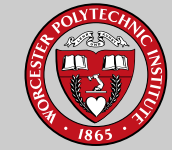
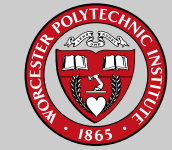
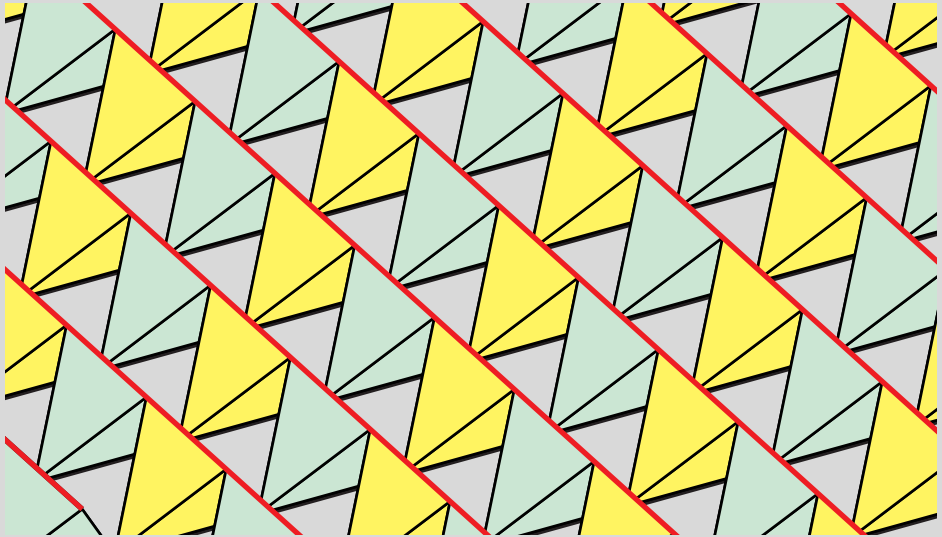


Auxetic behavior of 2-layer zeolites

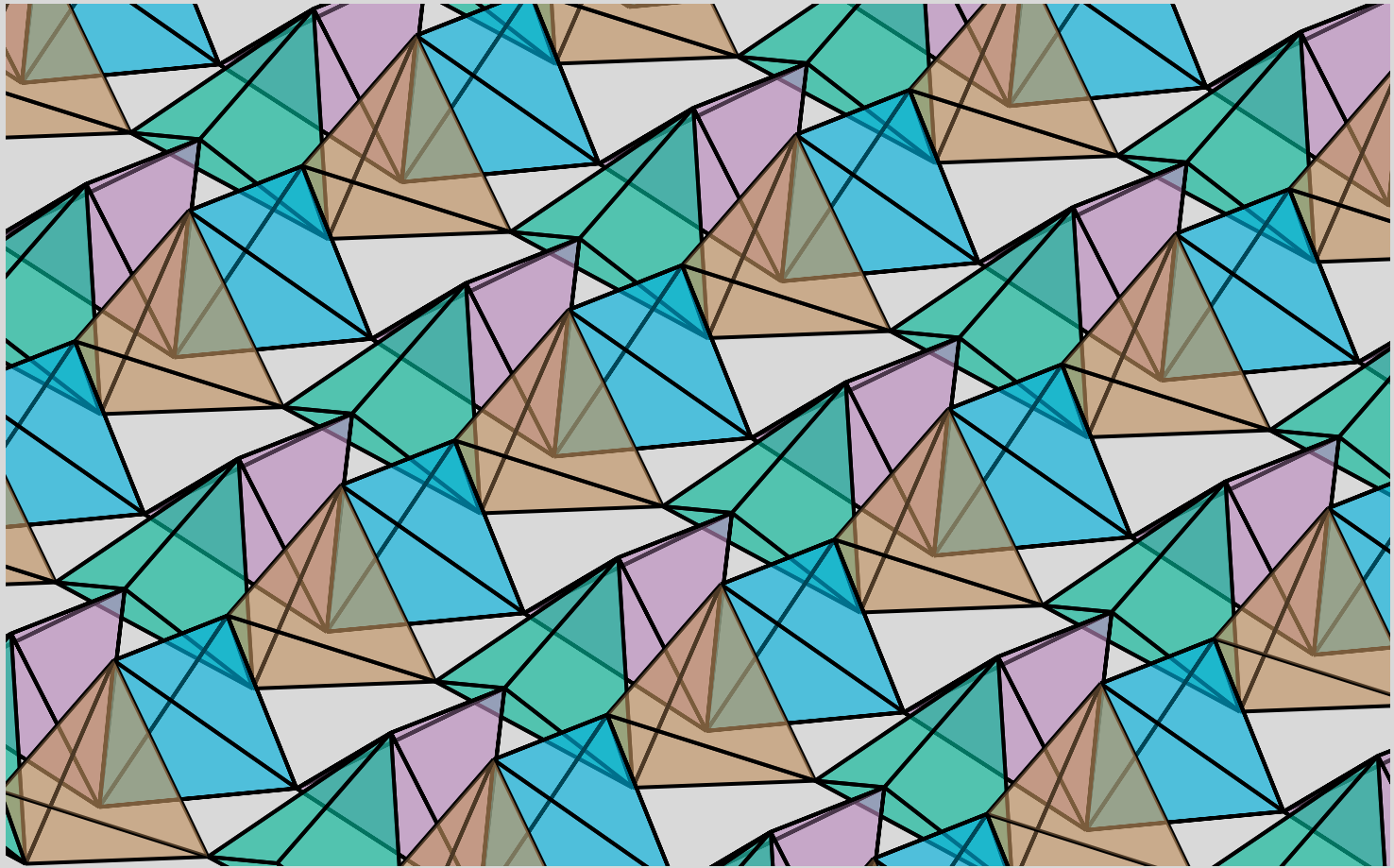
Brigitte Servatius — WPI



A one layer Zeolite

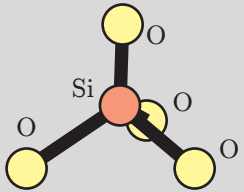


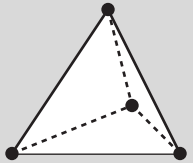
A one layer Zeolite



1. Chemical Zeolites

- crystalline solid
- units: $\mathrm{Si} + 4\mathrm{O}$





- two covalent bonds per oxygen

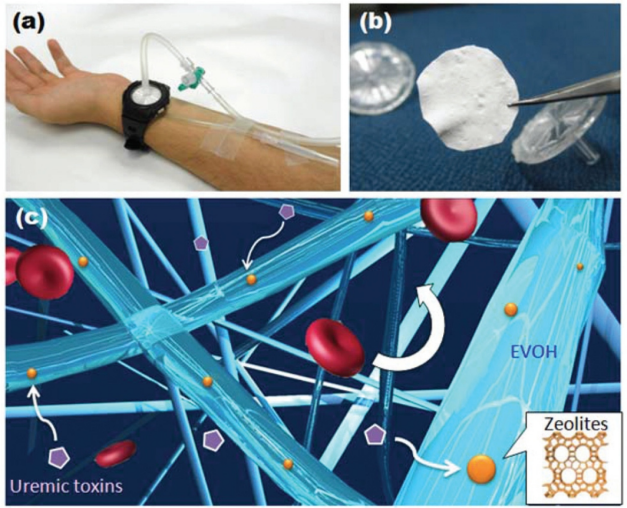


Fig. 1 Photographs of a wearable blood purification system (a) and a zeolite–polymer composite nanofiber mesh (b). (c) The nanofiber is composed of blood compatible poly(ethylene-*co*-vinyl alcohol) as the primary matrix polymer and zeolites which are capable of selectively adsorbing uremic toxins.

[7]

- naturally occurring
- synthesized
- theoretical

Zeolite membranes

[1], [8]

Simulating Large-Scale Morphogenesis in Planar Tissues

DMS2012330 (Wu PI). $200,000, 06/15/2020-05/30/2023. This project aims to improve tools for modeling a wide range of living tissues that are relatively planar and have been extensively studied experimentally.

2. Combinatorial Zeolites

Combinatorial d-Dimensional Zeolite

- A connected complex of corner sharing d-dimensional simplices
- At each corner there are exactly two distinct simplices
- Two corner sharing simplices intersect in exactly one vertex.

body-pin graph

Vertices: simplices (silicon)
Edges: bonds (oxygen)
There is a one-to-one correspondence between combinatorial d-dimensional zeolites and d-regular body-pin graphs.

Graph of a Combinatorial Zeolite

is obtained by replacing each d-dimensional simplex with K_{d+1}.

The graph of the zeolite is the line graph of the Body-Pin graph.

Whitney

(1932) proved that connected graphs X on at least 5 vertices are strongly reconstructible from their line graphs $L(X)$. [9]
Moreover, $Aut(X) \cong Aut(L(X))$.

3. Realization

A realization of a d-dimensional zeolite

An placement (embedding) of vertices of the the d-dimensional complex in $\mathbb{R}^d$. Equivalently a placement (embedding) of the vertices of the line graph of the body-pin graph.

