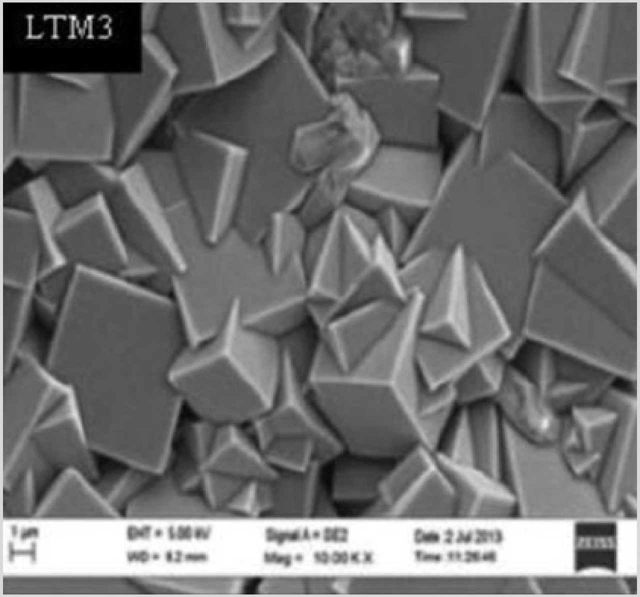
On saturated bi-layered disk shaped tetrahedral packings

Brigitte Servatius — WPI



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.

Curcumin nanodisks: formulation and characterization

Ghosh, M., Singh, A. T., Xu, W., Sulchek, T., Gordon, L. I., and Ryan, R. O. (2011)
Nanomedicine: nanotechnology, biology, and medicine, 7(2), 162167.
https://doi.org/10.1016/j.nano.2010.08.002

A process for synthesizing bilayer zeolite membranes

From the abstract [6]

A silicalite/mordenite bilayered self-supporting membrane with disc-shape was synthesized from a layered silicate, kanemite by two steps using solid-state transformation.
The mechanical strength (compression strength) of the membrane was greater than $10\frac{kg}{cm^2}$. Both sides of the membrane were much different in the morphology and SiO_2/Al_2O_3 ratio. One side (silicalite side) consisted of the intergrowth of prism-like crystals (ca. 12 μm), while the other side (mordenite side) was composed of scale-like crystals (ca. $> 1\mu m$).

Gas separation with zeolite membranes

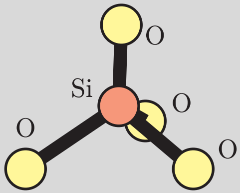
In [9] it is described how Zeolite membranes can be used to separate gases. Membrane technology constitutes an increasingly important, convenient, and versatile way of separating gas mixtures. Zeolite membranes are known to have high permeabilities in gas separations. Due to the well-defined pore structures, zeolite membranes can also offer high selectivities. In addition, zeolite-based membranes have high chemical, mechanical, and thermal stability, i.e. can potentially be used at both very high and very low temperatures, offering a great advantage over polymeric membranes.

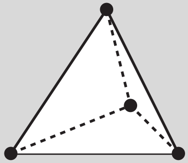
Mildred Dresselhaus (1930-2017), the queen of carbon science. Her research has been instrumental in the development of the nanotechnology field.

Mildred S. Dresselhaus holding a model of a carbon nanotube. Credit: Ed Quinn

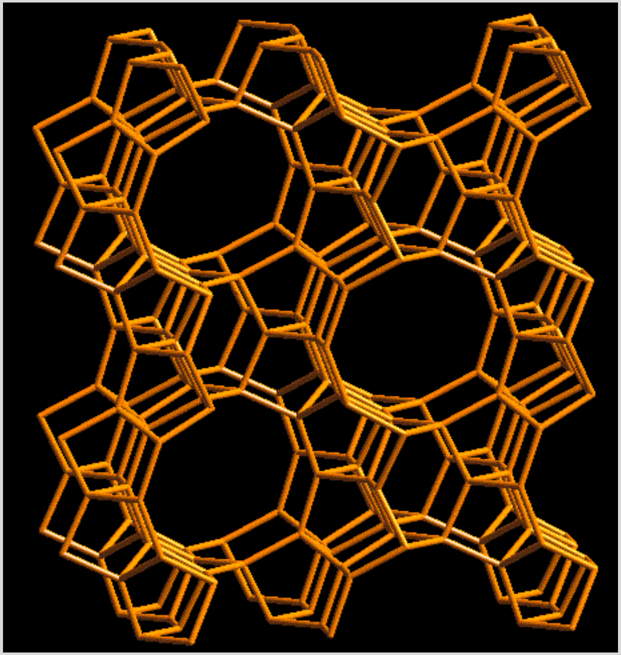
1. Chemical Zeolites

- crystalline solid
- units: Si + 4O





- two covalent bonds per oxygen



- naturally occurring
- synthesized
- theoretical

Used as microfilters.

