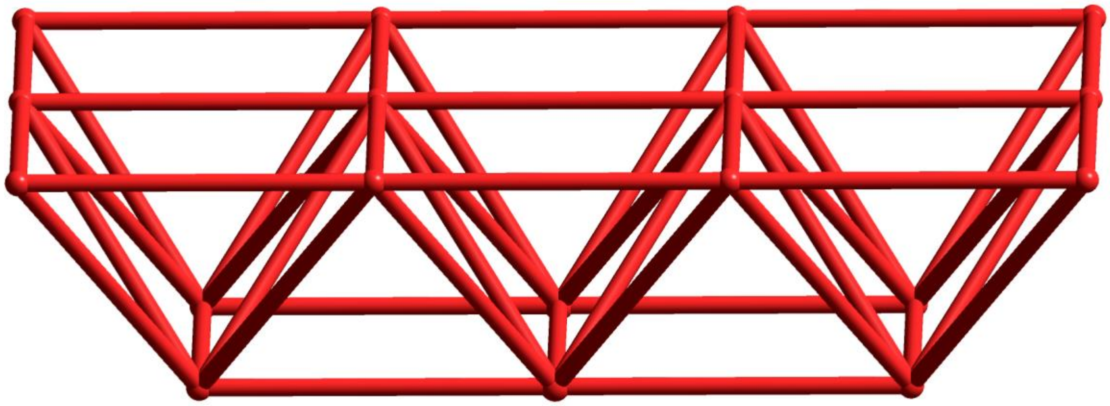


Figure 7. Tetrapodal view of space frame with multiple nodes.



In a sufficiently large structure (that is, if we neglect the surface of the structure and consider only the bulk) the ratio of struts to nodes is 6 to 1, because every strut connects 2 nodes, and every node is surrounded by 12 struts, each of which is shared with another node. To put it another way, our finished structure could be made from a single "monomer": a node pre-attached to 12 half-struts. A space frame is formed when these "monomers" form a three-dimensional "polymer" in which the half-struts bond to each other.

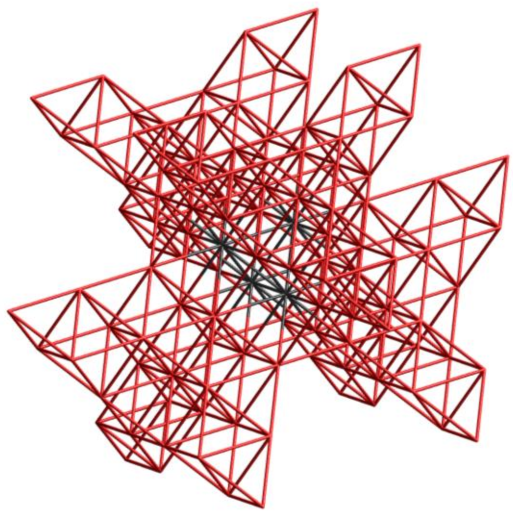
As it requires only 3 coordinates to specify the location of a point (neglecting singularities), the space frame, which "specifies" the location of a node using 6 struts, has a liberal ability to over-specify the location of each node. Put another way, the space frame architecture can distribute a load applied to any given node among multiple struts and nodes, and can degrade gracefully in the presence of weakness or even failure of individual struts or nodes. On the other hand, by eliminating superfluous struts and nodes, a space frame can be tailored to provide a three dimensional scaffolding of the desired shape with just the strength and stiffness that is required.

Meta-nodes

Meta-nodes are simply a larger example of the nodes involved in the space frame.

