Tetrahedra clusters serving as platform to foam-like structures design

Supplementary Information

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1. **Animations (*animated gif files to download*)**

Animation1:

https://drive.google.com/file/d/1pYXFC3Obx_IDvJW-f3DWhldGKmoU5xcl/view?usp=sharing

Animation2:

https://drive.google.com/file/d/1ZvgpKgxrvzZXULwW8zKy2vtS7jvxcliM/view?usp=sharing

Animation3:

https://drive.google.com/file/d/1hTPgoaH2gkiKU-KNEGvK8NzW21Mq4T8W/view?usp=sharing

Animation4a:

https://drive.google.com/file/d/1HhzJXtnixUZQfipjMyvHliVf8RyTscgH/view?usp=sharing

Animation4b:

https://drive.google.com/file/d/1_0Hn2BZp7hrVco-OAF_dWYYFgzCQt8A9/view?usp=sharing

Animation5a:

https://drive.google.com/file/d/1jL0V-kSHOkP_fOo8W-tI1xNppx76DQII/view?usp=sharing

Animation5b:

https://drive.google.com/file/d/1DMHN4DiZqXg-XiJmWQf3keLdC20w2dUG/view?usp=sharing

Animation6:

[*https://drive.google.com/file/d/1e_AD0fCwz7ryGW5HFX15pBBvCMXHt2lz/view?usp=sharing*](https://drive.google.com/file/d/1e_AD0fCwz7ryGW5HFX15pBBvCMXHt2lz/view?usp=sharing)

Animation7:

[*https://drive.google.com/file/d/1F1_3p-c_-9RN9Tw-yrOAfwYXqROupeU1/view?usp=sharing*](https://drive.google.com/file/d/1F1_3p-c_-9RN9Tw-yrOAfwYXqROupeU1/view?usp=sharing)

2. Construction of clusters

Initially, one central tetrahedron was specified to satisfy two conditions: a) its centre is positioned at {0,0,0} in a Cartesian coordinate system, b) its height $h=1$. See Fig. S1 below.

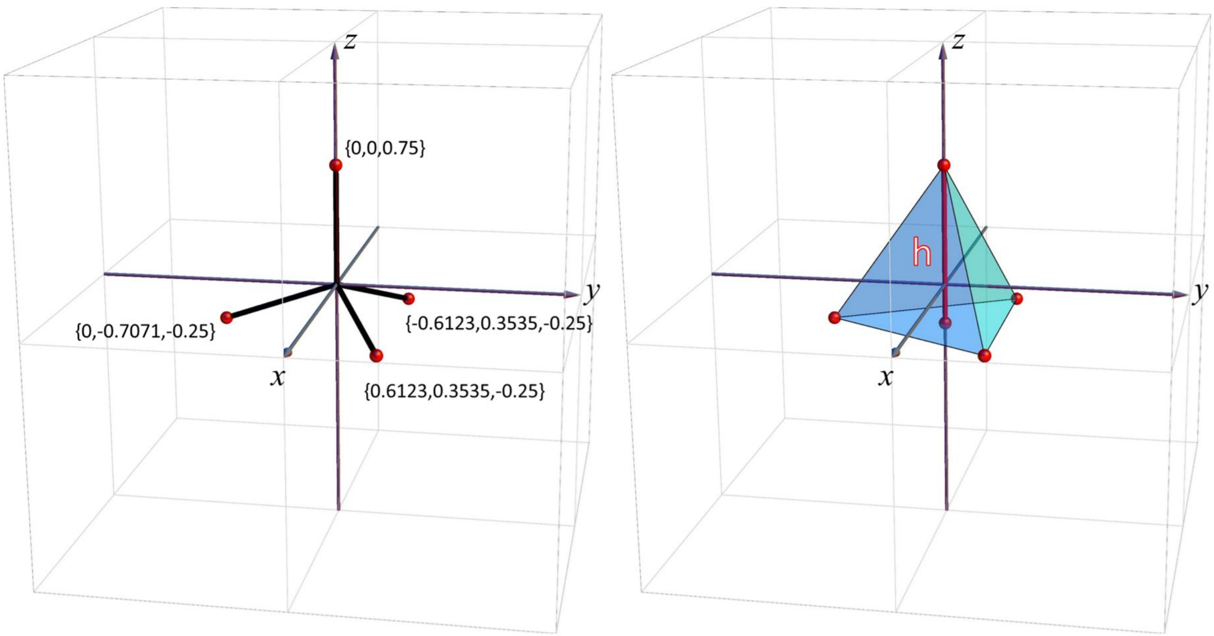

Fig. S1. Initially specified tetrahedron.

Knowing coordinates of one particular tetrahedron it is relatively simple to find coordinates of adjacent tetrahedra taking into consideration that each tetrahedron has the height $h=1$. As an example let us find coordinates of point *D{z,y,z}* (presented in Fig.S2), which is the fourth vertex of adjacent tetrahedron. First, one has to specify normal vector $\vec{n}$ to the triangular face determined by points ABC. It can be done by a calculation of the cross product $\vec{n} = \vec{a} \times \vec{b}$ where $\vec{a} = \vec{B} - \vec{A}$ and $\vec{b} = \vec{C} - \vec{A}$. Here, coordinates A, B, and C are treated as a free vectors. Subsequently, one has to calculate unit vector $\hat{n} = \frac{\vec{n}}{|\vec{n}|}$ and translate it using a free vector $\vec{O}$ which points at the centre of a triangle ABC. Accordingly, the terminal point of the translated unit vector $\hat{n}_T$ identifies coordinates of point *D{z,y,z}*.

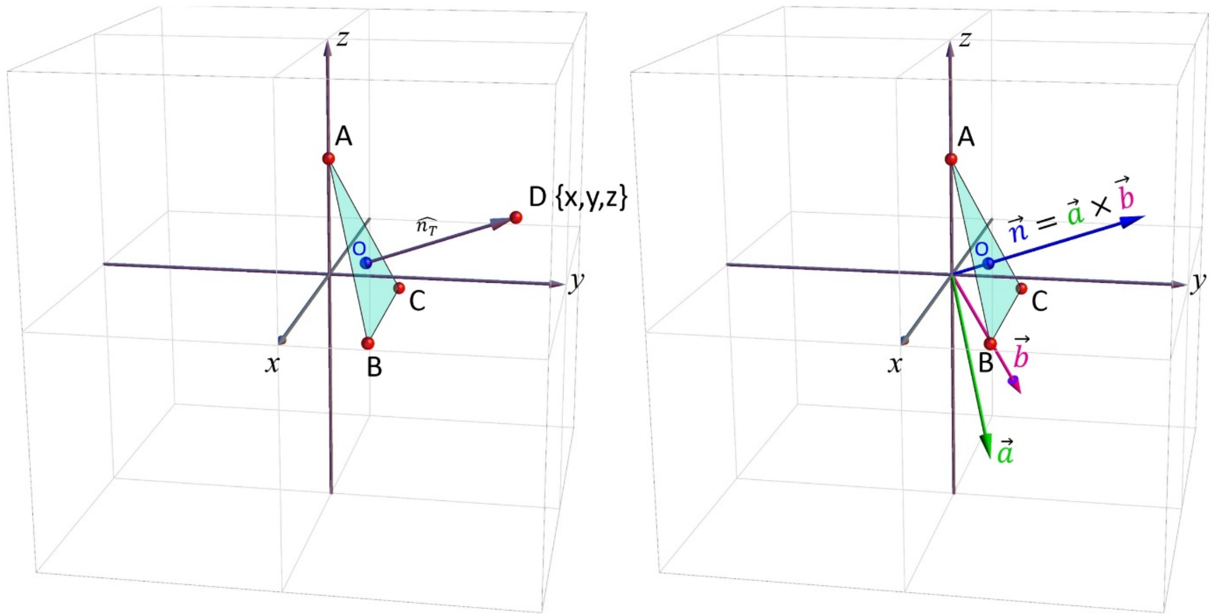

Fig. S2. Determination of adjacent tetrahedron coordinates.

Above mentioned procedure can be used to construct any tetrahedra clusters, which grow via simple face-face joint steps (i.e.where two adjacent tetrahedra always share one common face). Following this protocole (see Fig. S3) one can initially construct a four-armed tetrahedral star, N=5 cluster and subsequently decorate it with additional layer of tetrahedra to finally reach N=17 cluster, which is also discussed in the paper.