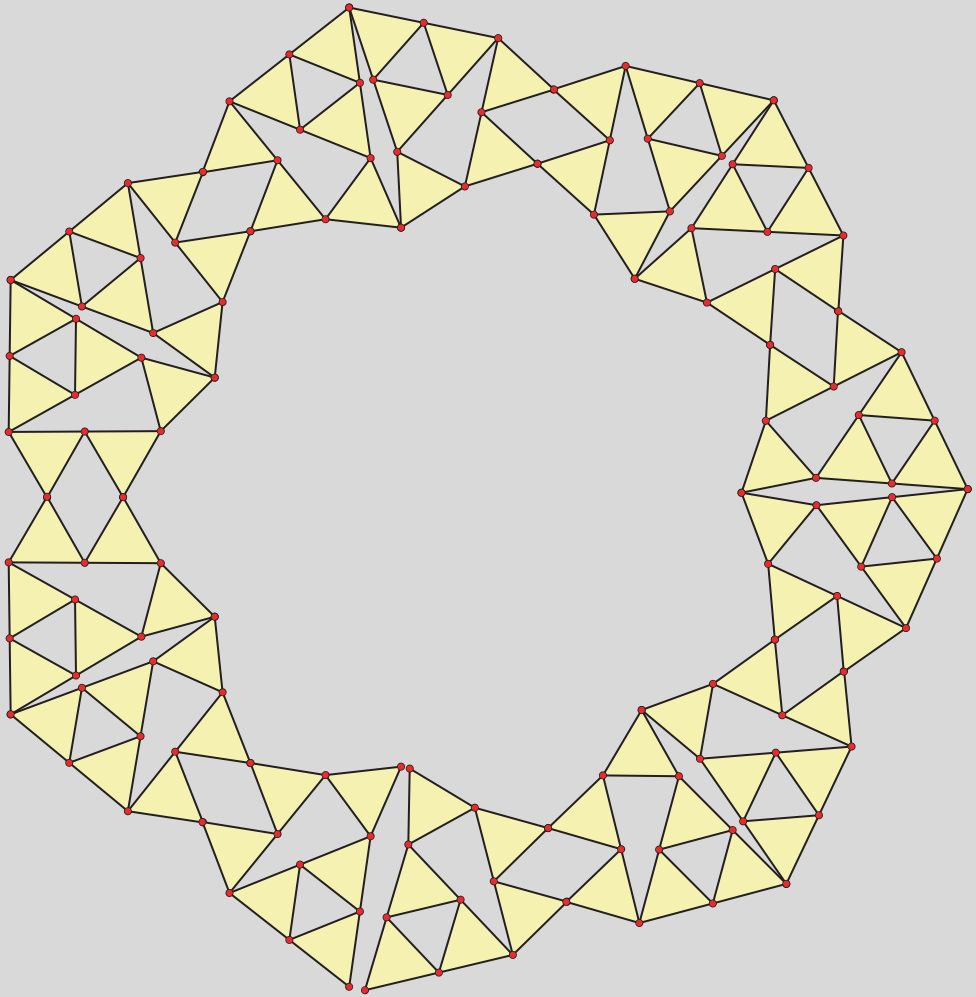
unit-distance realization

A realization where all edges join vertices distance 1 apart in $\mathbb{R}^d$.

non-interpenetrating realization

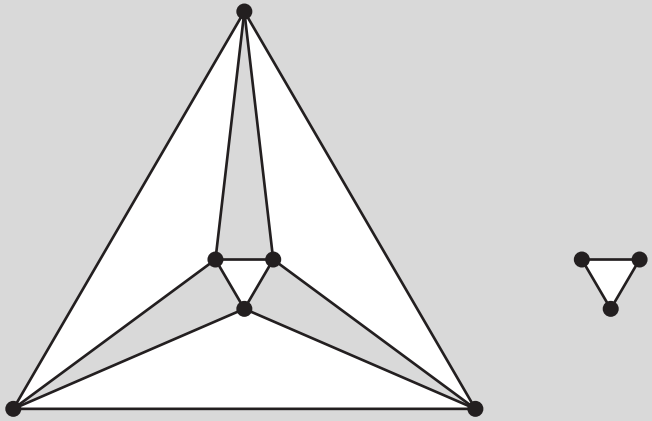
A realization where simplices are disjoint except at joined vertices.

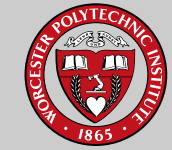
The typical situation: Not unit distance realizable.



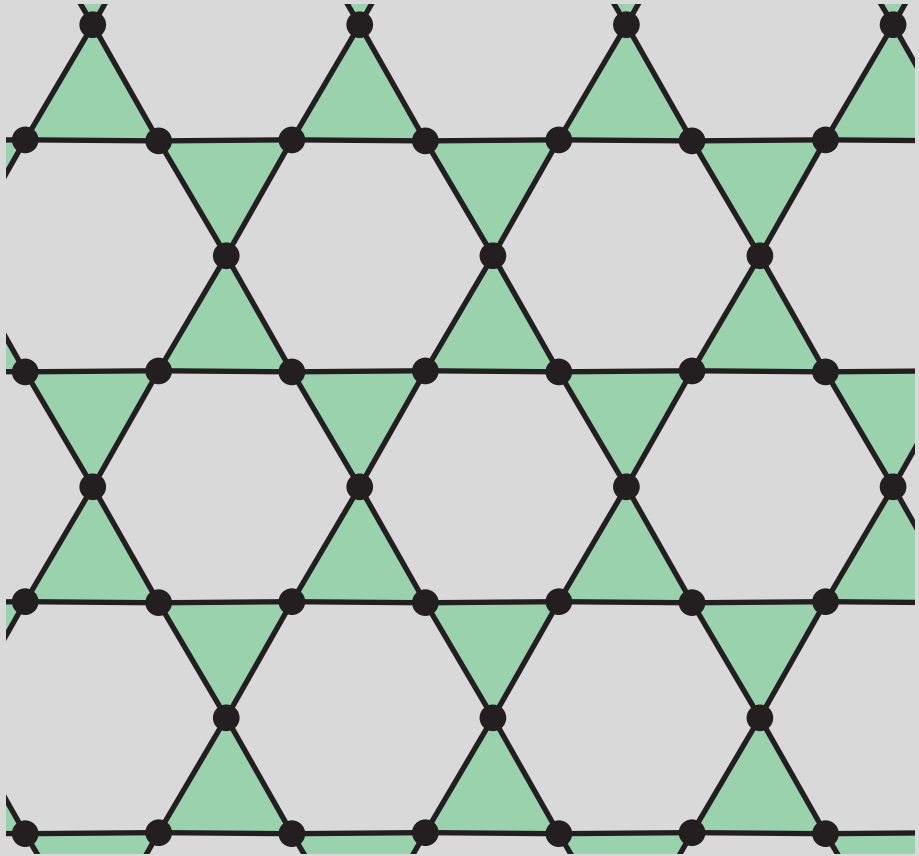
4. 2d Zeolites

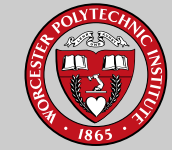
Smallest 2d zeolite is the line graph of K_4: The graph of the octahedron with four (edge disjoint) faces.
For body-pin graphs on more than 4 vertices, the zeolite can be recovered uniquely from the line-graph.