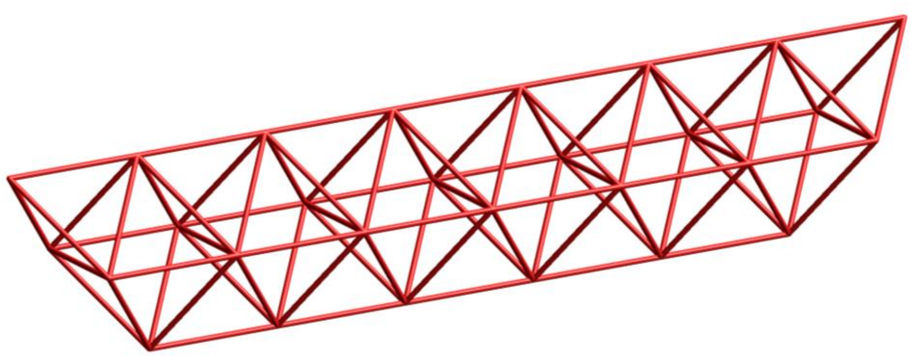
In **Fig. 8**, we can see a meta-node. The heart of the meta-node is a tetrahedron shown in black, composed of four nodes connected by four struts, the four nodes being otherwise indistinguishable from any other node in the structure.

Figure 8. Example of a meta-node (black) inside a space frame (red).



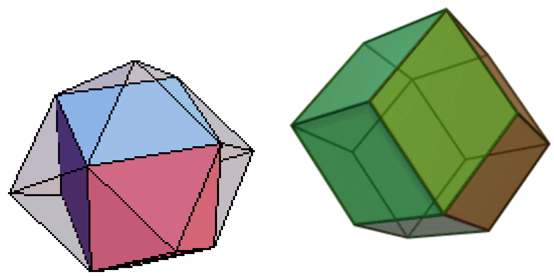
Meta-nodes can be spaced as close together or as far apart as might be needed, consistent with the need to avoid buckling and to maintain some degree of rigidity between the meta-nodes. Fractal structures based on this approach are a generalization of the approach described by Rayneau-Kirkhope et al.[4]

Figure 9. A meta-strut.



[4] Meta-nodes can be used to build a meta space frame, which can in its turn be used to build meta meta-nodes, which can be used to build a meta meta space frame, etc. This fractal hierarchy could in principle span length scales from microns to very large macroscale structures.

Figure 10. Geometry of the rhombic dodecahedron.



Rhombic dodecahedrons can, by themselves, tessellate 3-space,[5] just like a cube.

The volume of a single rhombic dodecahedron V_{rd} that is part of a tessellation of a region is $V_{rd} = D^3/\sqrt{2}$, where *D* is the distance between two adjacent rhombic dodecahedrons (or between the centers of two rhombic dodecahedrons along a line normal to their common face, technically defined as twice the radius of an inscribed sphere tangent to each of the rhombic dodecahedron's faces).[6]

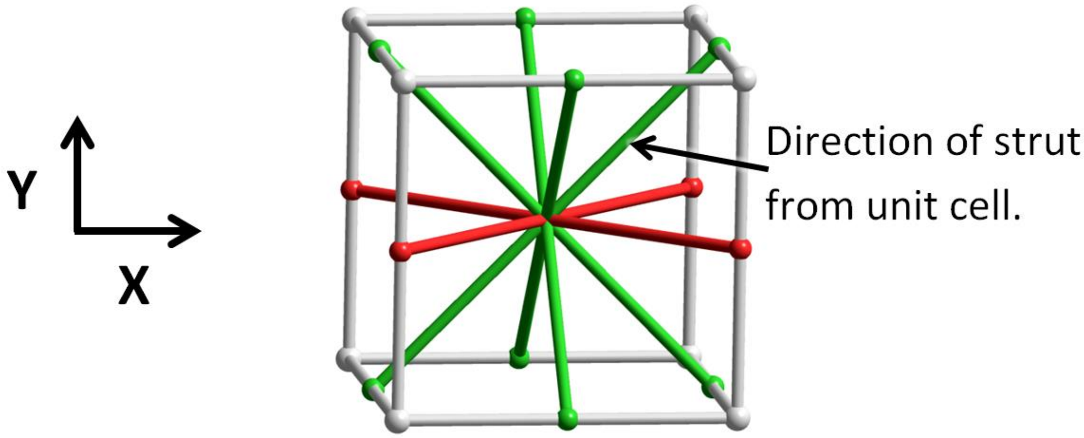
Molecular struts

If we wish to create a molecular strut from some material which forms a crystal, then we can start from the unit cell. For simplicity, we assume that the unit cell is a cube and has hexoctahedral[7] symmetry.