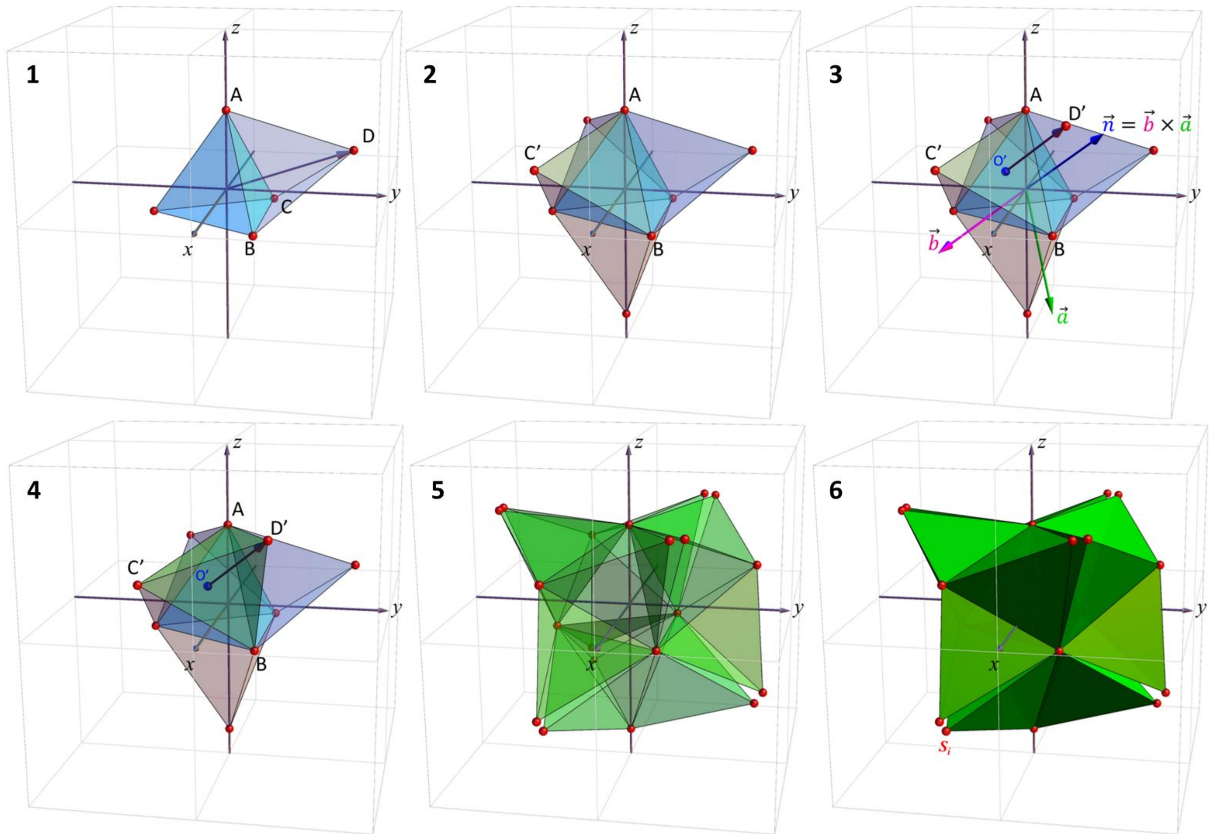

Fig. S3. tetrahedra clusters construction scheme.

In order to construct N=41 cluster (see Fig. S4) ona has to decorate N=17 cluster with additional 24 surface tetrahedra employing the same procedure as before.

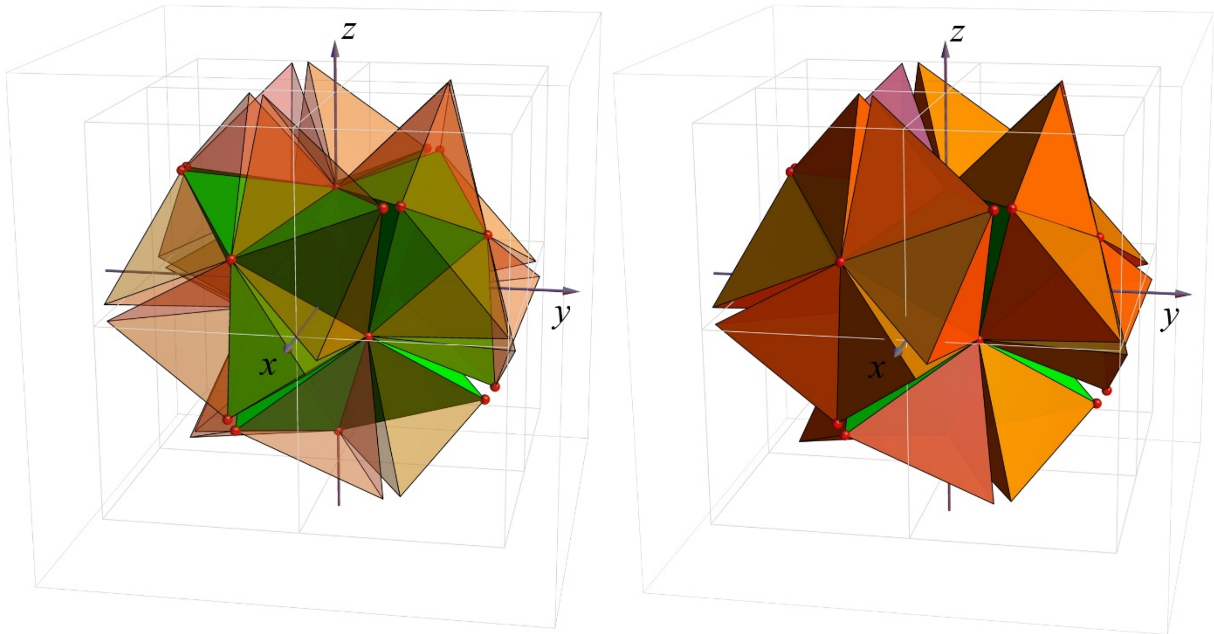

Fig. S4. N=41 cluster (orange) constructed via ”decoration” of N=17 cluster (green) with additional 24 surface tetrahedra.

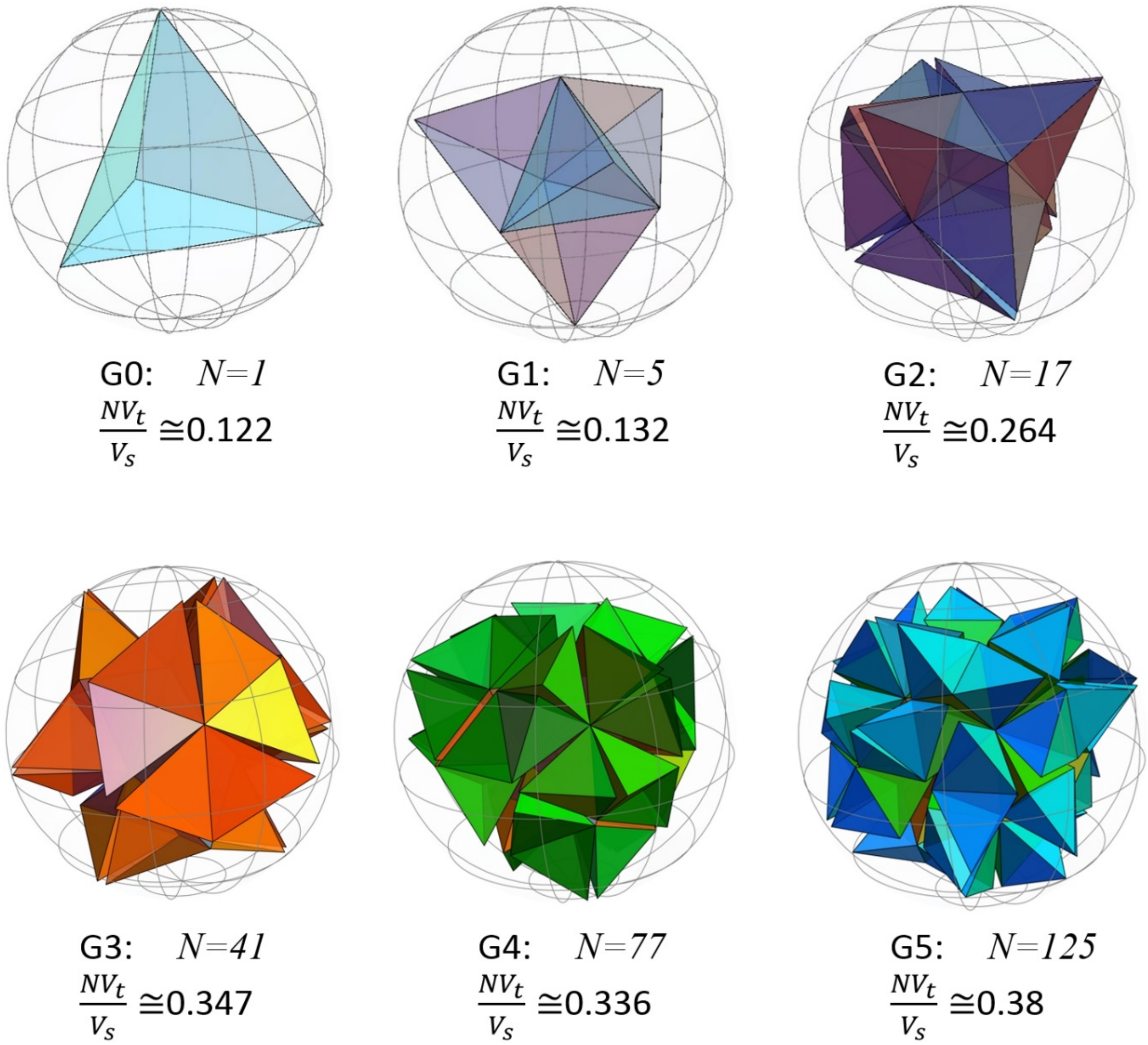

Fig. S5. Generations from G_1 to G_5. N signifies number of tetrahedra involved in the cluster. V_t signifies the volume of one tetrahedron, V_s signifies the volume of the sphere in which the cluster is embodied.