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

[8](1932) proved that connected graphs X on at least 5 vertices are strongly reconstructible from their line graphs $L(X)$. Moreover, $Aut(X) \cong Aut(L(X))$.

3. Realization

A realization of a d-dimensional zeolite

A placement (embedding) of the vertices of 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

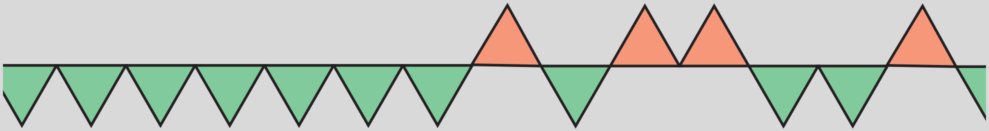
A realization where all edges join vertices distance 1 apart in $\mathbb{R}^d$.

non-interpenetrating realization

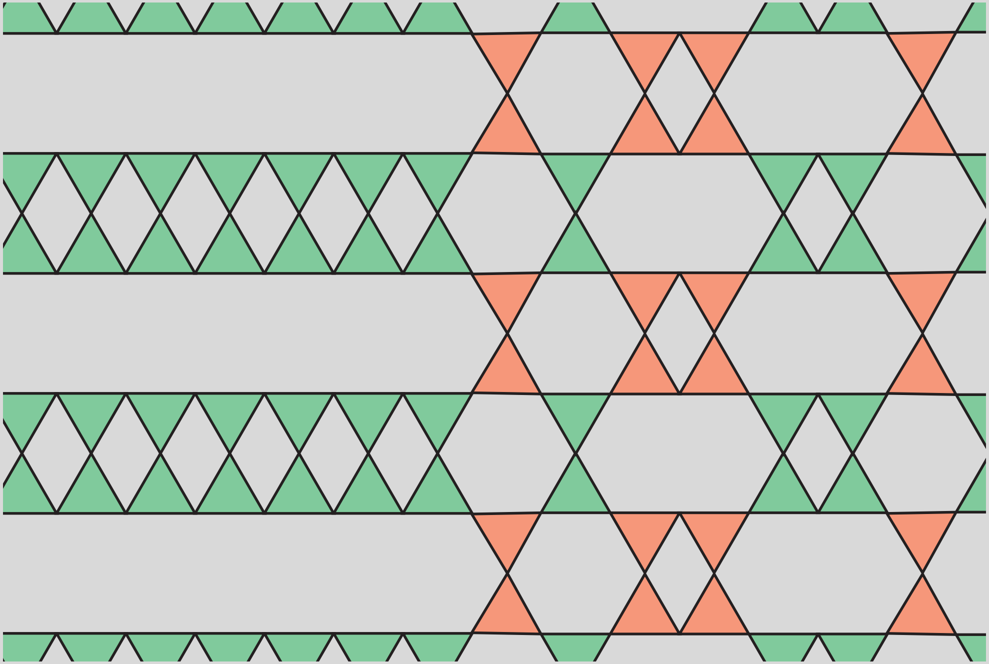
A realization where simplices are disjoint except at joined vertices.

The Layer Construction

The Layer Construction

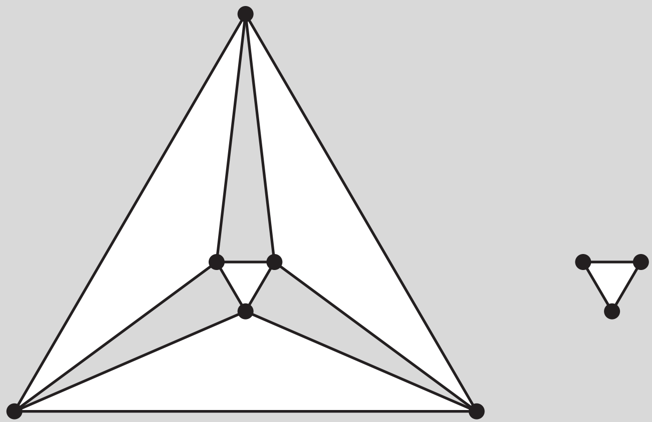


The Layer Construction



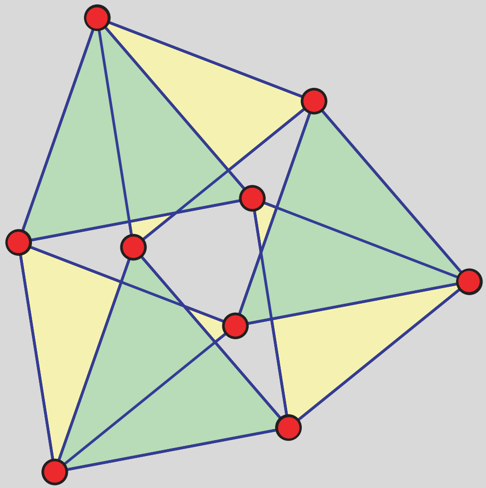
Finite 2d Zeolites

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.