A strut from a unit cell will extend from the center of the unit cell along a line towards the center of an edge of the unit cell, as illustrated below in Figure 11:

[5] Freitas, *Nanomedicine*, Fig. 5.6 and Section 5.2.5, http://www.nanomedicine.com/NMI/5.2.5.htm.
[6] See Wikipedia, https://en.wikipedia.org/wiki/Rhombic_dodecahedron, and some algebra.
[7] In essence, having all possible symmetries available for a cube. See https://en.wikipedia.org/wiki/Crystal_system.

Figure 11. A strut emerging from a unit cell.

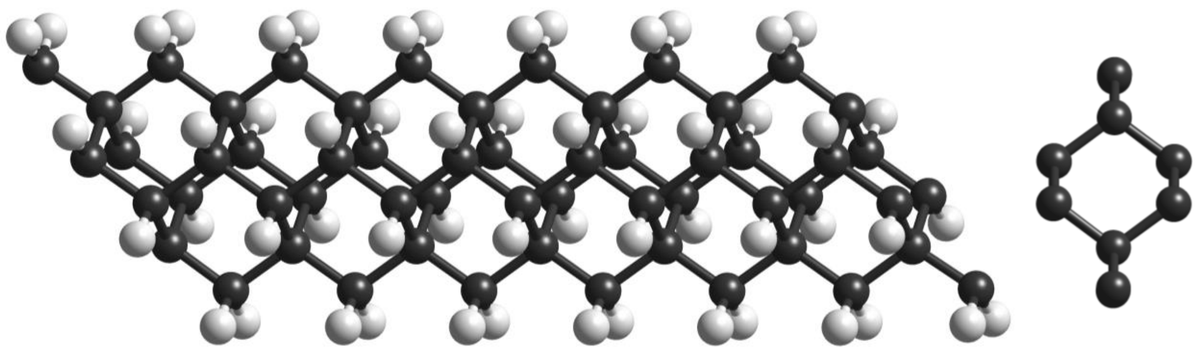


As can be seen from inspection, the designated strut is in the 110 direction. The other three upward pointing green struts are 011, 01-1, and -110. The four red struts are 101, 10-1, -101 and -10-1. The four downward pointing green struts are 1-10, 0-11, 0-1-1, and -1-10.

To make a molecular strut that is n unit cells long, we create a block of the material in a suitable computer modeling program that is ~n unit cells on a side. We then orient the block so that we are looking directly down on the 110 surface of the block, cut out the outline of the strut, and remove all atoms outside the outline. Rotating the strut, we will now be able to see its full length. The strut will be chemically unstable (have dangling bonds) because simply removing atoms will leave surface atoms on the strut that are not suitably terminated. In addition, the strength of the strut might be insufficient because bonds along the length of the strut might be insufficient to provide the desired strength. Examine the strut and determine if the bonding pattern along the length of the strut is likely to provide sufficient strength for the intended purpose. If it is, terminate the dangling bonds so that they are chemically inert. The simplest approach is to add hydrogens wherever there are dangling bonds. This might cause steric congestion. If steric congestion is a problem, modification of the structure to relieve steric congestion can be attempted. The simplest approach is to substitute larger groups for smaller groups, or to remove two adjacent hydrogens that are in close contact and bond the atoms to which the two hydrogens are bonded to a single atom, such as oxygen. Other atoms, such as sulfur, or groups, such as CH_2, can also be used. Ultimately, any local change involving replacement of a small number of atoms with some other small number of atoms which stabilizes the local structure can be utilized. Should this process produce a satisfactory result, then further efforts are not needed. If, however, the strut is not strong enough, or stabilization of the strut surface is problematic, then the original n x n x n block of material should be reloaded and a second strut outline cut onto the 110 surface of the block. Repetition of this process several times might be required before a satisfactory strut has been produced.