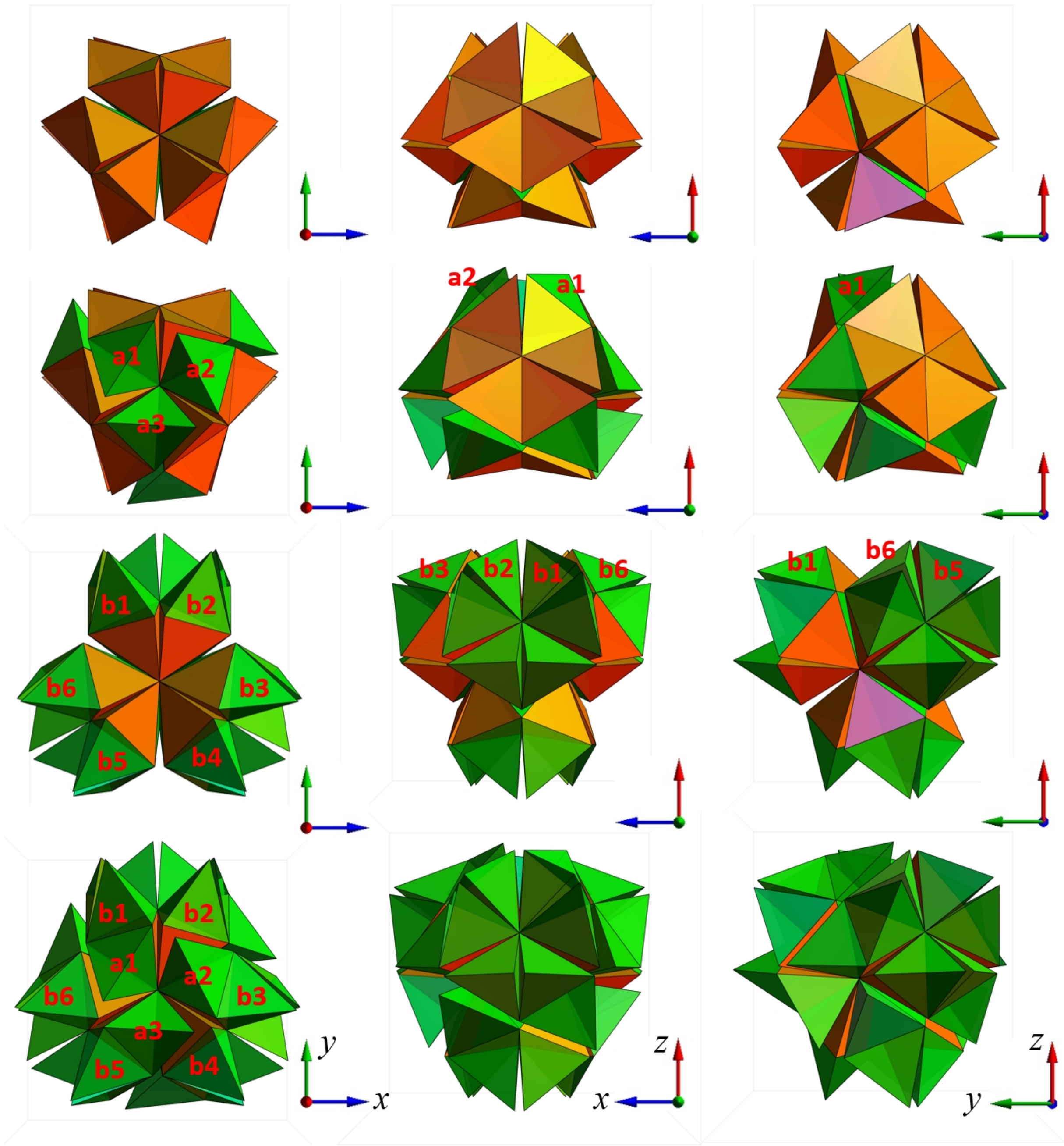

Fig. S6. Illustrates decoration of G_3 cluster to reach G_4. Top line represents three orthogonal, spatial projections of G_3 cluster. The very bottom line shows the same three projections of G_4 cluster. In between are shown two sub-populations of surface tetrahedra (12a+24b), which have to be added to reach G_4.

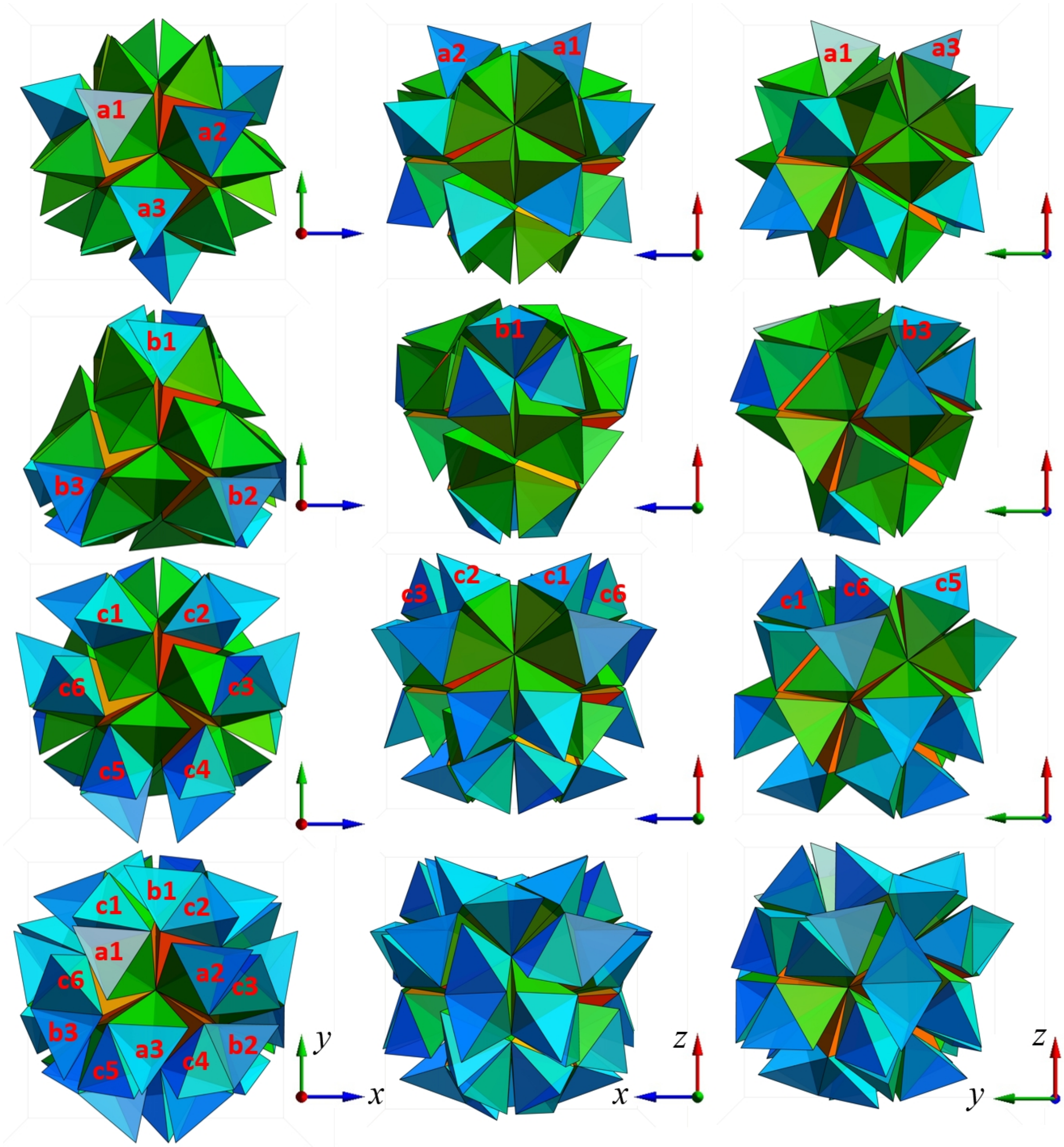

Fig. S7. Illustrates decoration of G_4 cluster to reach G_5. The very bottom line shows three orthogonal, spatial projections of G_5 cluster. Above are shown three sub-populations of surface tetrahedra (12a+12b+24c), which have to be added to reach G_5.