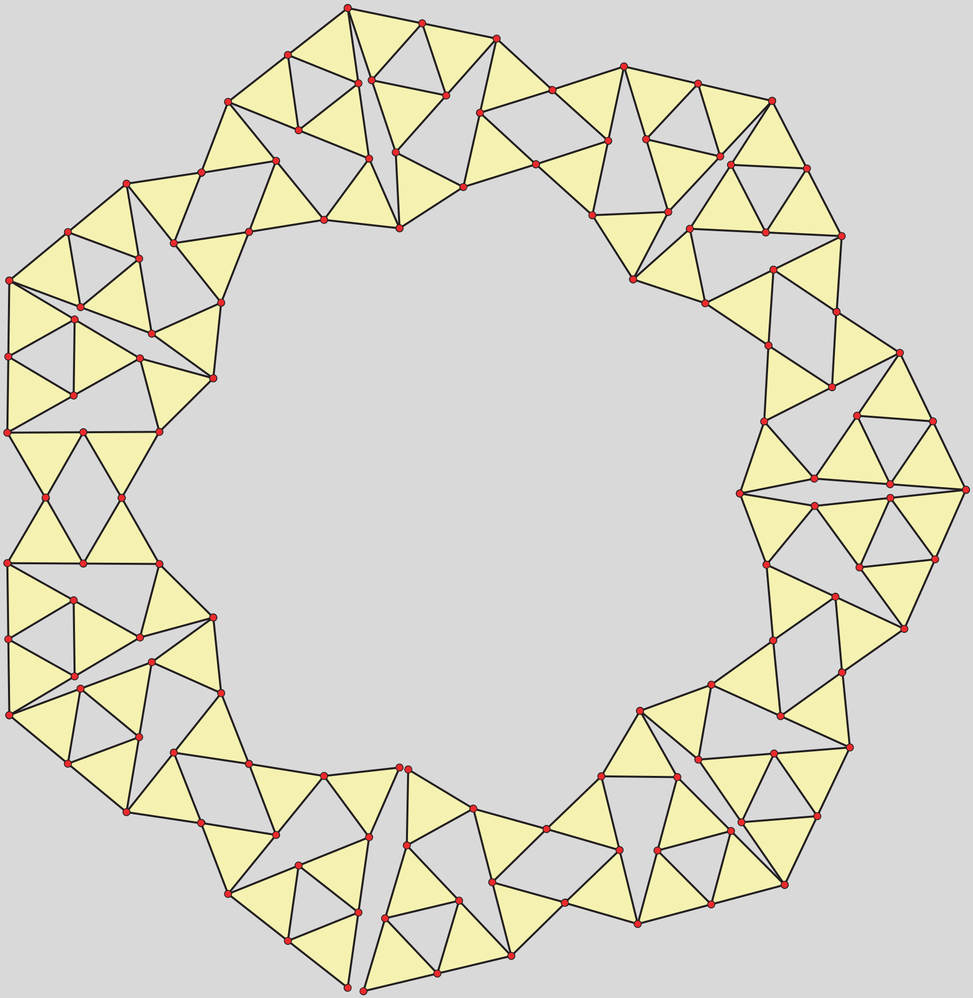


4. Finite 2d Zeolites

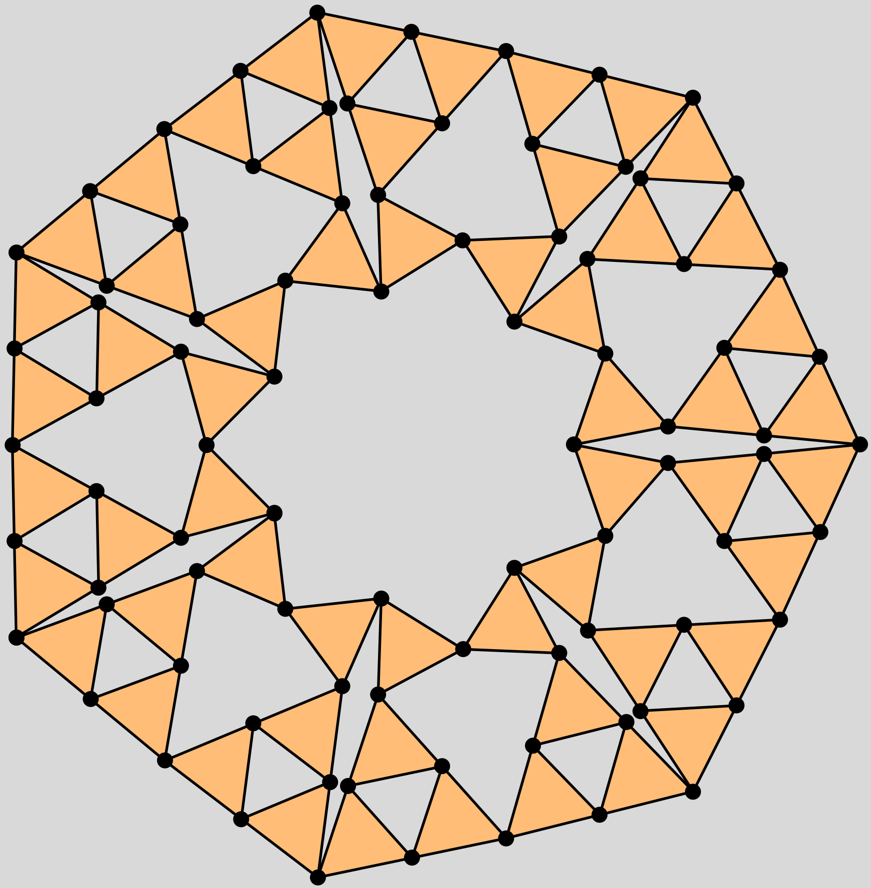
Body pin graph: $K_{3,3}$. Since the body pin graph is not planar, the resulting zeolite cannot be planar. Its underlying graph is generically globally rigid. However, it has a unit distance realization in the plane which is a mechanism.