The results of this process for diamond are shown below:

Figure 12. A molecular strut for diamond. The strut outline is shown at right.



The resulting strut seems satisfactory for distances of a few nanometers. This strut would likely be too flexible for longer distances, which would require either a larger strut cross section (drawing a larger outline on the 110 surface in the process described above) or alternatively using a meta-strut (a strut that was itself made of smaller struts, either as described by Rayneau-Kirkhope et al., or by making struts carved out of a uniform space frame. These are two distinct approaches, as Rayneau-Kirkhope describe structures that are not built purely from nodes that are rhombic dodecahedron – their struts can depart the node at other angles).

Molecular nodes

The advantage of struts made by this technique is that a "node" in the space frame can be simply a solid block of the material defined by the unit cell used in making the strut. That is, 12 struts meeting at a node can seamlessly fuse into a single crystal, because all 12 struts share the same crystal structure and orientation.

Put another way, we could make a space frame from a single block of a crystal, such as diamond, simply by removing atoms where we want empty spaces to be located. This process would create a structure which was all one single crystal. If we built a space frame according to the algorithm given here, (1) all the struts pointing in a given direction and all the nodes will be identical, and (2) the result could also have been achieved by carving it from a single crystal. For crystals with a cubic unit cell and appropriate symmetry (such as diamond) all the struts will be identical. For crystals that are not cubic (hexagonal, tetragonal, orthorhombic, monoclinic, triclinic) the resulting space frame will not be uniform (some struts will be longer than other struts), but all struts pointing in a given direction *will* be identical, both in their structure and length.

A node without struts is shown in Figure 13. The diamond node created by attaching 12 struts like the molecular struts shown in Figure 12 is illustrated in Figure 14.

Figure 13. A molecular node for diamond. The view on the left shows the node straight on. The view on the right is rotated a few degrees. All carbon atoms are part of a strut going through the node. All oxygen atoms replace two hydrogen atoms that would otherwise have made a hard contact.

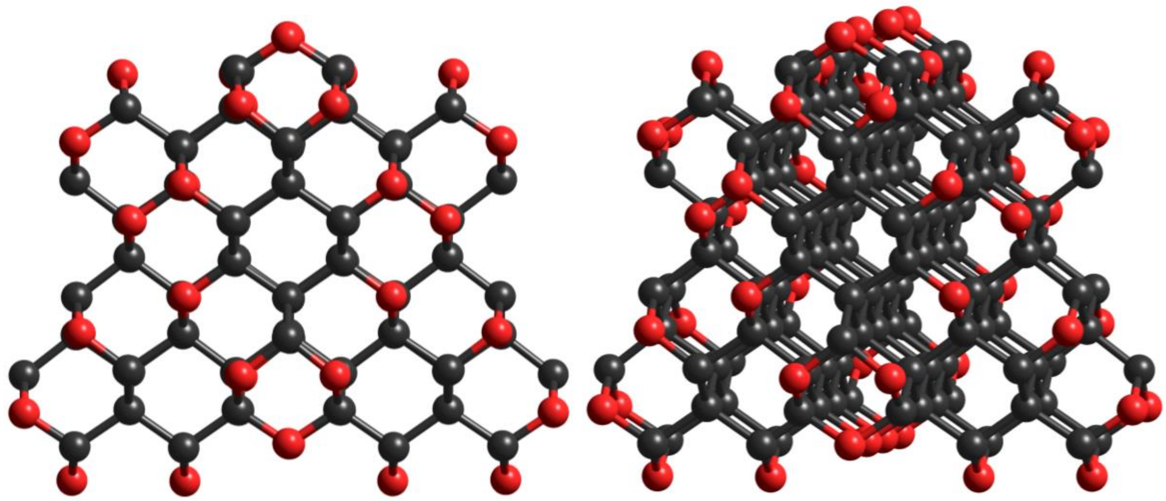


Figure 14. A molecular node for diamond, with stubbed struts. View A shows the node straight on. View B shows the node rotated a few degrees.