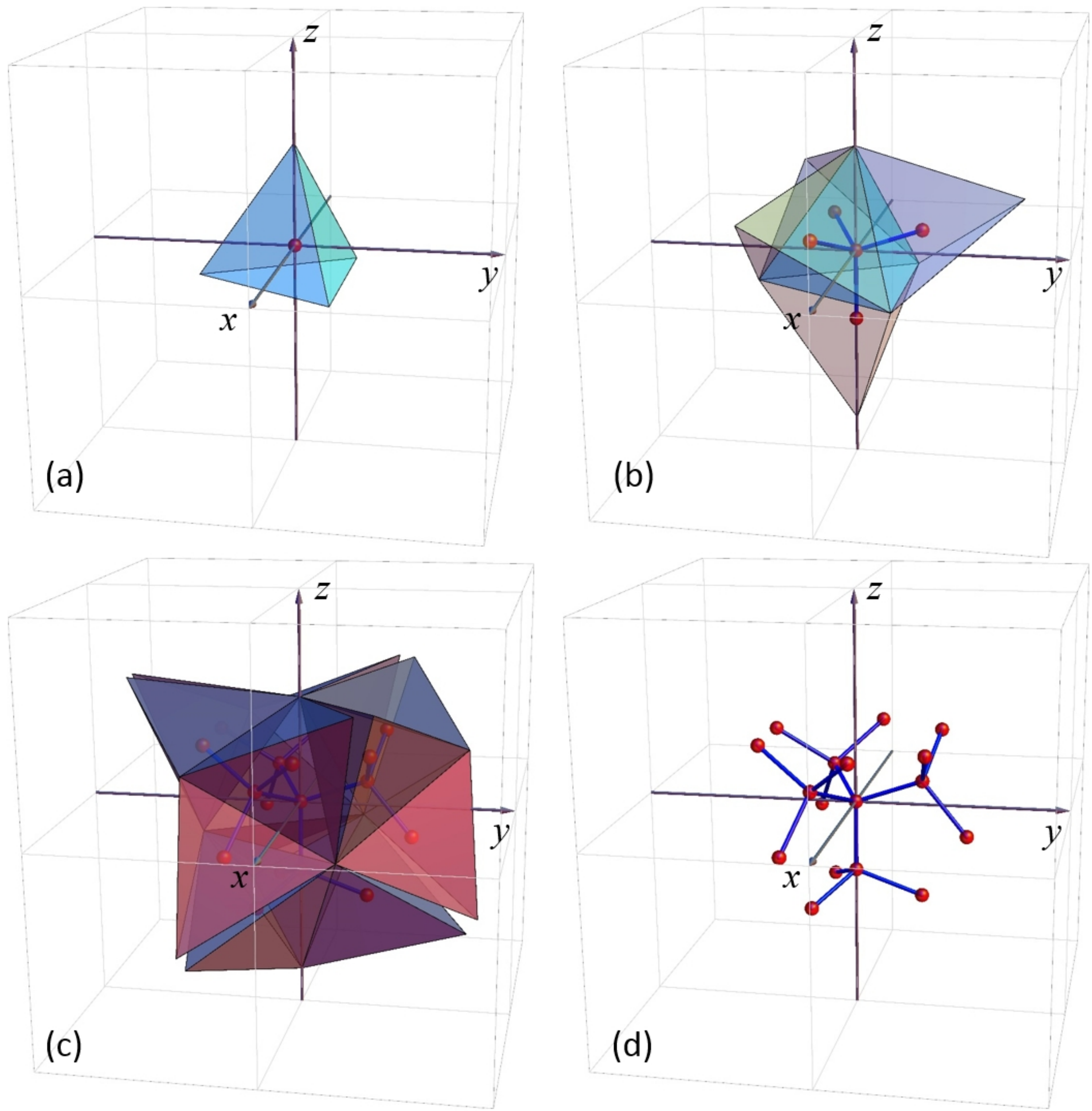

Fig. S8. Sequential dendrimer formation protocole exemplified on G_1 and G_2 clusters. Initially, all central points (centres of gravity) of individual tetrahedra have to be specified and, subsequently, the connections are constituted only between those tetrahedra which share one common face.

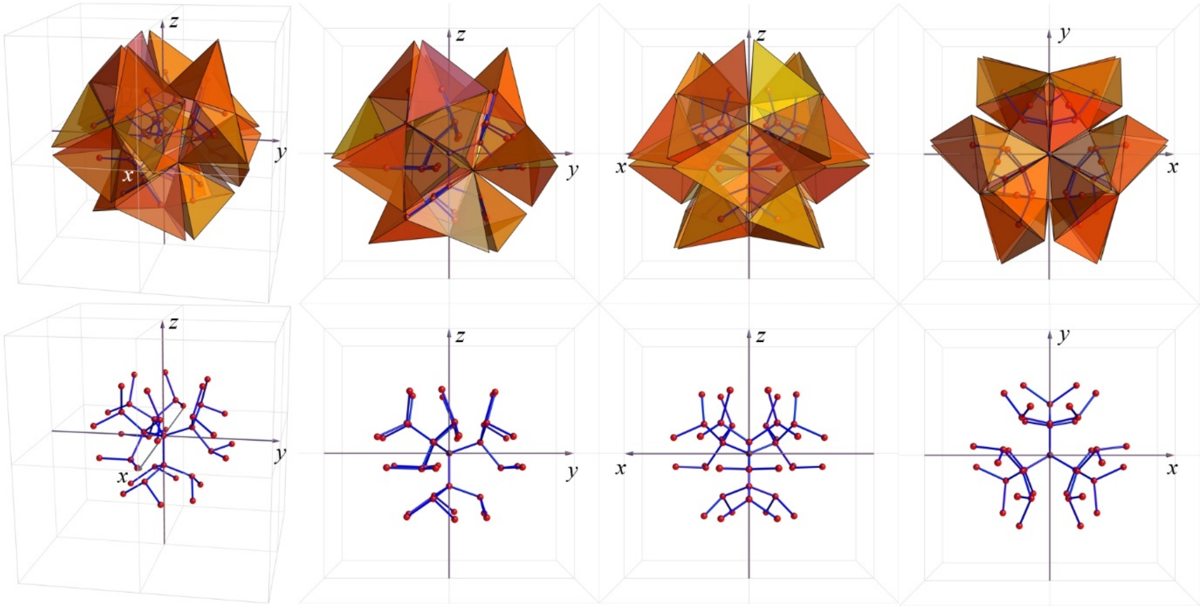

Fig. S9. G_3 dendrit. *Top*) illustrates four different projections of G_3 cluster, *bottom*) illustrates the same four different projections of the corresponding tetrahedral dendrit.

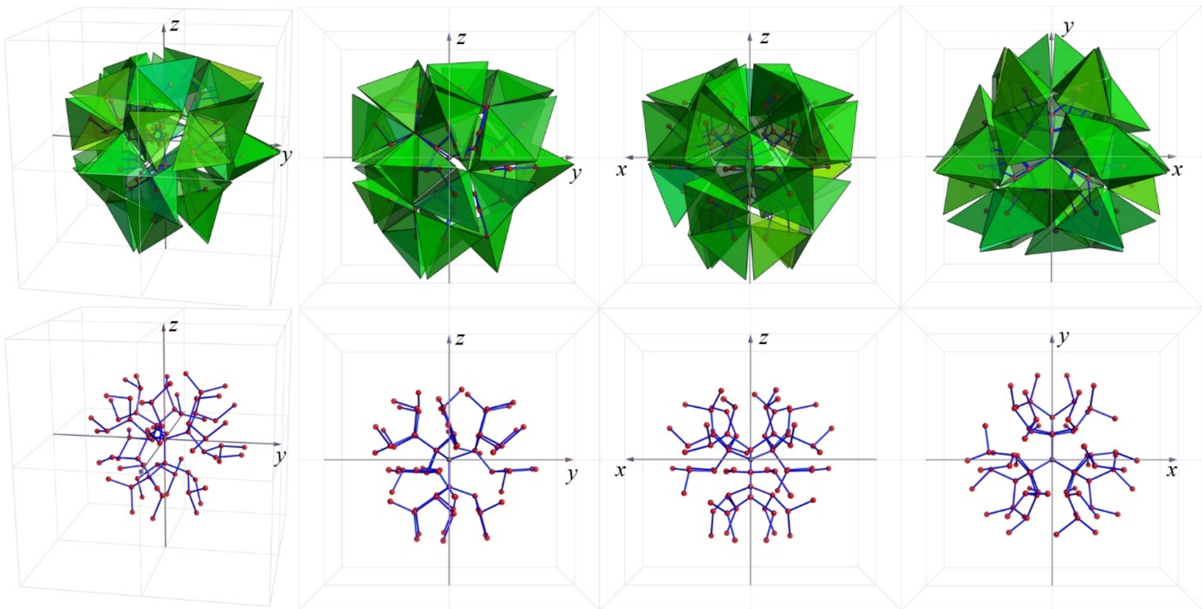

Fig. S10. G_4 dendrit. *Top*) illustrates four different projections of G_4 cluster, *bottom*) illustrates the same four different projections of the corresponding tetrahedral dendrit.

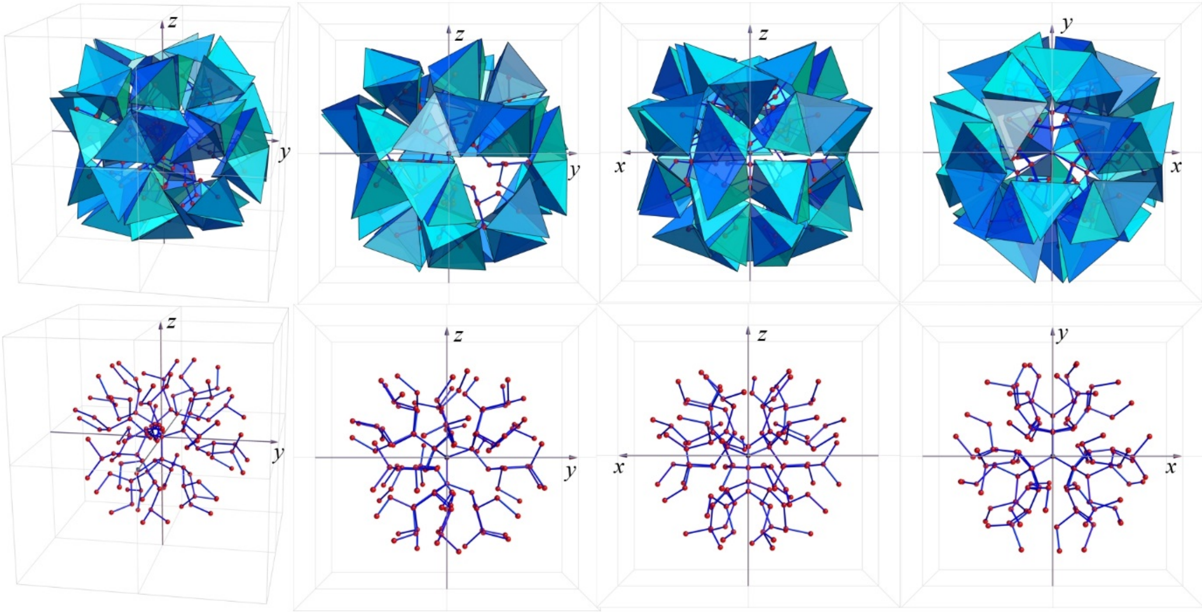

Fig. S11. G_5 dendrit. *Top*) illustrates four different projections of G_5 cluster, *bottom*) illustrates the same four different projections of the corresponding tetrahedral dendrit.