The typical situation: Not unit distance realizable.

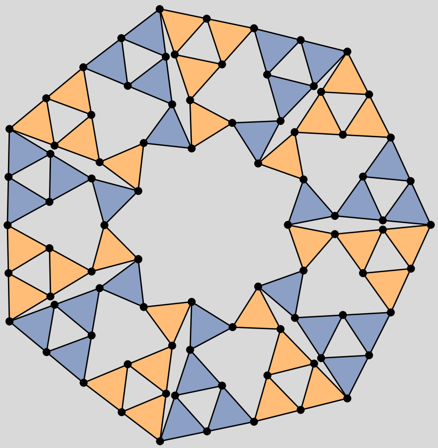


Harborth's Example [4, 3]



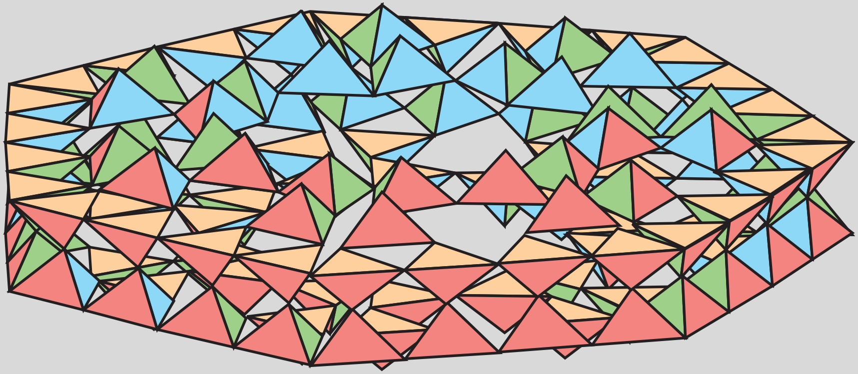
The Layer Construction

$Z = (T, C)$ 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 $\mathbb{R}^{d+1}$.

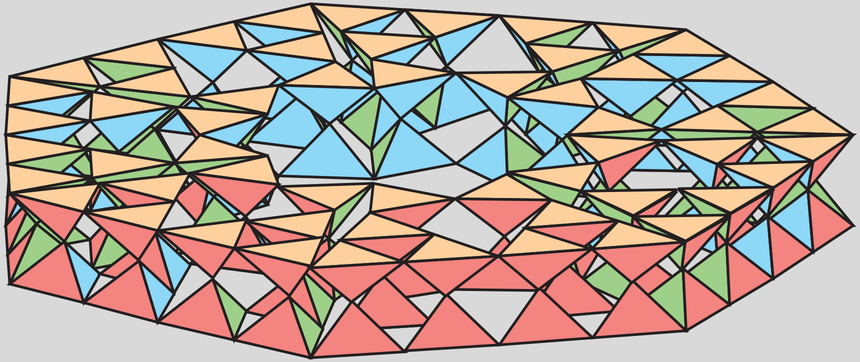
The general case starting from a finite zeolite.