Figure 14, View A

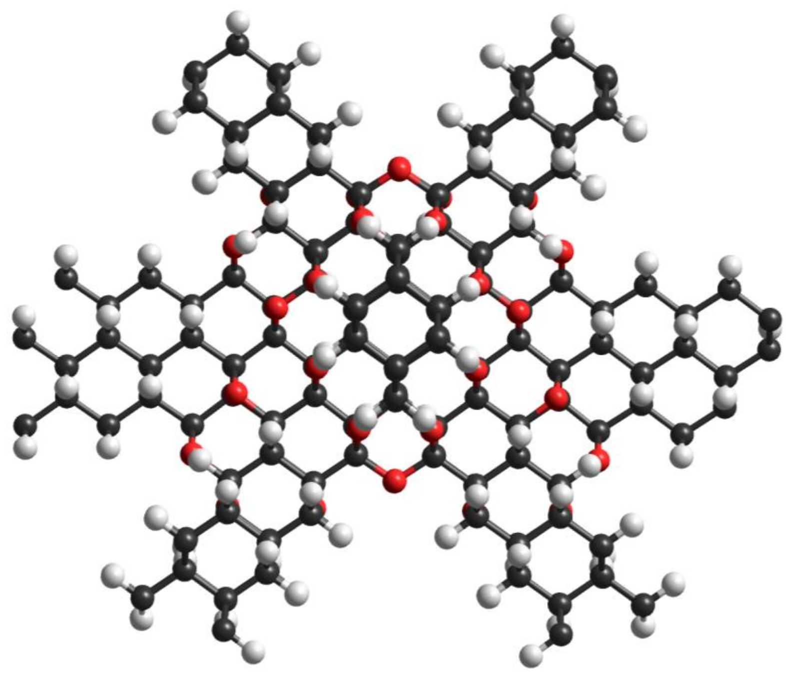
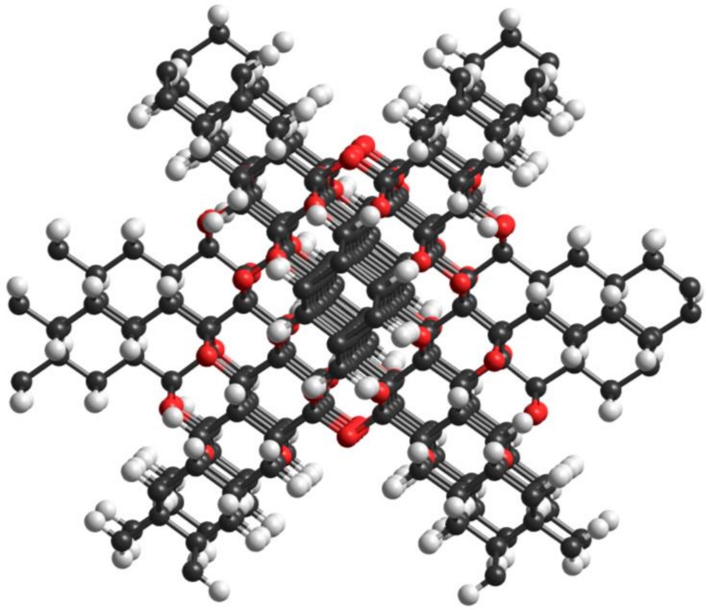