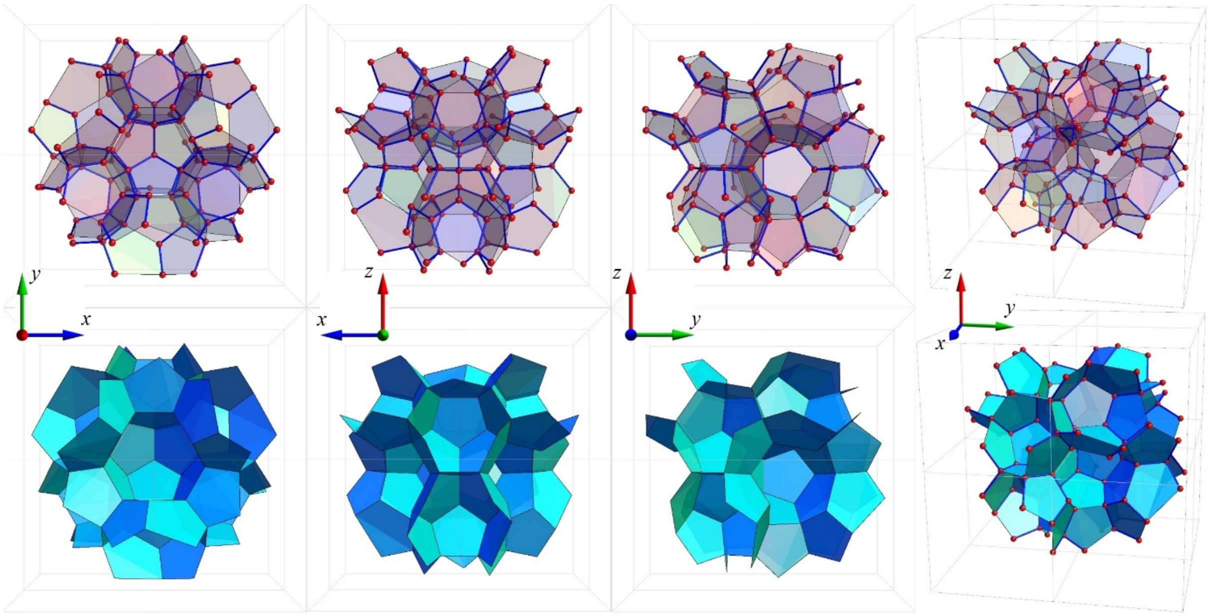

Fig. S12. *top*) shows tetrahedral dendrit viewed from four different angles. *Bottom*) illustrates solely the pentagonal membranes streatched onto the dendrit.

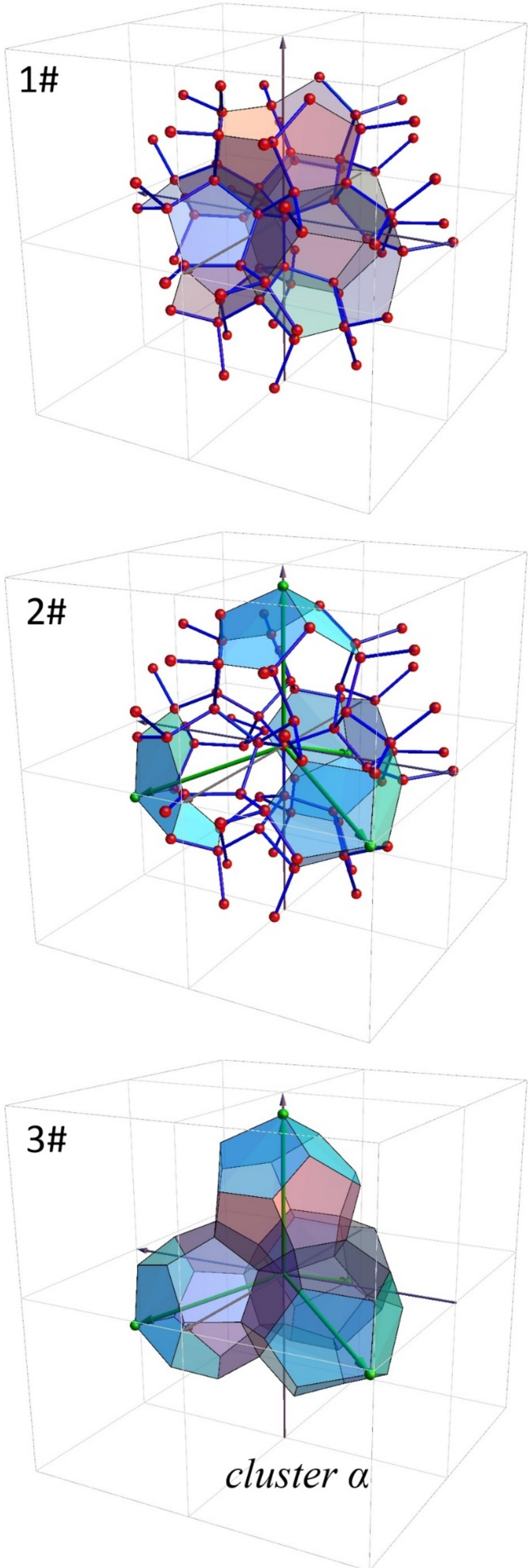

Fig. S13 open cells are „artificialy" closed using additional pentagonal membranes taking into account tetrahedral symmetry. Green vectors are tetrahedrally coordinated.

3. **Various foam-like, periodic structures**

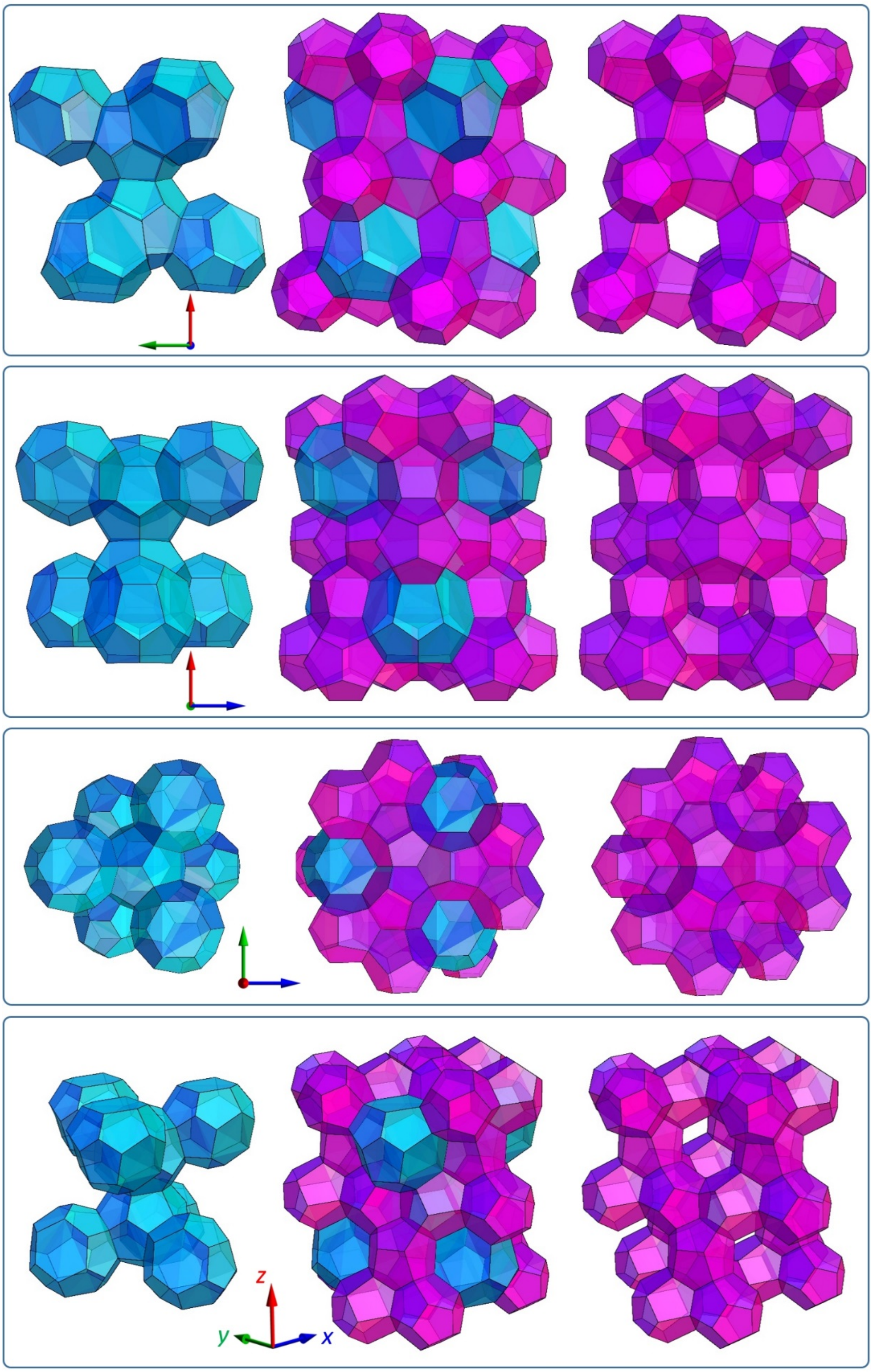

Fig. S14. Four different projections displaying Structure A, which resembles sII framework typical for hydrates.