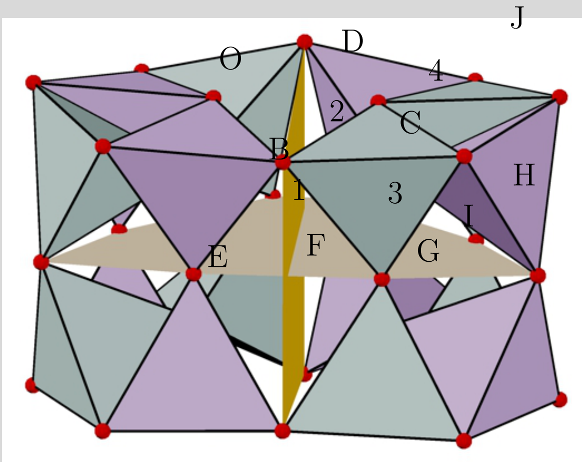
Theorem: There are uncountably many isomorphism classes of unit distance realizable zeolites in $\mathbb{R}^3$.
(actually in any dimension $d > 1$. [7])

5. Disk shaped zeolite

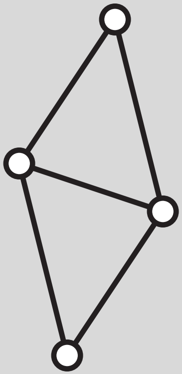
Labels all +1
A two layered zeolite.

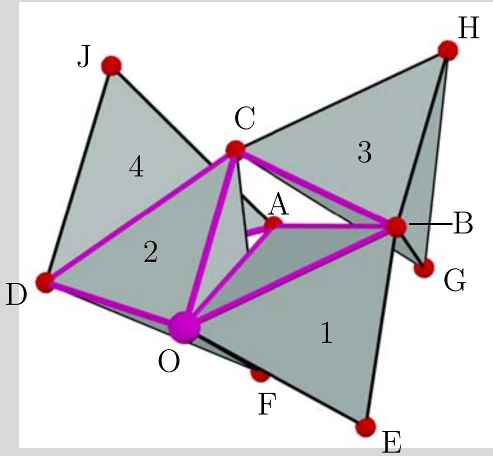


A finite 3-D symmetric example:



Model with its two planes of symmetry

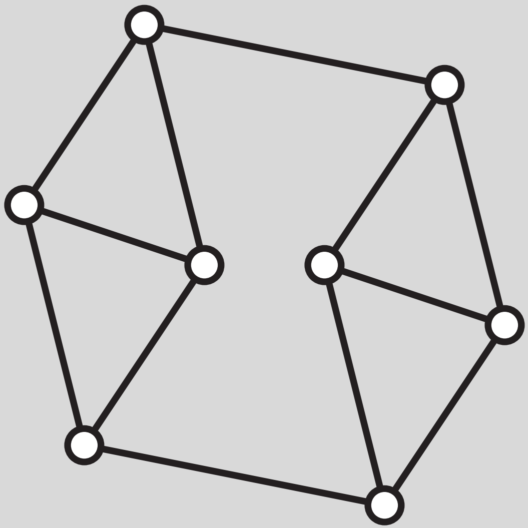




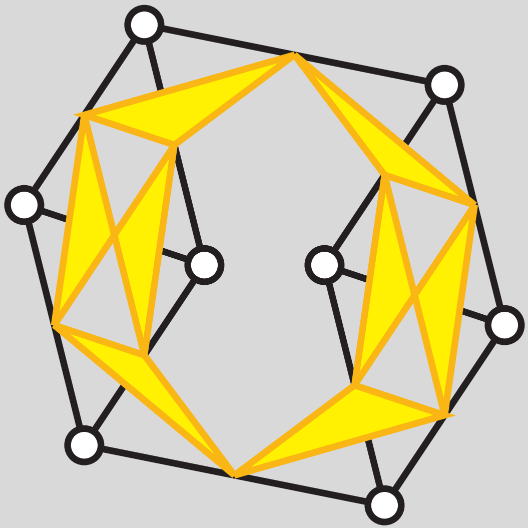
[1]

This 16 Tetrahedra model of Harborth and Möller can be thought of as a bi-layer.