Figure 14, View B

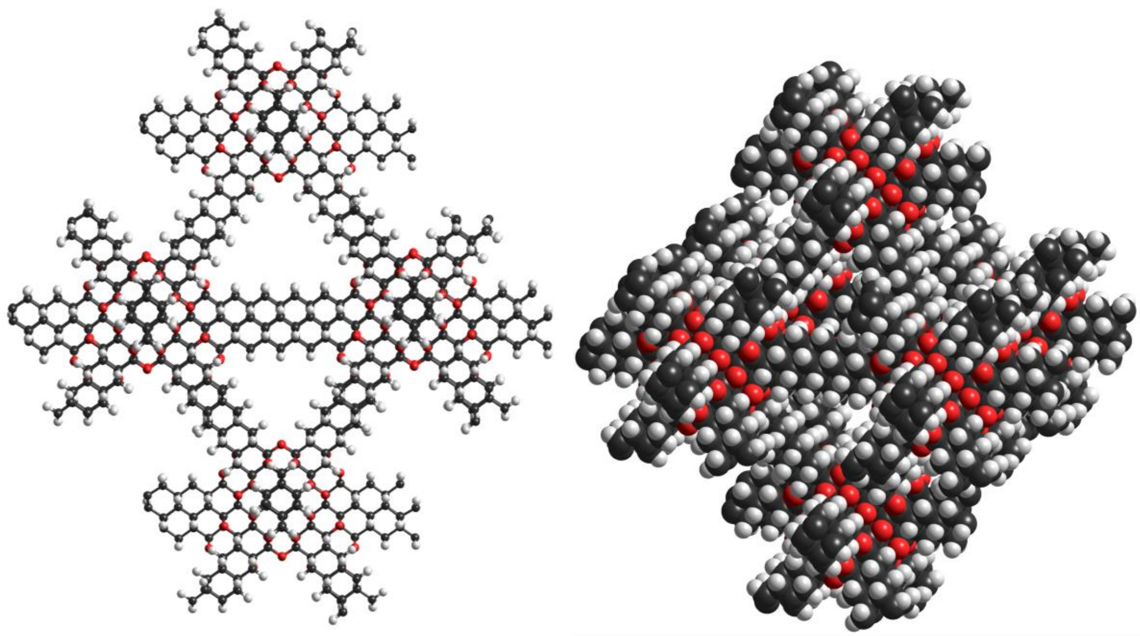


The node was created (conceptually) by taking six struts, intersecting them at their midpoints in a common crystal lattice, and then using the carbon atoms common to all six. Surface hydrogens that made hard contacts with other surface hydrogens were replaced with an oxygen bonded to the two supporting carbons. As hard contacts only occur when the two supporting carbon atoms would have been bonded to a common carbon atom in a six membered ring, replacing the missing carbon atom with an a —O— provides an approximately correct substitution while preventing the steric congestion that a —CH_2— would have created. As can be seen, the diamond crystal structure extends through the node, which also bonds seamlessly to the 12 struts of the space frame.

Assembling node-plus-12-half-struts into structures

Six of these node-plus-12-half-struts can be combined to create a meta-octahedron, illustrated in Figure 14.

Figure 15. A meta-octahedron seen in ball-and-stick view straight on (left) and space-filling at a small angle (right).



The following observations are in order:

First, figures 13, 14 and 15 show structures which, if the hydrogens were removed and the oxygens were replaced with carbon, would be part of a single diamond crystal. That is, the carbon atoms would have the bonding pattern of carbon atoms in a diamond, except that some carbon atoms from that diamond would be missing.