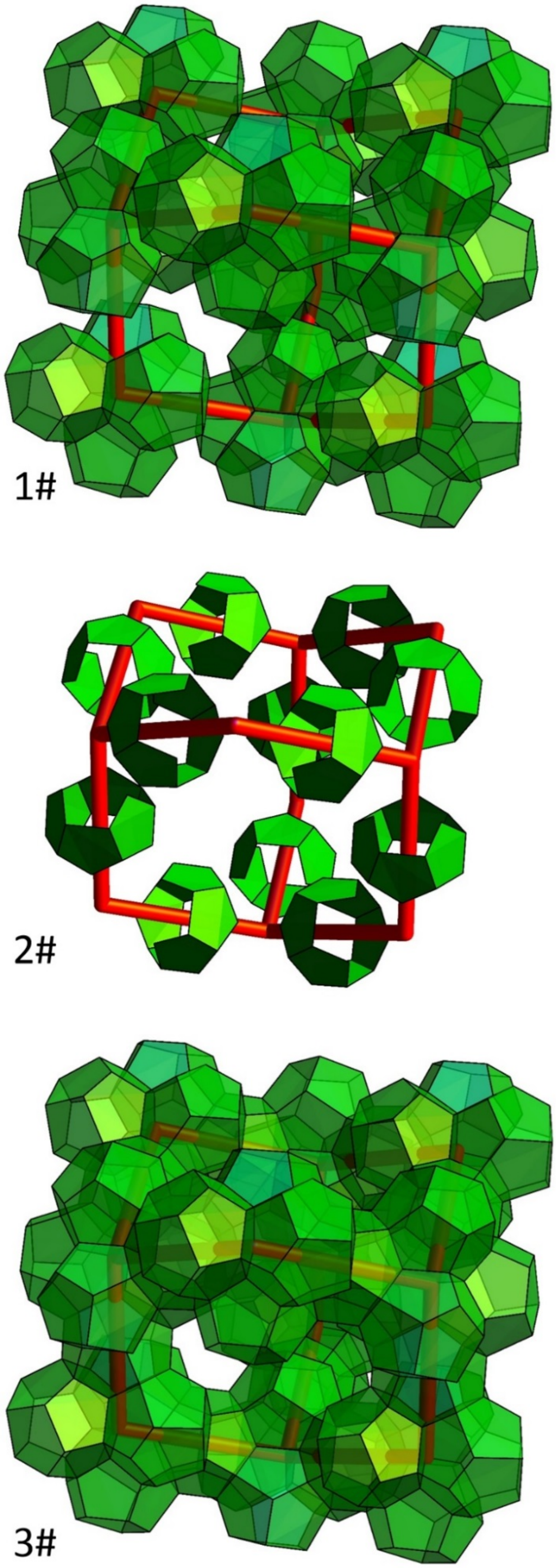

Fig. S15. Design of structure B – linkers geometry. 1#) 10 *α clusters* positioned onto adamantane cage-like scaffold, 2#) *α clusters* are interconnected via dodecahedra.

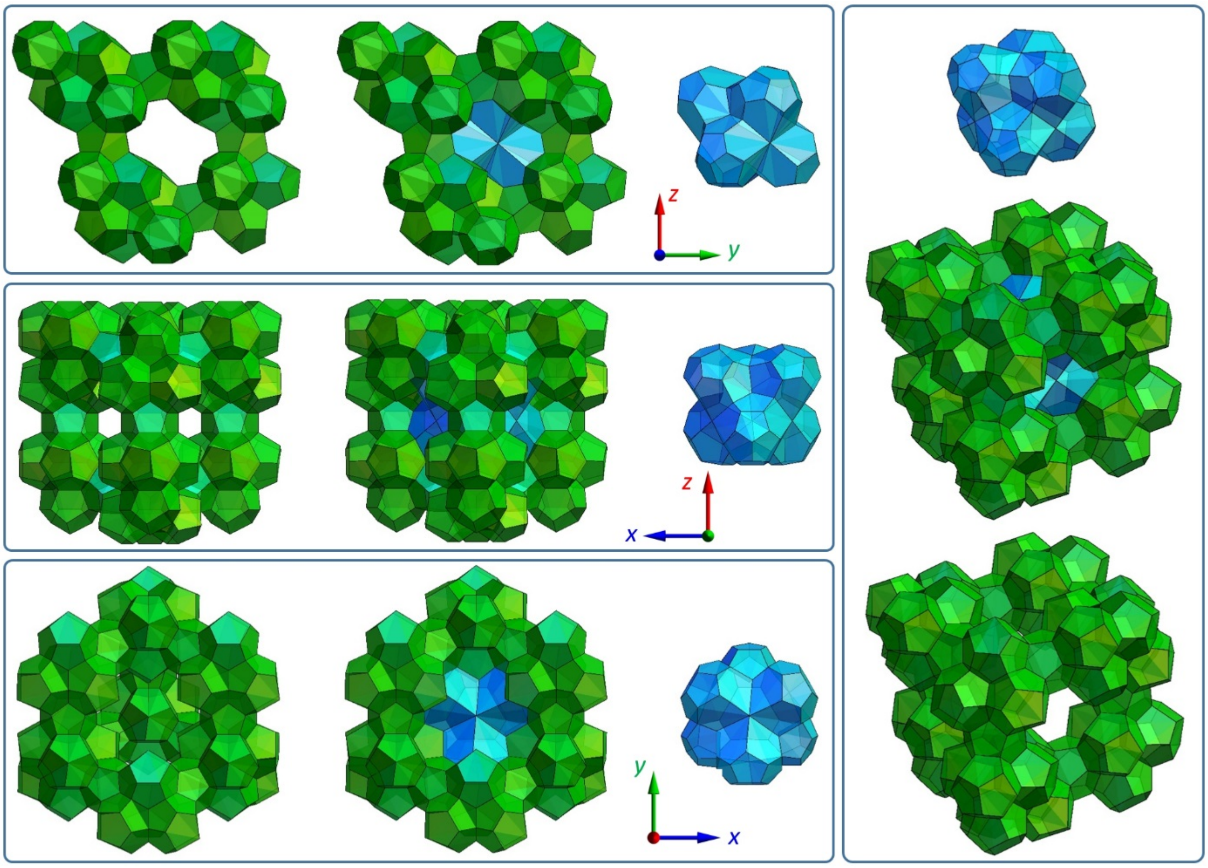

Fig. S16. Structure B – geometry of void – four different projections shown.