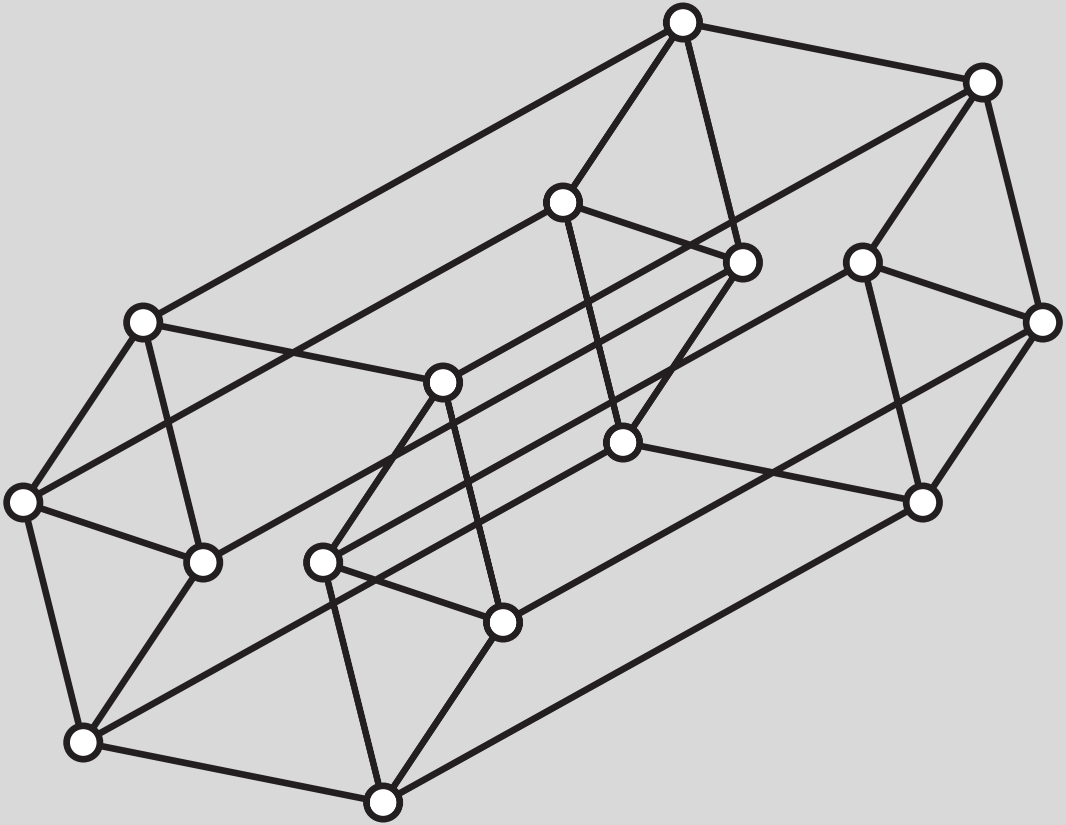
A 3-regular graph



A 3-regular graph with line graph



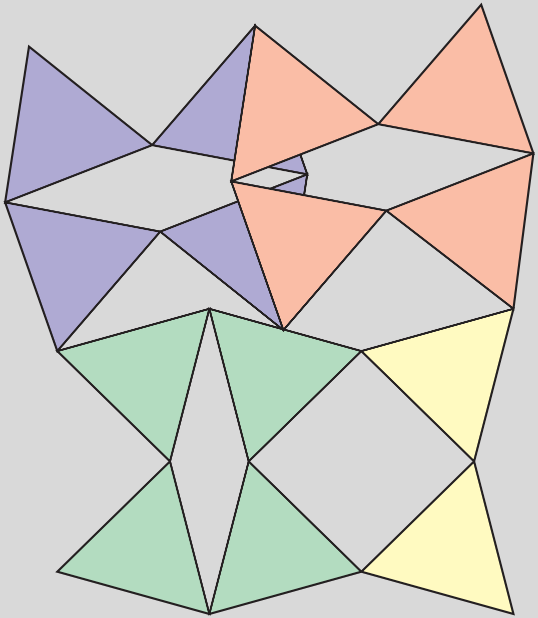
The Harboth-Möller model



The body pin graph of the Harborth-Möller Model.

Excluding triangular holes

Strip 02



Chemical Zeolites
Combinatorial . . .
Realization
Finite 2d Zeolites
Disk shaped zeolite
Holes in Zeolites
Motions
Vertex transitive . . .