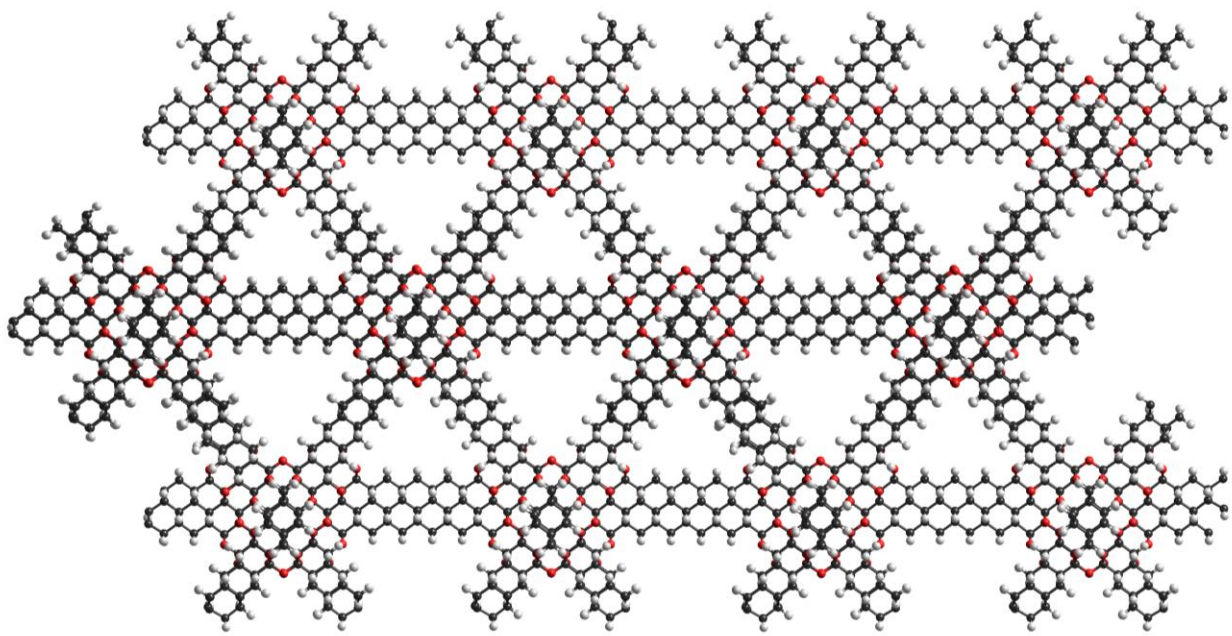
Second, the termination of the struts is not chemically stable. It is intended to show a truncated termination that could, logically, be connected to another strut. The actual physical mechanism for coupling nodes and struts is not specified here. Further work is required to define a convenient mechanism for coupling nodes and struts.

Third, self-assembly of a building block with 12 strut-stubs which had rhombic dodecahedron symmetry, but in which the ends of the struts had been modified to link to the ends of other struts, is a potentially valuable area of research. If such a molecule could be designed and synthesized, under appropriate conditions it would presumably self-assemble into a molecular space frame. Synthesis of a molecule with 12 linking groups using existing technologies might be challenging. However, molecules with 6 linking groups, such as cyclohexanehexacarboxcylic acid, appear quite feasible.[8]

Fourth, positional assembly of a rhombic dodecahedron building block should also be feasible, and would allow construction of 3 dimensional molecular structures of considerable strength. The use of positional assembly would presumably allow the use of simple struts and rhombic dodecahedron nodes, whose synthesis could be envisioned with existing technology. Note that molecules with the symmetry of dodecahedrons, including dodecahedrane and C60, are different from rhombic dodecahedrons and appear less suited to the construction of space frames. The possibility of stable molecules with the symmetry of rhombic dodecahedrons has been discussed in the literature.[9]

Fifth, the nodes can be combined into meta-struts, as illustrated in Figure 16, and these meta-struts can then be used in combination with meta-nodes to build a meta-space frame.

Figure 16. A meta-strut.



Higher order space frames

The meta-structures illustrated here can be viewed as first order meta-structures. Second order meta-structures would be built from first-order meta-structure components. Third order meta-structures

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[8] *Molecular building blocks and development strategies for molecular nanotechnology*, by Ralph C. Merkle, Nanotechnology **11** (2000) 89-99.