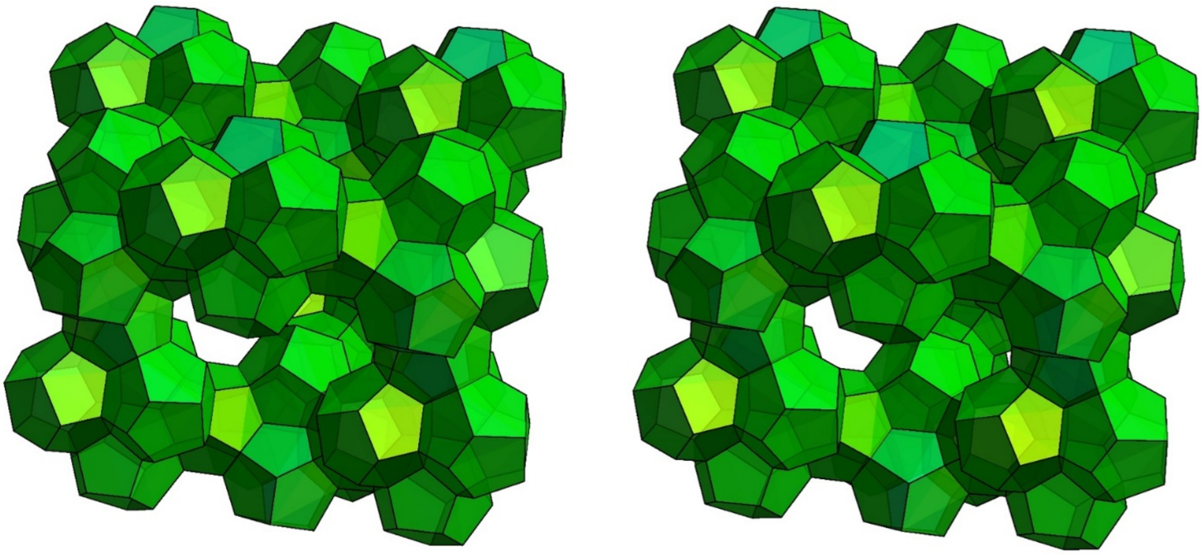

Fig. S17. Structure B - stereoscopic view

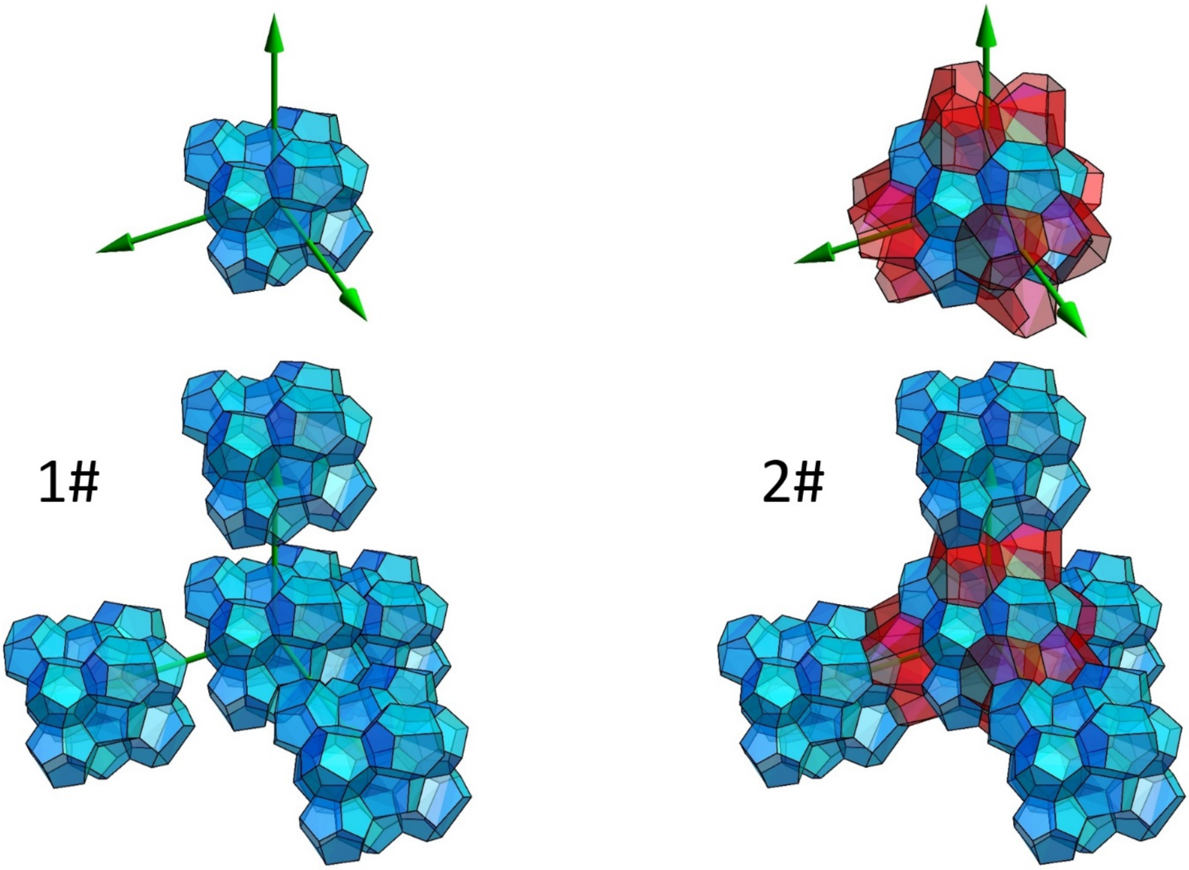

Fig. S18. Structure Γ (single diamond) based on γ cluster– linkers geometry. Green vectors are tetrahedrally coordinated.

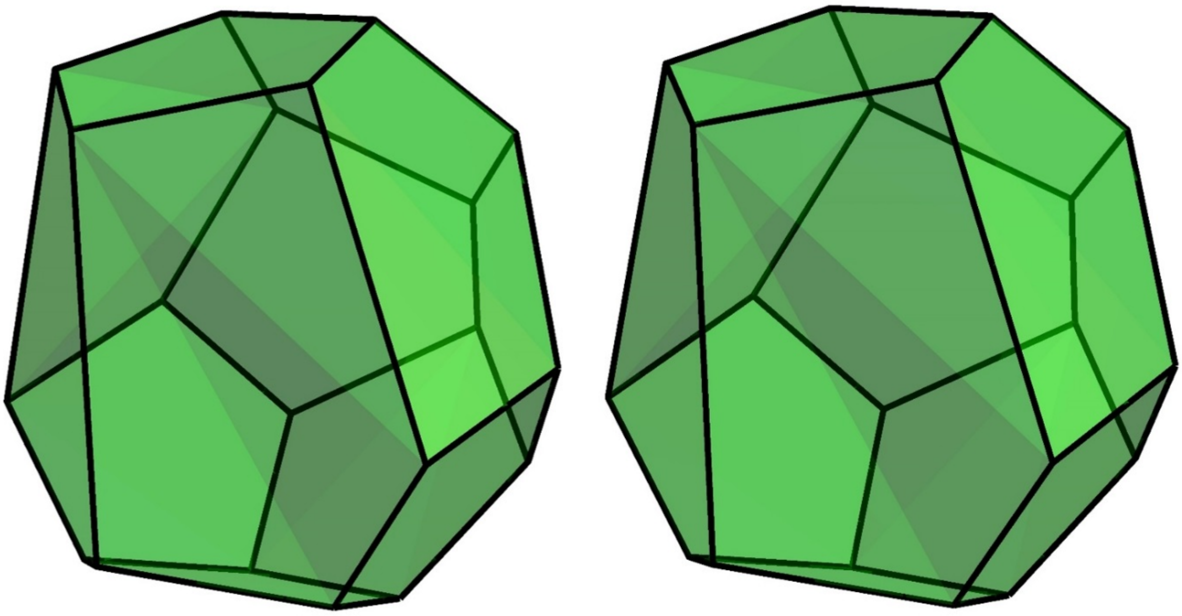

Fig. S19. Linker geometry (used in structure Γ and Δ) - stereoscopic view

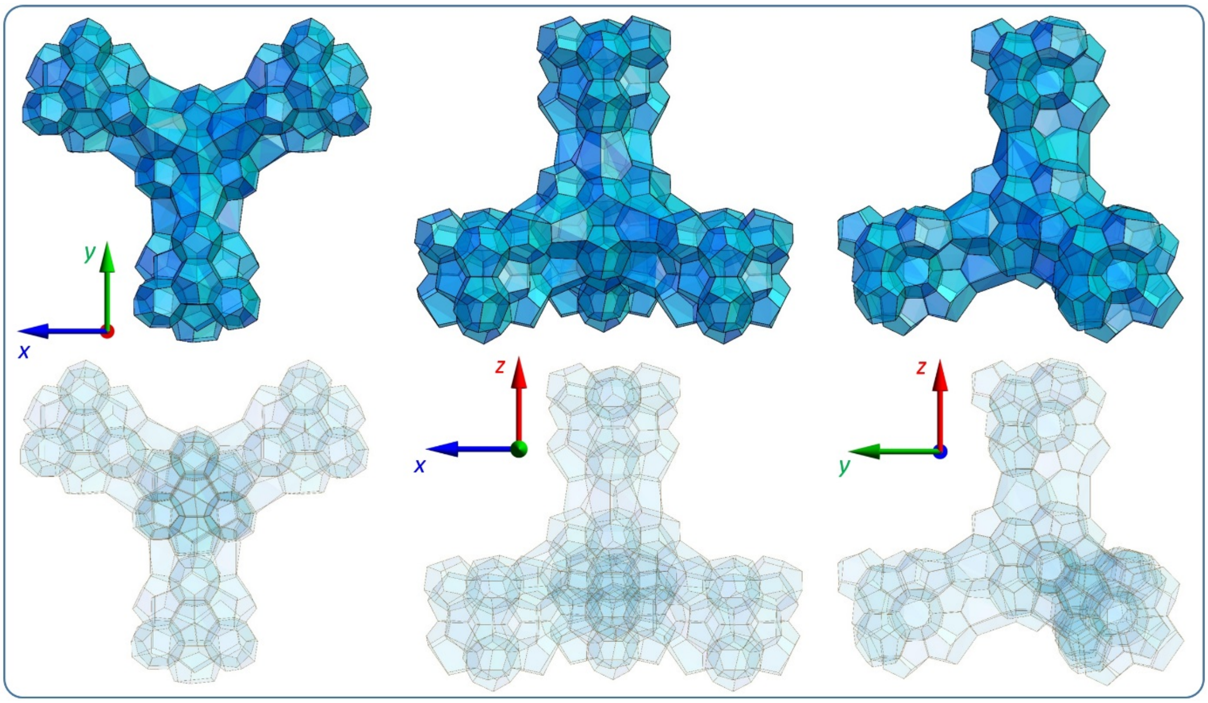

Fig. S20. Structure Γ (single diamond) – three different points of view.