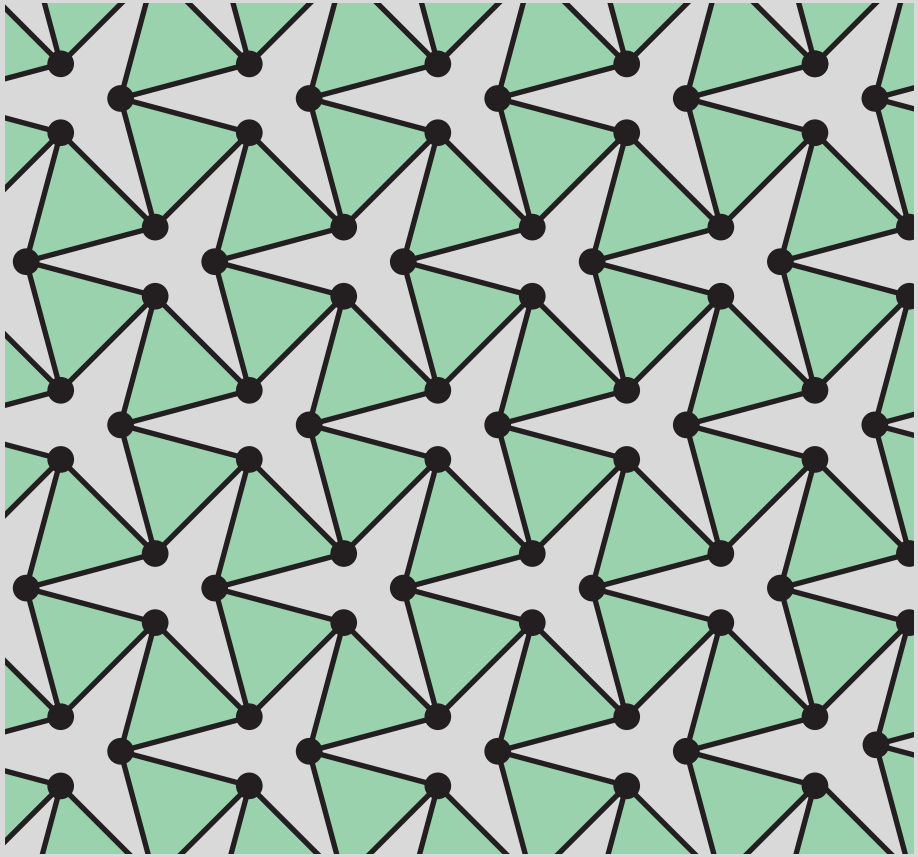


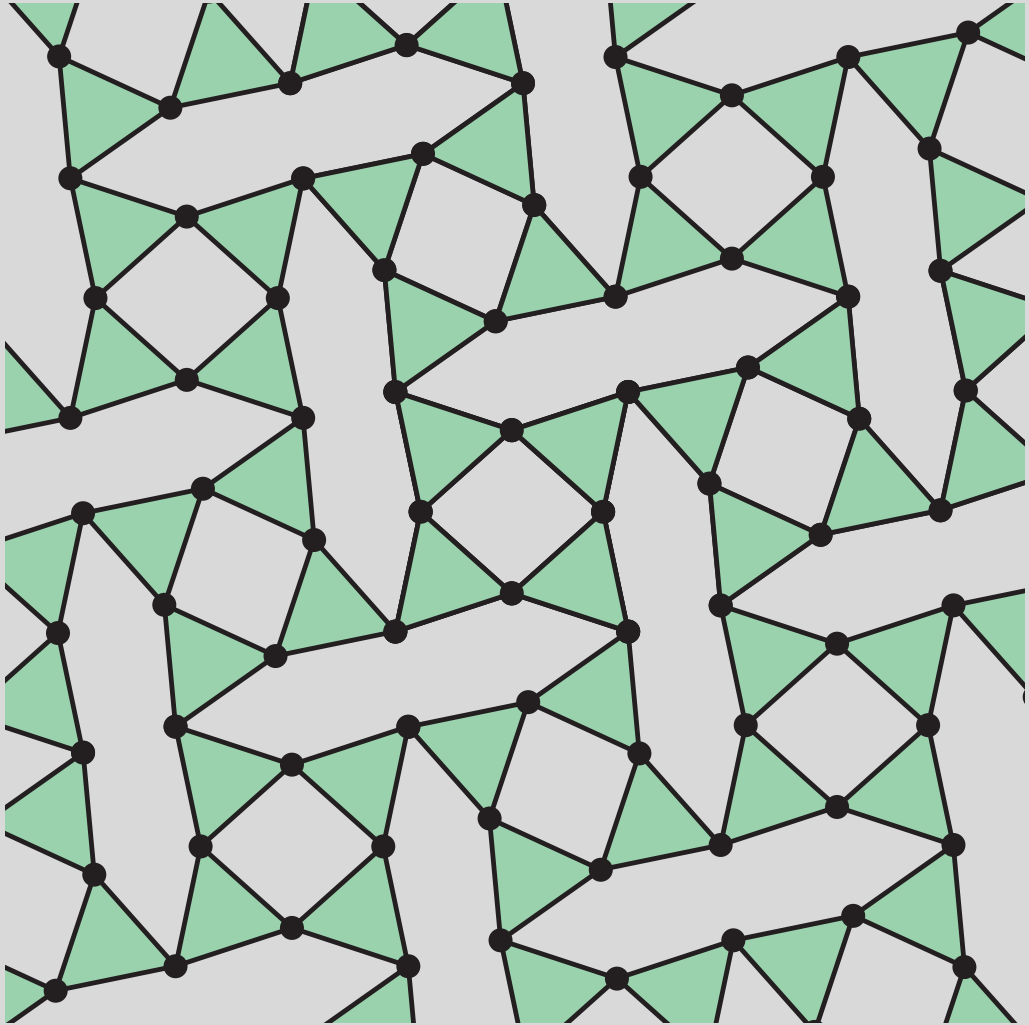
It is just as easy to construct infinite symmetric examples:

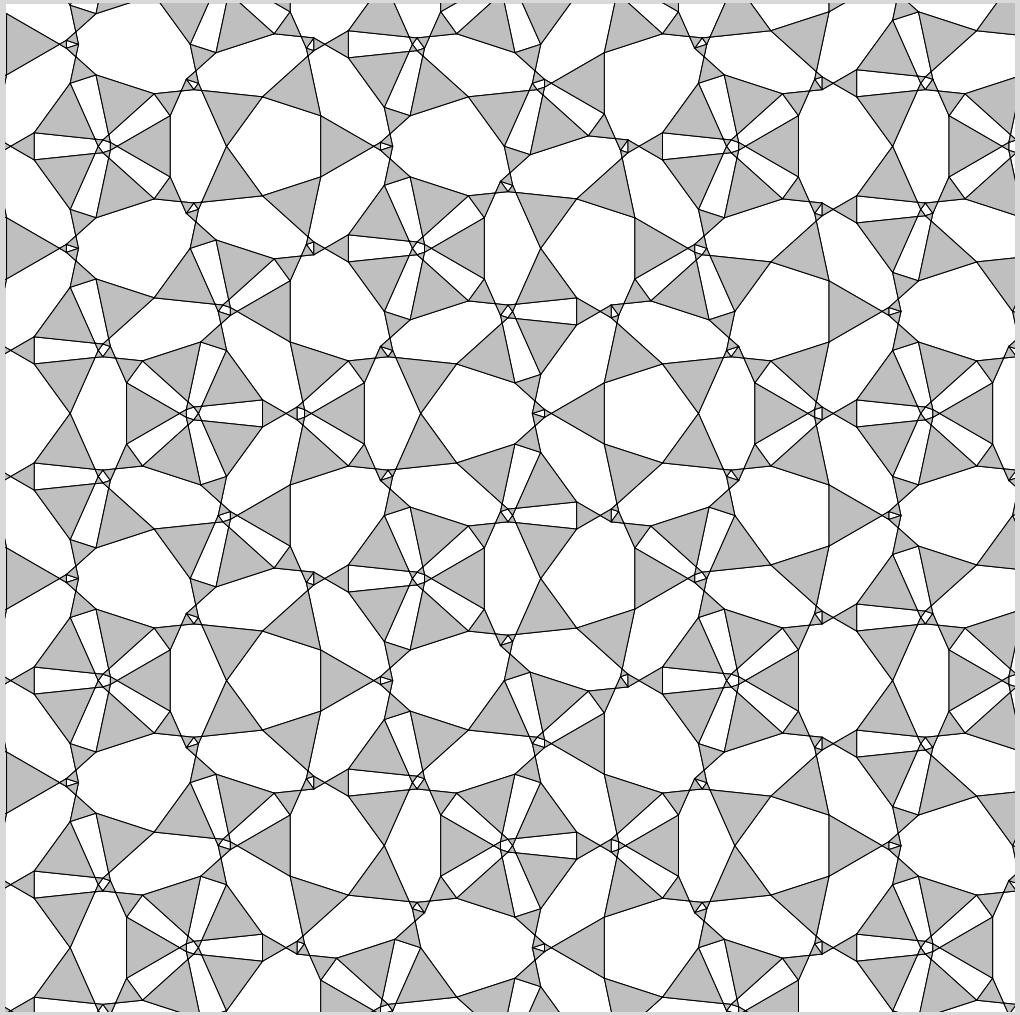




Showing a different symmetry

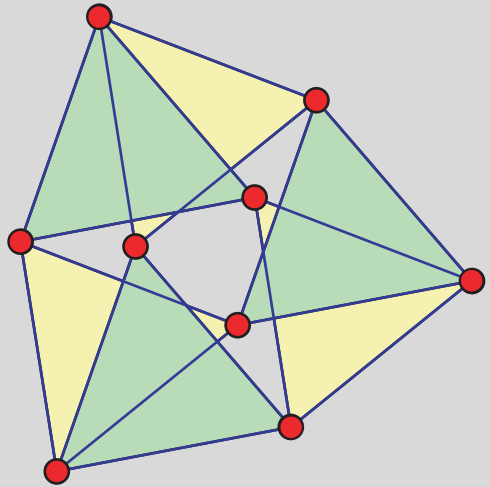


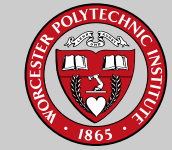




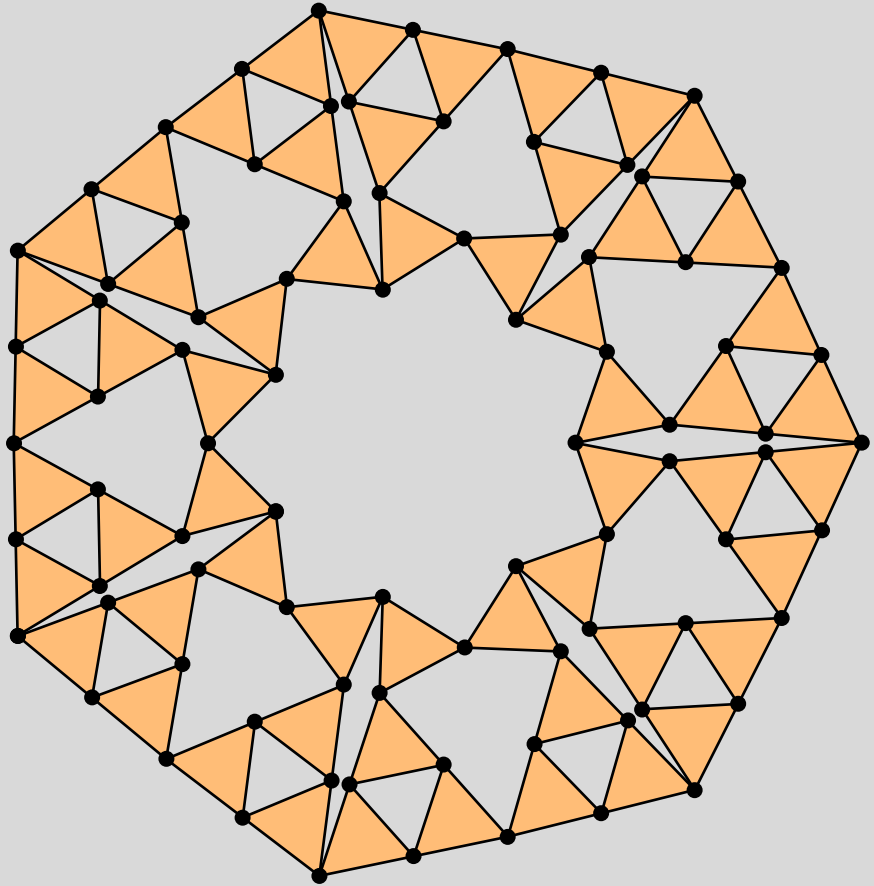
5. Finite Zeolites

Body pin graph: $K_{3,3}$. Since the body pin graph is not planar, the resulting zeolite cannot be planar. Its underlying graph is generically globally rigid. However, it has a unit distance realization in the plane which is a mechanism.