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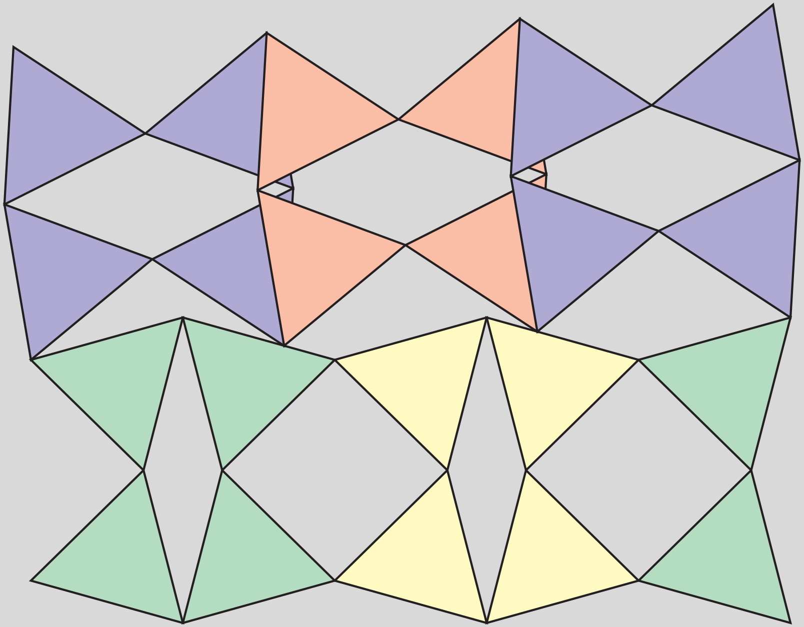
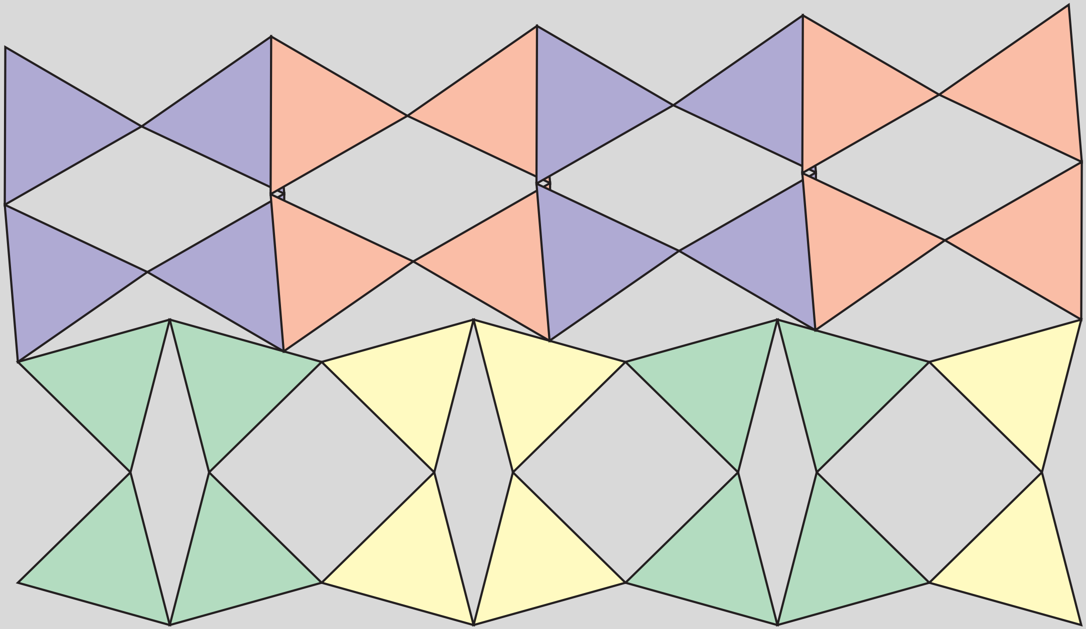
Strip 04