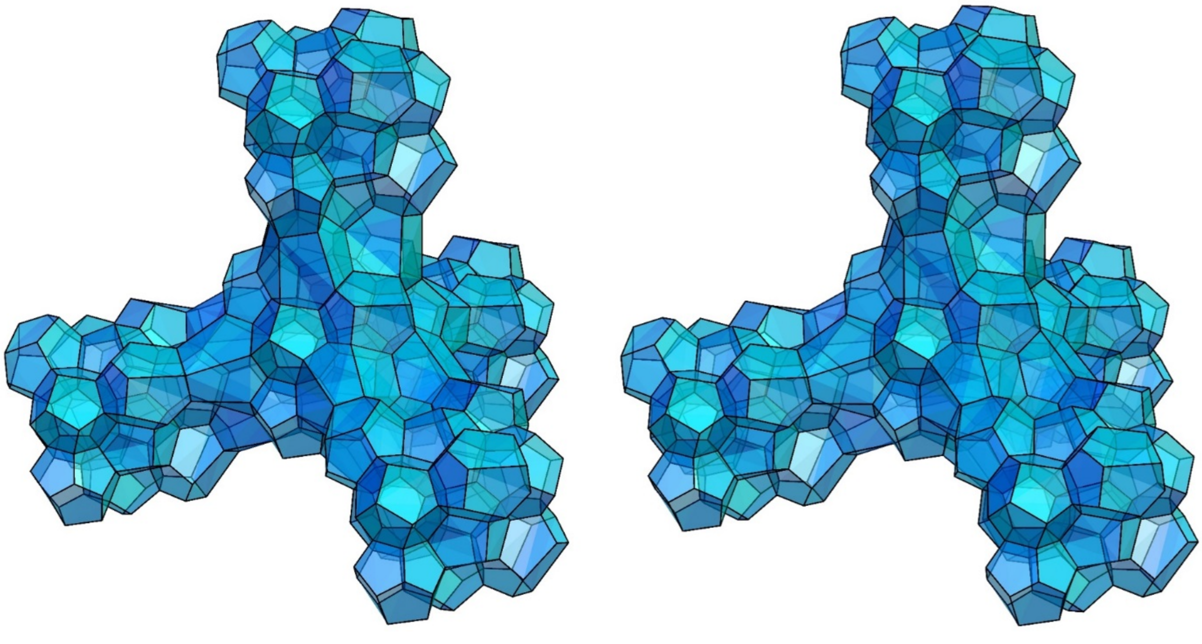

Fig. S21. Structure Γ (single diamond) - stereoscopic view

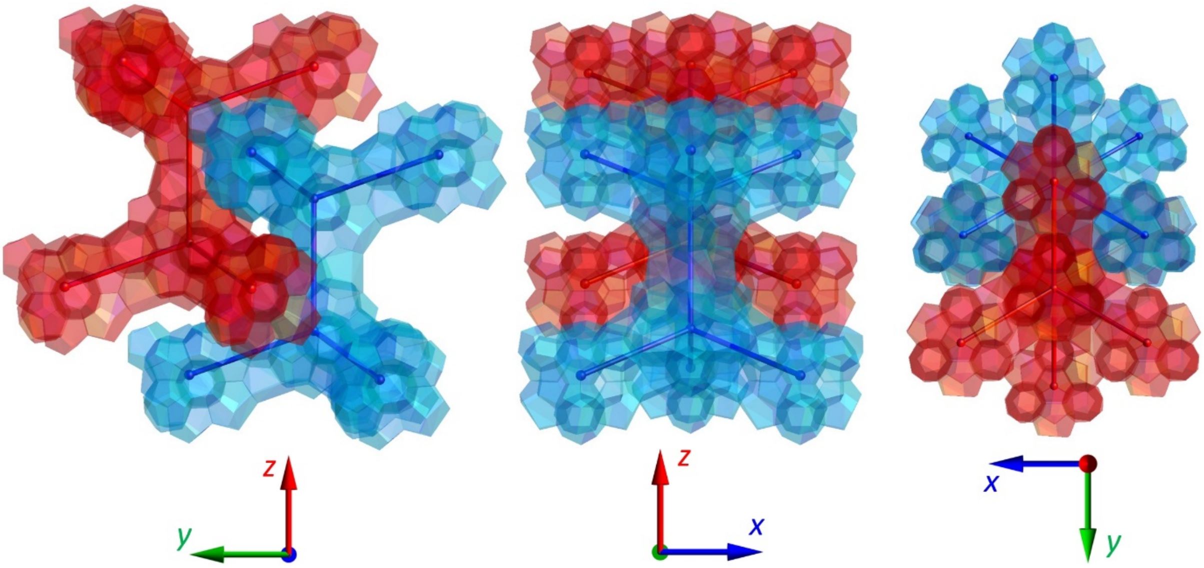

Fig. S22. Structure Γ (DD) - three different points of view.

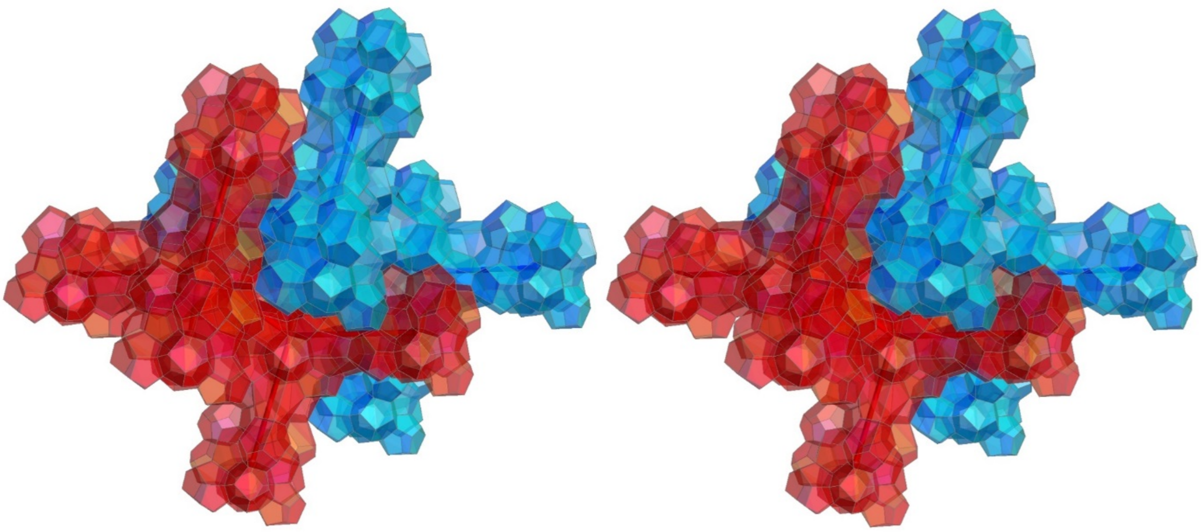
Fig. S23. Structure Γ (DD) -stereoscopic view

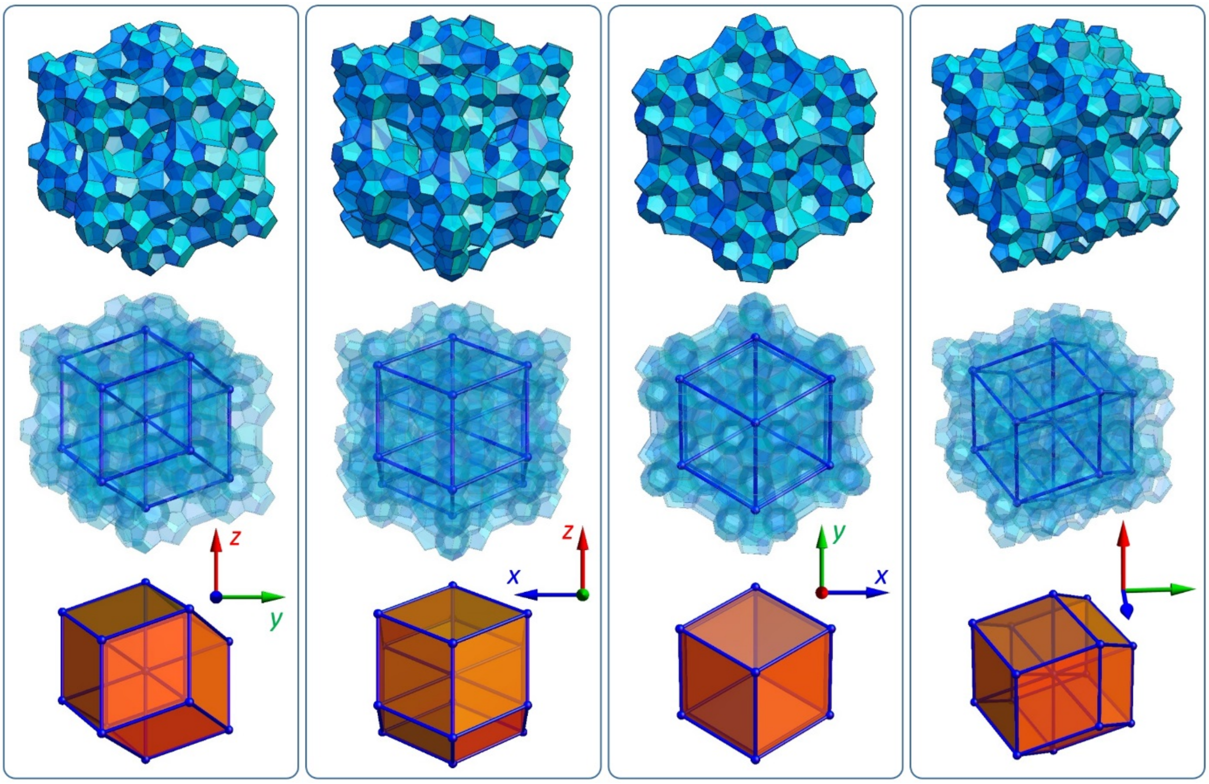

Fig. S24. Structure Δ - four different points of view.

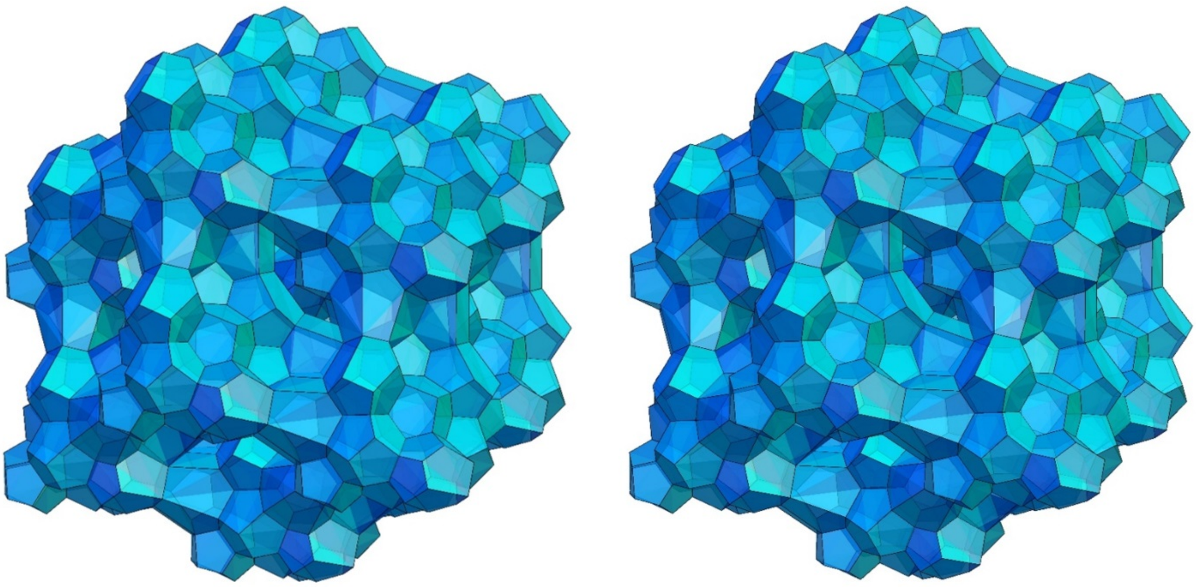

Fig. S25. Structure Δ - stereoscopic view