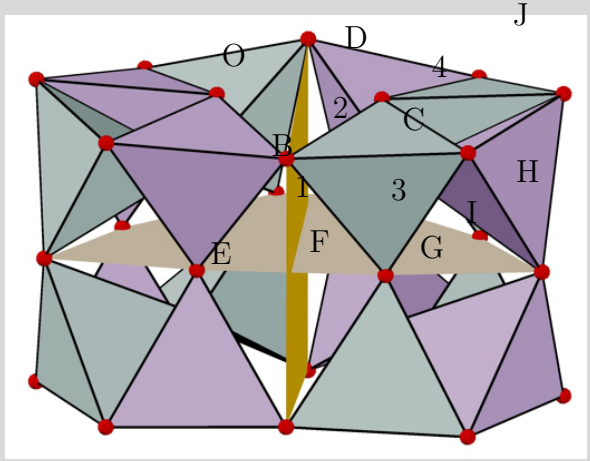




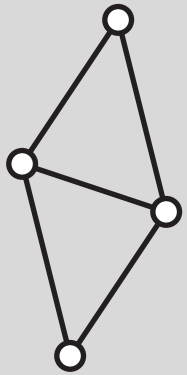
Harborth's Example

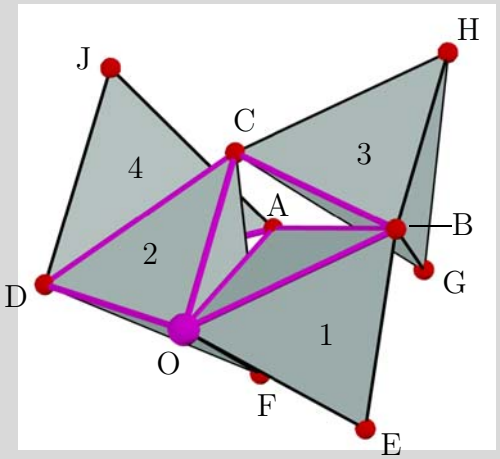


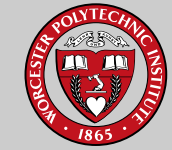
A finite 3-D symmetric example:



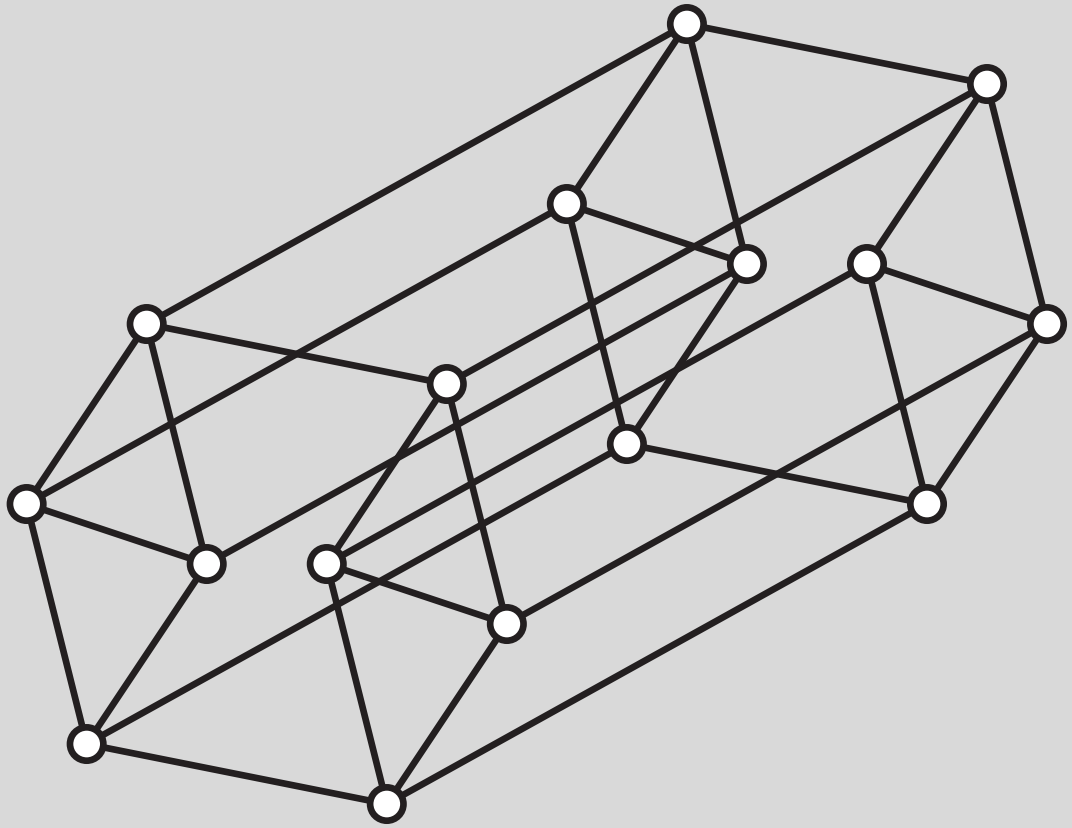
Model with its two planes of symmetry



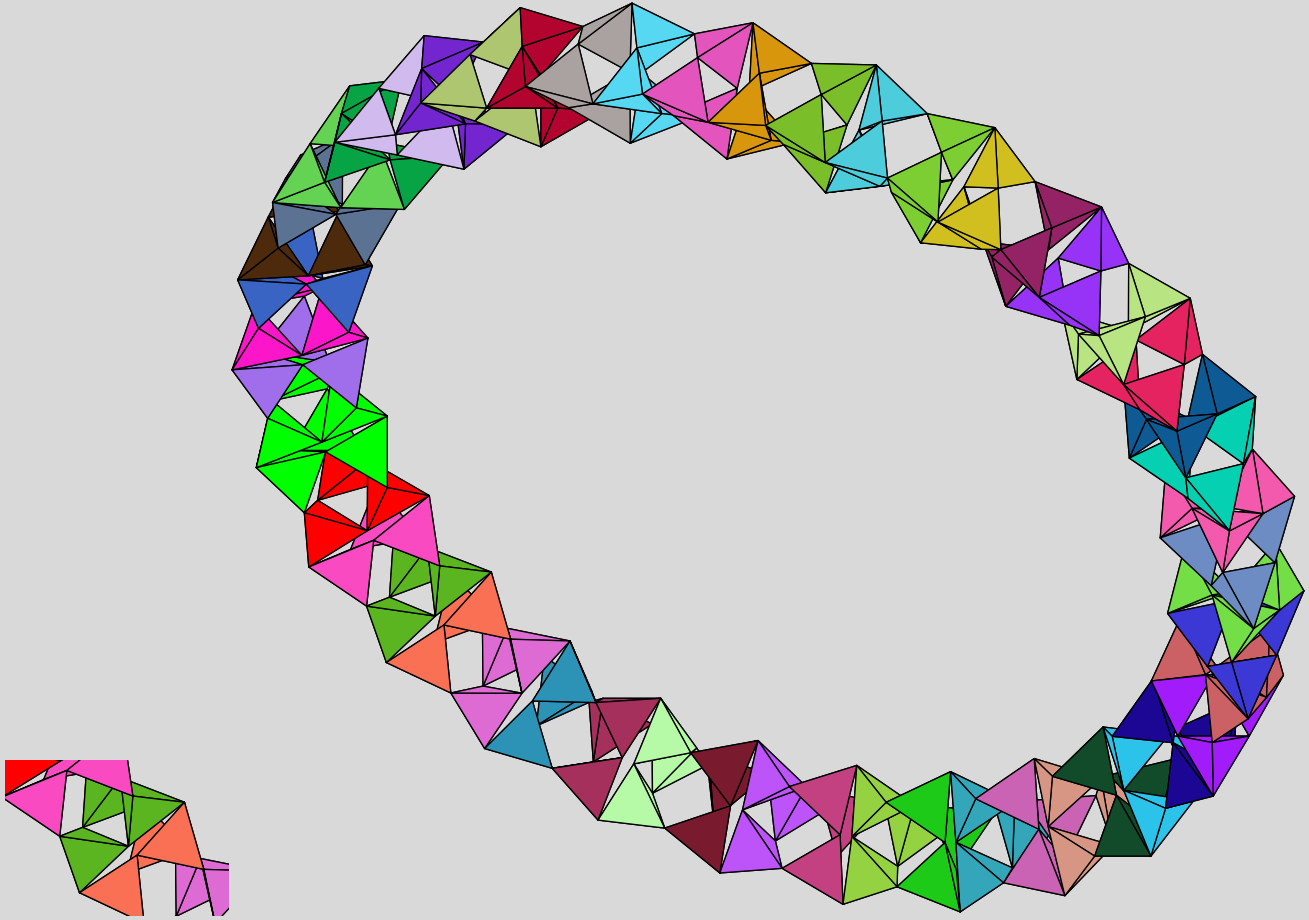


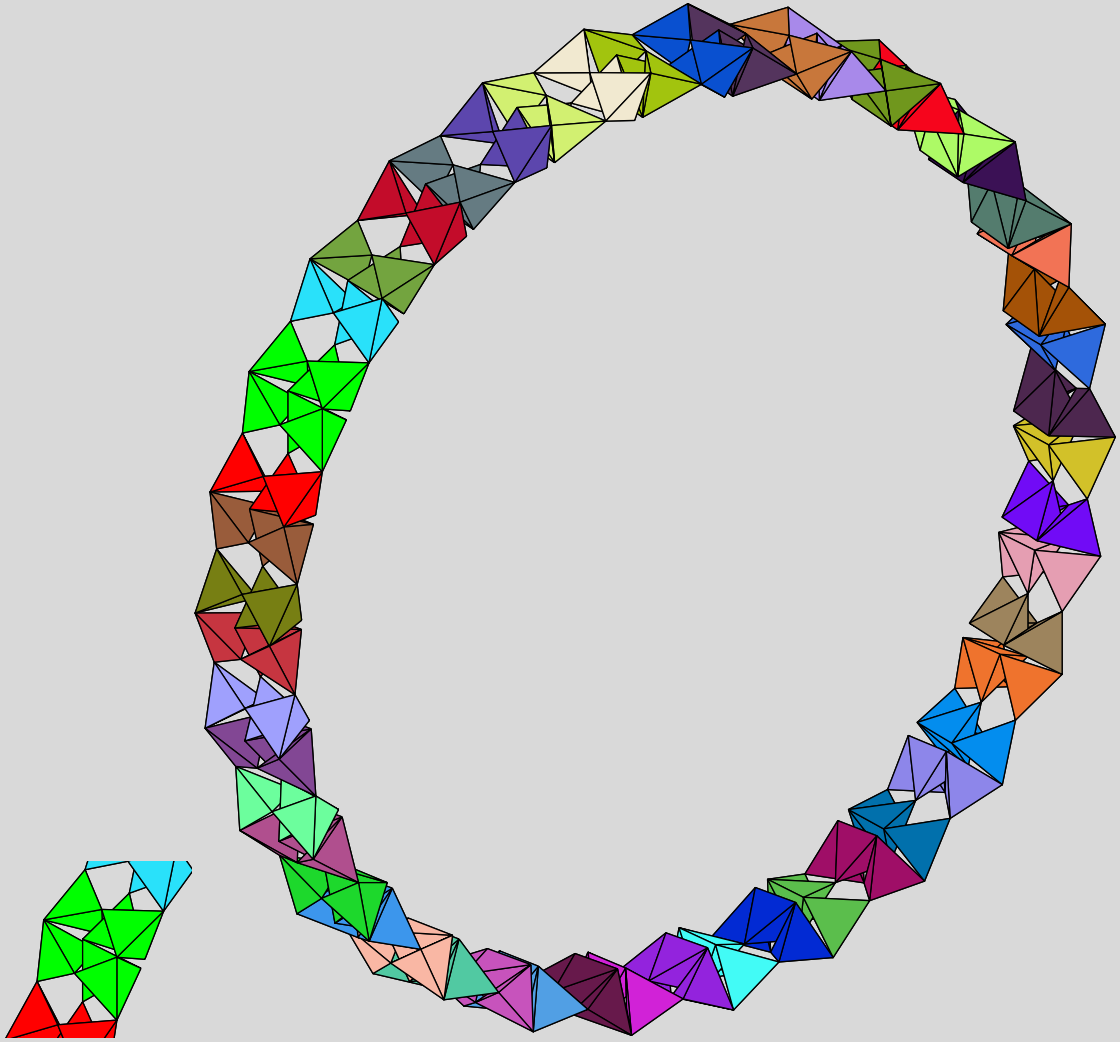


The Harboth-Möller model



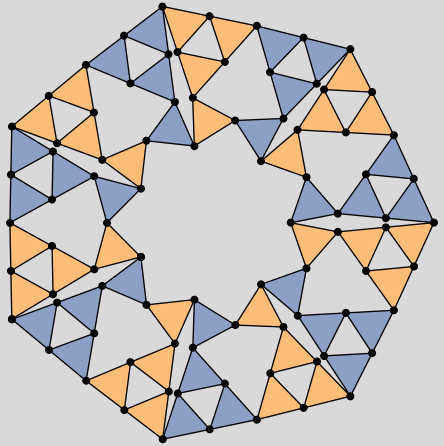
The body pin graph of the Harborth-Möller Model.



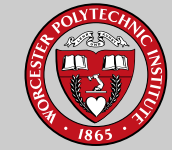


6. The Layer Construction

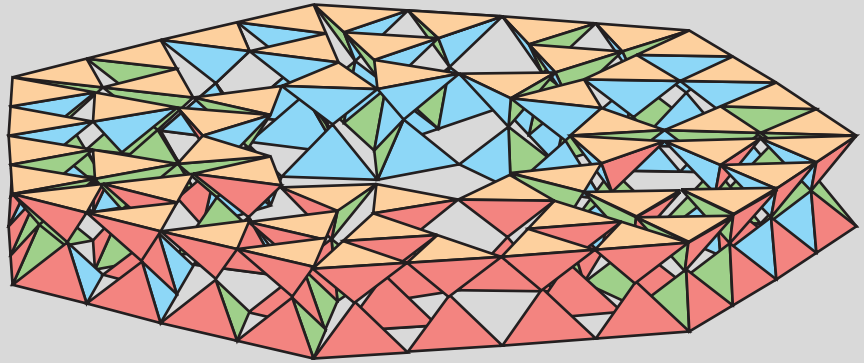
$Z = (T, C)$ is a combinatorial zeolite realizable in dimension d.
$\mathbb{R}^d \subseteq \mathbb{R}^{d+1}$
Label each $t \in T$ arbitrarily with ± 1.
For $+1$, erect a $d+1$ dimensional simplex in the upper half space,
For -1, erect a $d+1$ dimensional simplex in the lower half space,
Call the Complex Z_a and its mirror image Z_b.

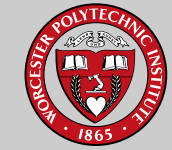


Alternately staking Z_a and Z_b gives a *layered Zeolite* in $\mathbb{R}^{d+1}$.

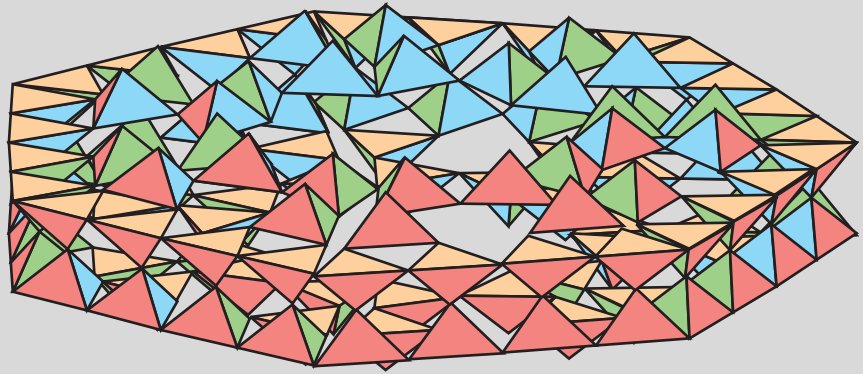


Labels all +1
A two layered zeolite.



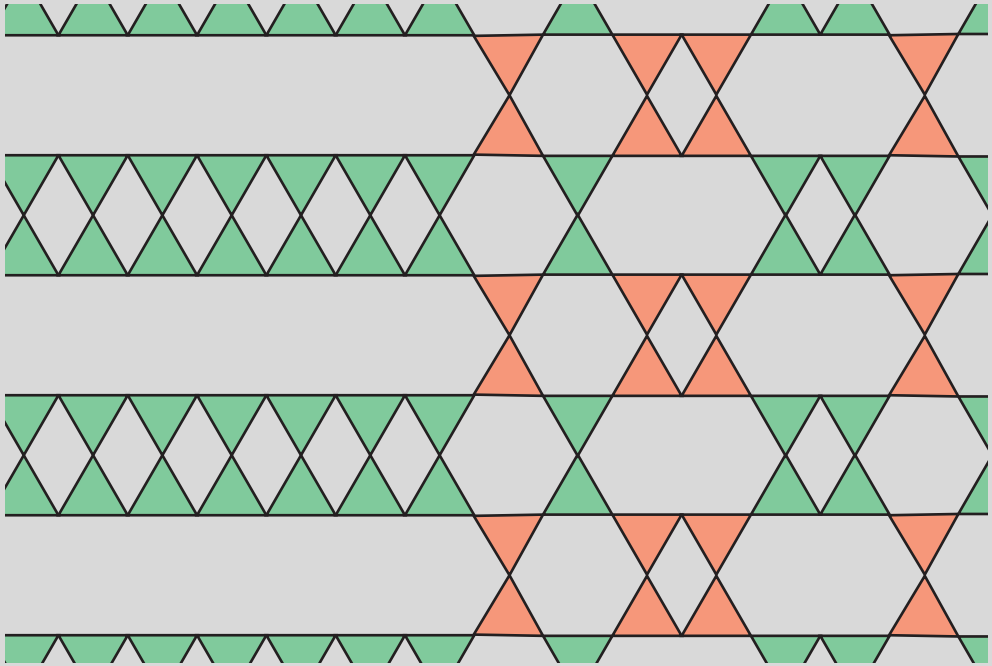


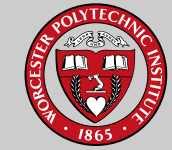
The general case starting from a finite zeolite.