[9] Boldyrev et al. say "we show computationally that two molecules, Mg2Al4O8 and Na4Mg4O6, have very stable distorted rhombic dodecahedron structures", *Polyhedral Ionic Molecules*, Alexander I. Boldyrev and Jack Simons, *J. Am. Chem. Soc.*, 1997, 119 (20), pp 4618–4621; DOI: 10.1021/ja964063m.

would be built from second order meta-structure components. This process can be continued until some limit is reached. The most obvious limit would be gravitational: at some point, an Nth-order meta-structure would collapse under its own weight. This would be less of a problem in a micro-gravity environment, but even in space a large enough meta-structure might eventually collapse under its own self-induced gravitational forces.

Very light and strong structures of entirely arbitrary shape could in principle be made using this approach. The closest structural analogy might be today's aerogel's, which have little mass, yet still have significant strength.

Distortions, defects, and dislocations

A variety of crystal dislocations or distortions can be introduced into a molecular space frame and would increase the range of possible designs this approach encompasses. Most simply, individual struts could be lengthened or shortened in the design in a coordinated manner to create smooth curves into the finished structure. Crystal defects, such as twinning or dislocations could be introduced. The design of a stable dislocation in a solid material can be challenging. However, the design of a stable dislocation in a space frame should be substantially easier, as it might involve only moderate bending of struts that were relatively tolerant of strain.

It would also be possible to relax the constraints suggested here on the structure of individual nodes. While 12 struts of identical length emerging from a node with rhombic dodecahedral symmetry provides a simple and easy way to assemble a space frame, the length, structural make up, number, and angle of emergence of struts from a node can all be varied to a greater or lesser extent. Further, the static nature of the molecular space frame can be altered. Struts could be lengthened or shortened dynamically, in response to commands and powered by, for example, molecular electrostatic motors. Struts could even be detached and reattached dynamically. This line of reasoning leads to Utility Fog.[10] Clearly, it would be possible to select any point along a continuum from an entirely static molecular space frame made from a single crystal, to a molecular space frame that introduces dislocations and defects to achieve desired geometrical, structural and load bearing objectives, to a more dynamic structure that can adjust the length of some or all of its struts to respond to external loads and conditions, to full Utility Fog: which can dynamically adapt its shape, density, strength, and other properties as it actively interacts with its environment.

Conclusion

Space frames are a well-known architectural structure. The basic components of space frames (struts and nodes) can be made from molecules. Molecular space frames can be used to make structures of any desired shape, including, inter alia, struts and nodes. These "meta-struts" and "meta-nodes" can be

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[10] *Utility Fog: The Stuff that Dreams Are Made Of*, by J. Storrs Hall, originally published 1993, published July 5, 2001 on KurzweilAI.net, http://www.kurzweilai.net/utility-fog-the-stuff-that-dreams-are-made-of

used to make “meta-space frames”. First order meta-struts and first order meta-nodes can be used to make first-order meta-space frames. First order meta-space frames can be used to make second order meta-struts and second order meta-nodes, which can be used to build second order meta-space frames. This process can be continued to higher and higher orders.

By appropriate design, an arbitrary cubic crystal structure can be used as the basis for a molecular space frame all of whose nodes are identical, and all of whose struts are identical in length, and whose molecular structure is the same as a solid block of the original crystal with appropriate hollows carved into it, and with appropriate terminations of surfaces to provide for chemical stability. For cubic crystal structures of appropriate symmetry, all struts can be identical.

For triclinic or other non-cubic crystal structures, a non-uniform molecular space frame can be designed with all struts pointing in the same direction having the same length, but with struts pointing in different directions possibly differing in length, but otherwise with properties similar to those described.

Very light and strong structures which have very little mass could in principle be made in this fashion.