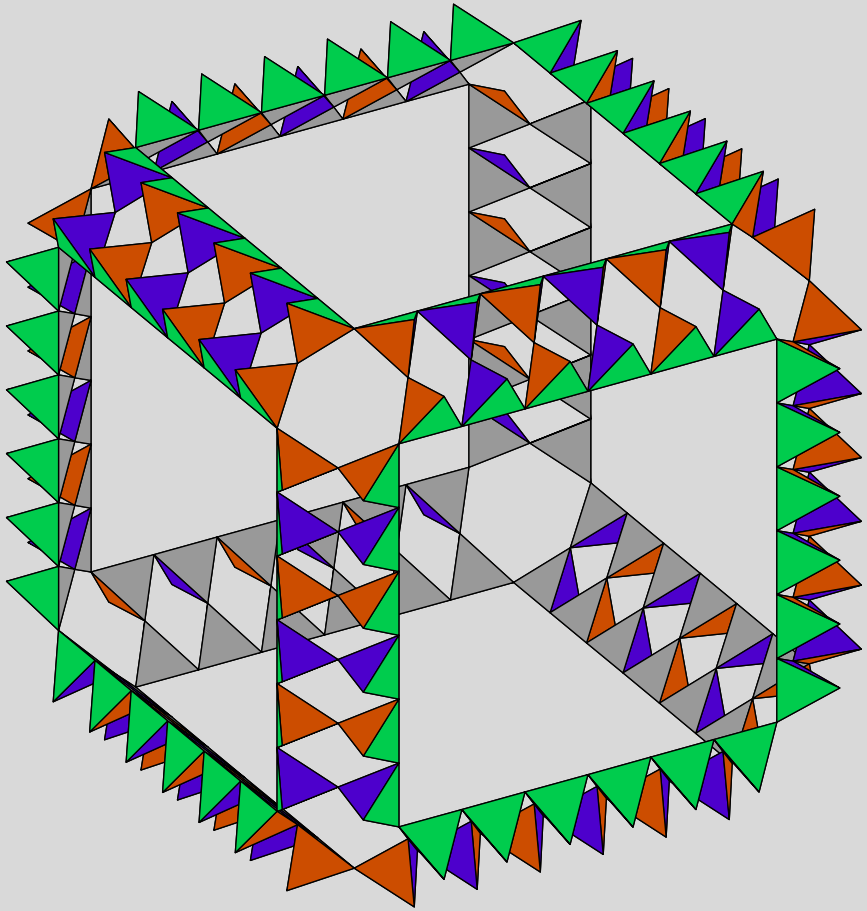
Theorem: There are uncountably many isomorphism classes of unit distance realizable zeolites in $\mathbb{R}^3$.
(actually in any dimension $d > 1$.)

Proof:





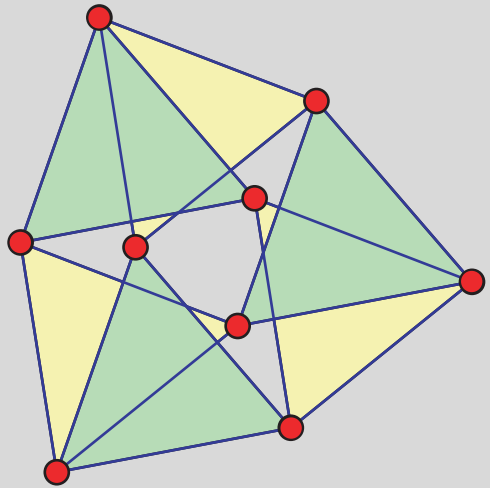
7. Holes in Zeolites



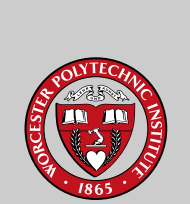
8. Motions

Degree of Freedom

Each simplex d-dimensional simplex has $d(d+1)/2$ degrees of freedom
Each contact of the $d+1$ contacts removes d degrees.
By a naïve count, a zeolite is rigid - (overbraced by $d(d+1)/2$.)

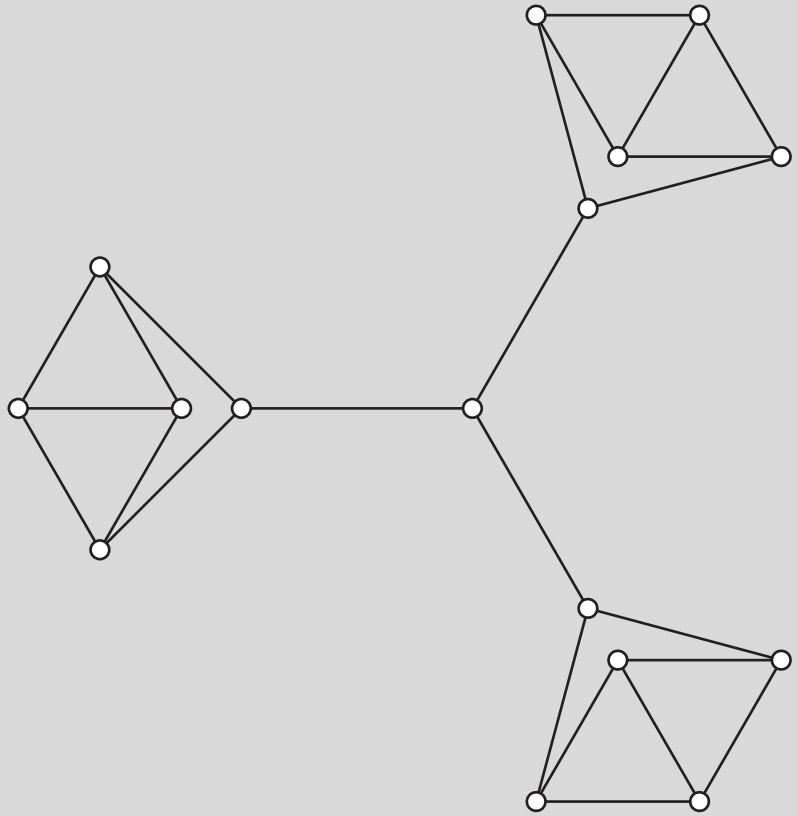


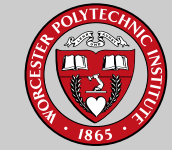
A 4-regular vertex transitive graph is globally rigid unless it has a 3-factor consisting of s disjoint copies of K_4 with $s \geq 3$ [4].



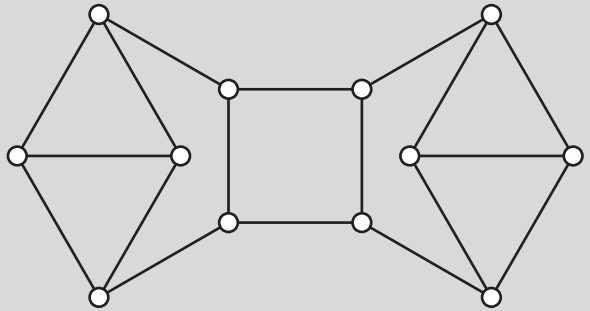
Are there finite generically flexible 2D Zeolites?

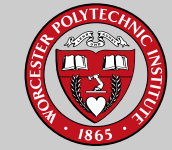
Yes, line graphs of 3-regular graphs with edge connectivity less than 3.





Are there finite generically rigid but not globally rigid 2D Zeolites?
Yes, line graphs of 3-regular graphs with edge connectivity less than 3.





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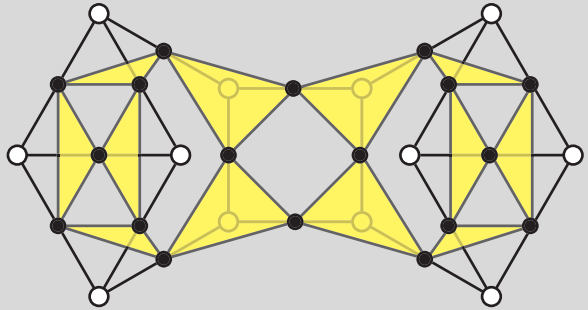
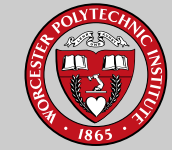
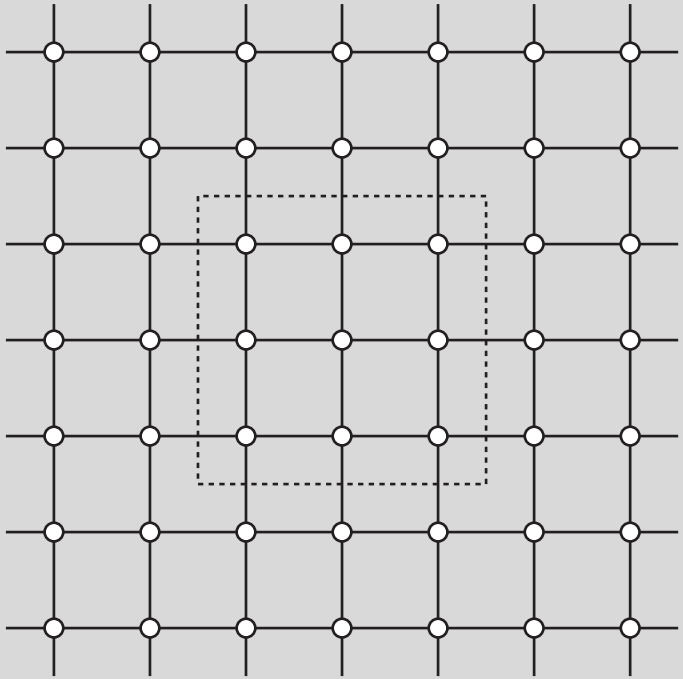
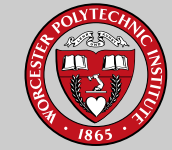


Generically globally rigid 2-d Zeolites were characterized by Jordan [5].

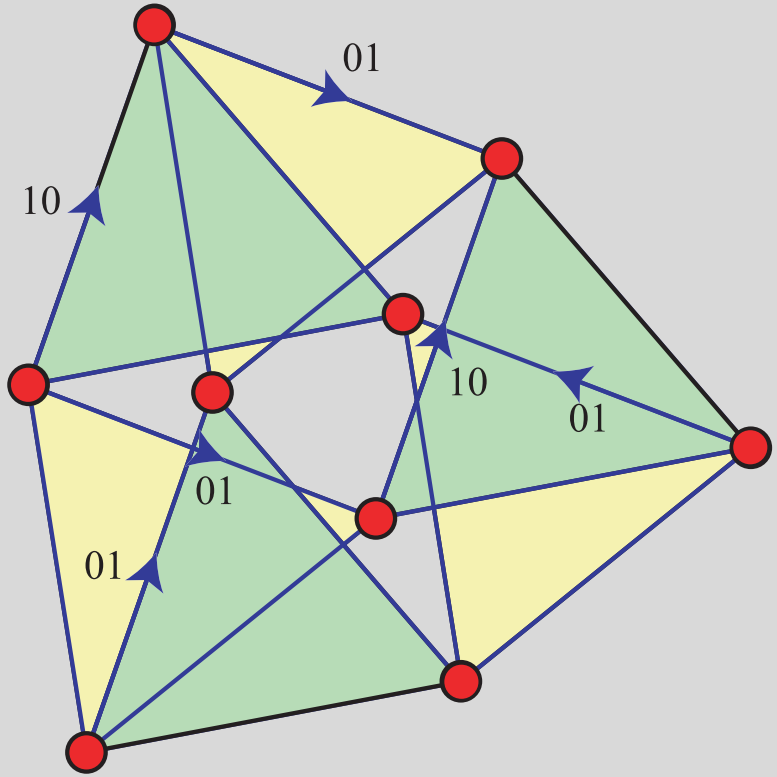


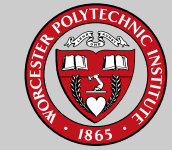
9. A geometric approach



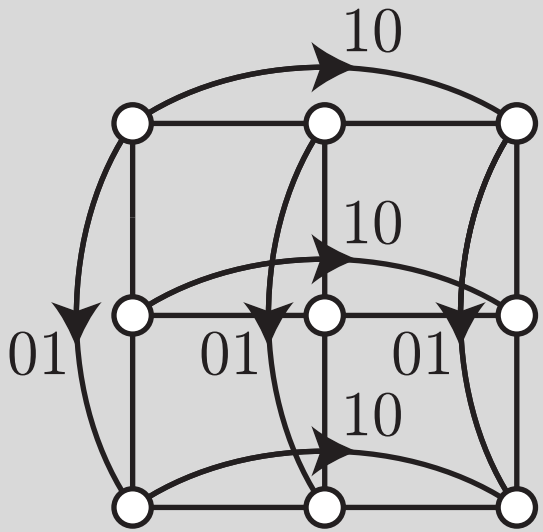


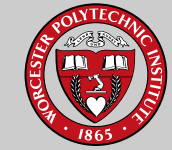
Combinatorial version of the gain graph



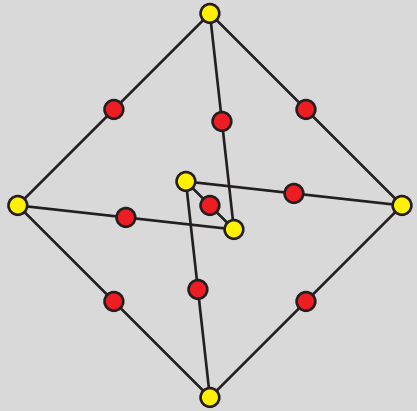


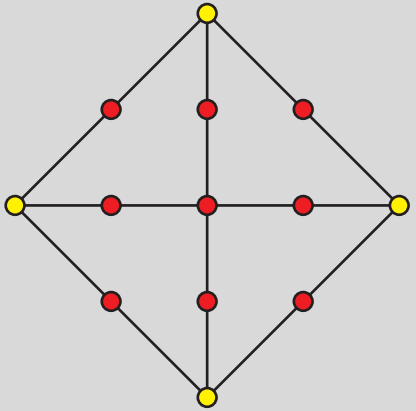
Geometric version of the gain graph

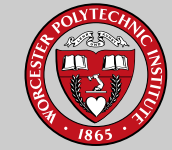




It's a geometric line graph!

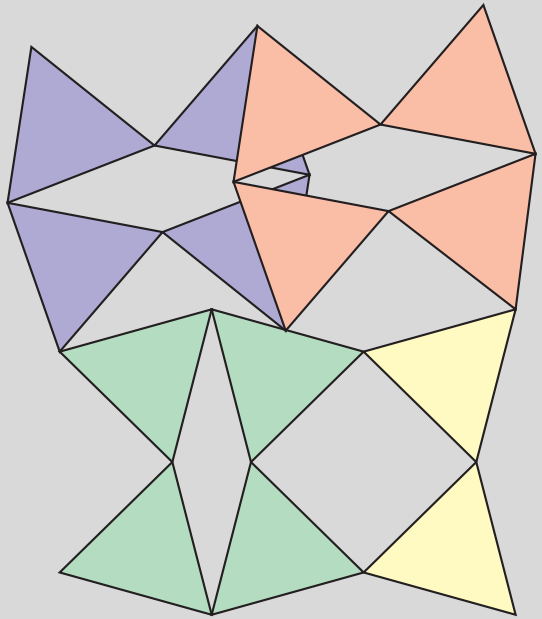


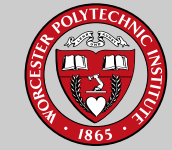




Harbort's construction of a 2-d zeolite without triangular holes

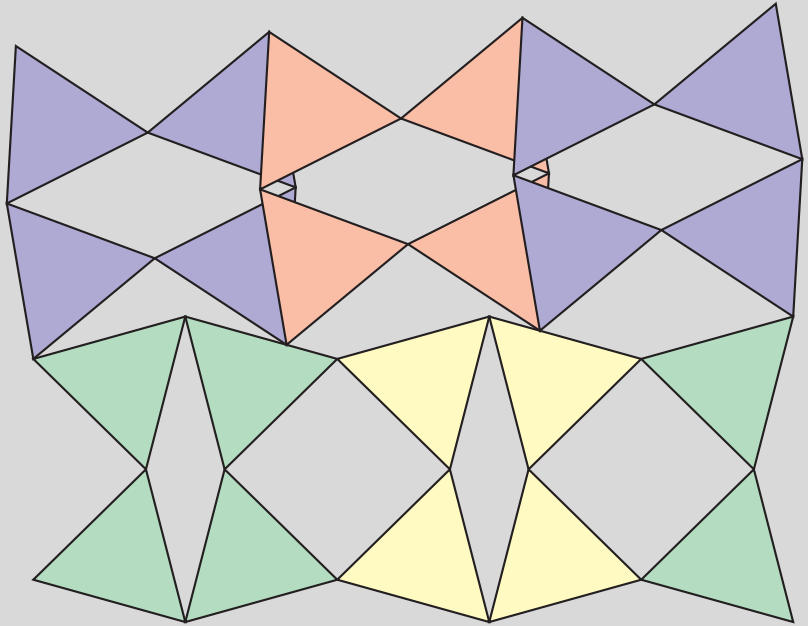
Strip 02

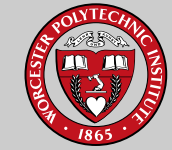




Harbort's construction of a 2-d zeolite without triangular holes

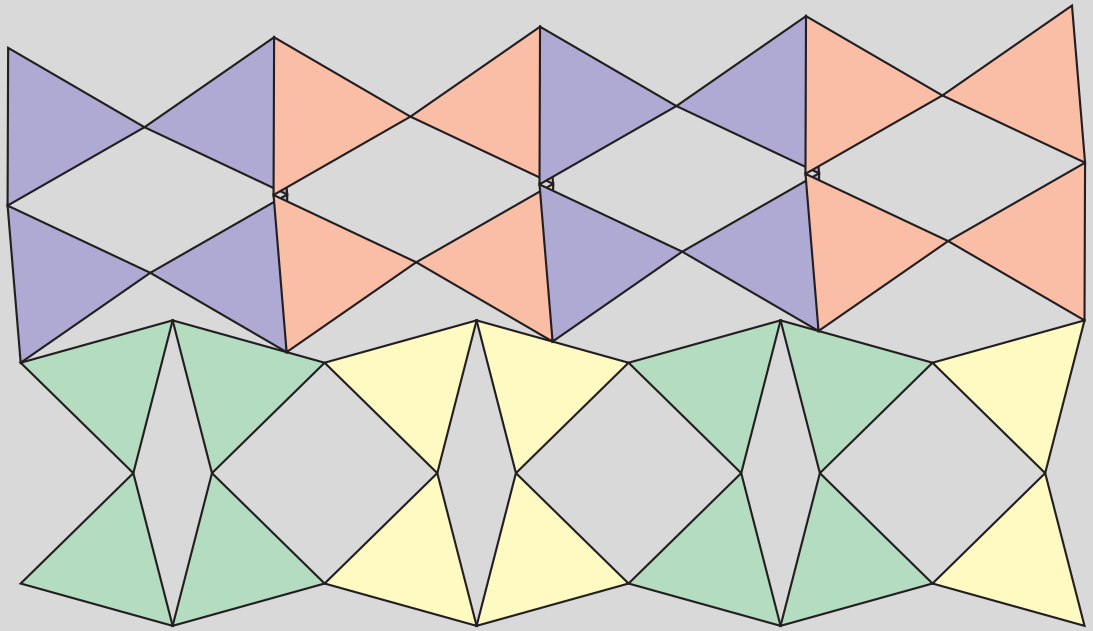
Strip 04

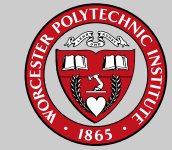




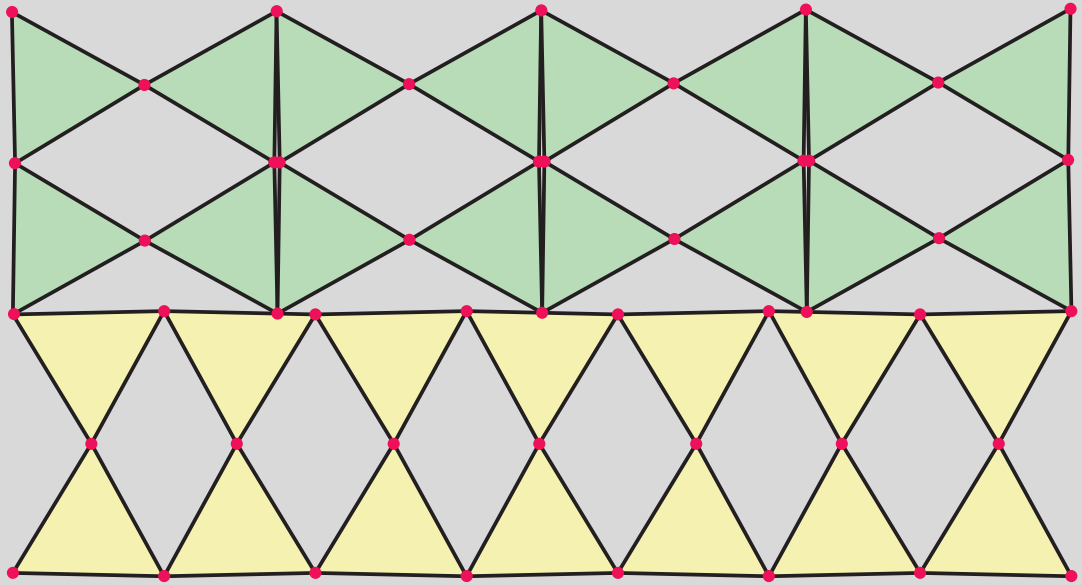
Harbort's construction of a 2-d zeolite without triangular holes

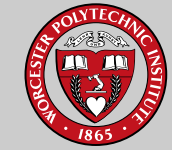
Strip 06





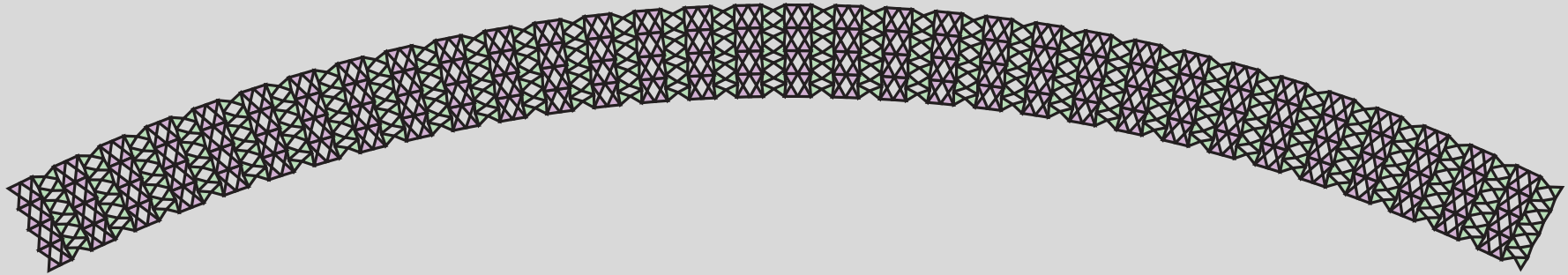
Harbort's construction of a 2-d zeolite without triangular holes



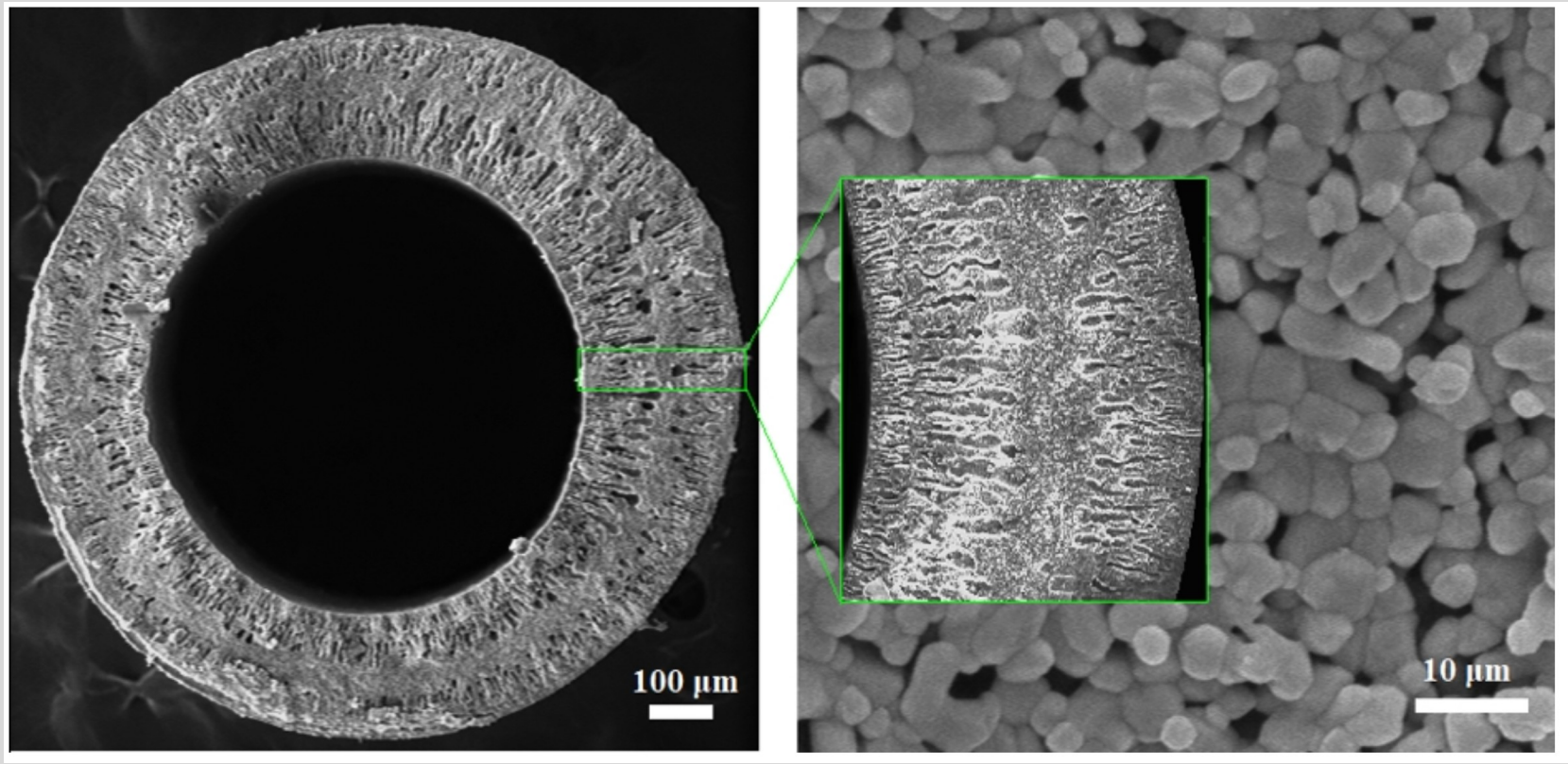


Harbort's construction of a 2-d zeolite without triangular holes

Ring



The smallest possible ring graph has 3800 triangles [3]. Subsequently the 2-layer Zeolite has 7600 tetrahedra!



[6]

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