Excluding triangular holes

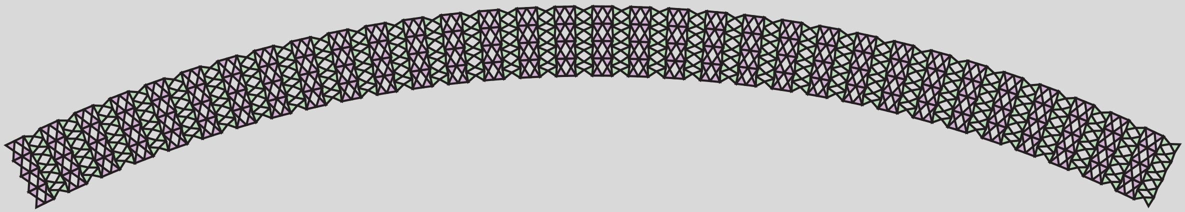


Excluding triangular holes

Strip 06



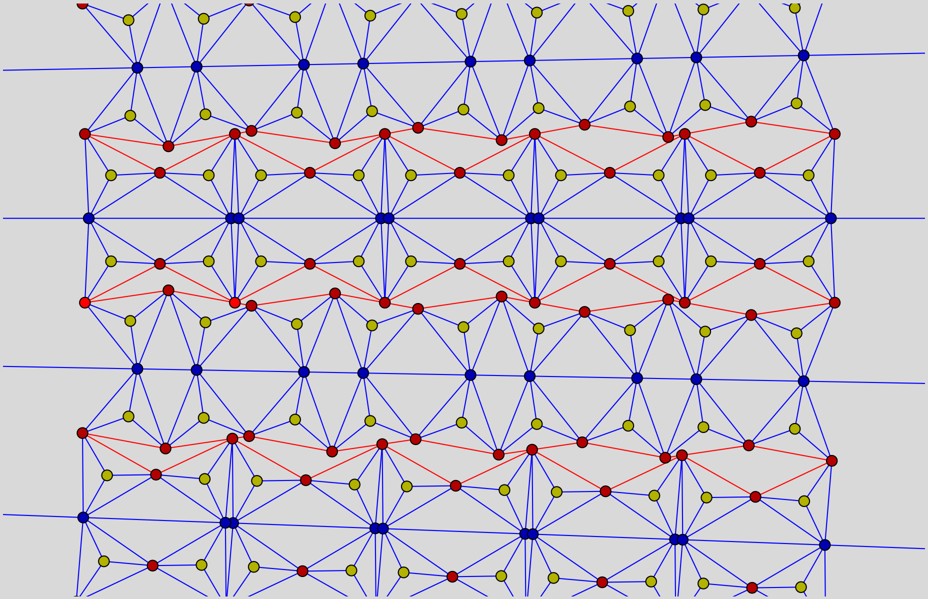
Ring



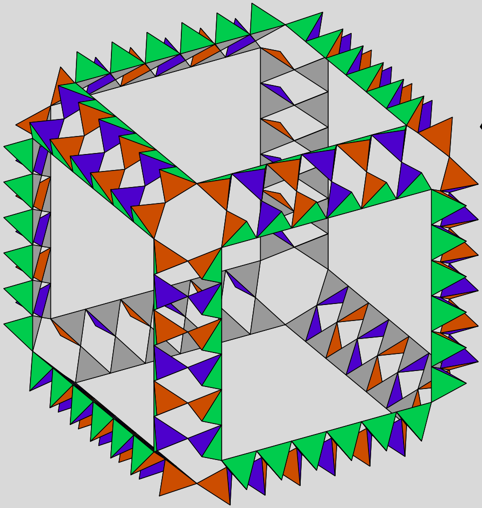
Harborth [2] showed that the number of triangles in a ring graph is at least 3800.

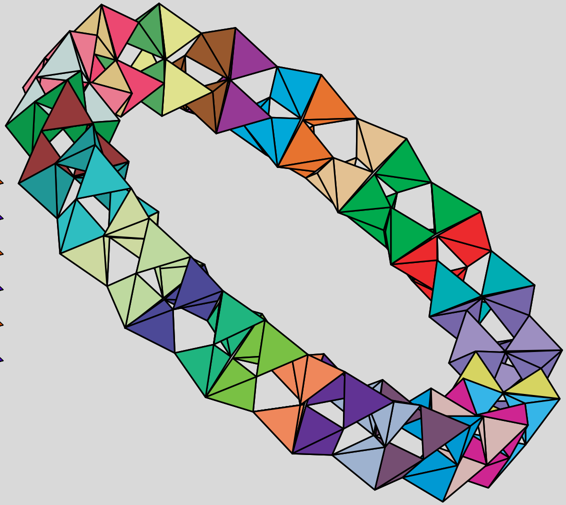
Ring bilayer

Does it move?



6. Holes in Zeolites

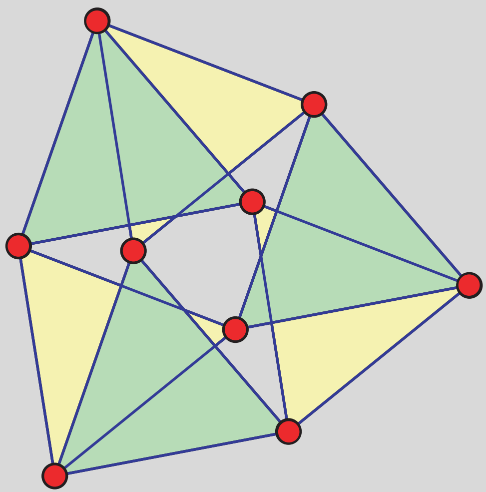




7. Motions

Degree of Freedom

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



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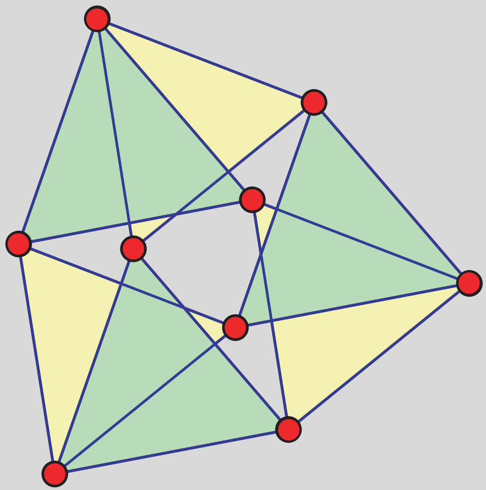
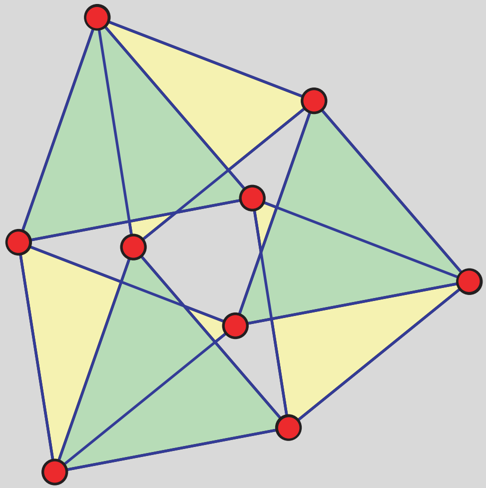
Generically globally rigid in the plane.

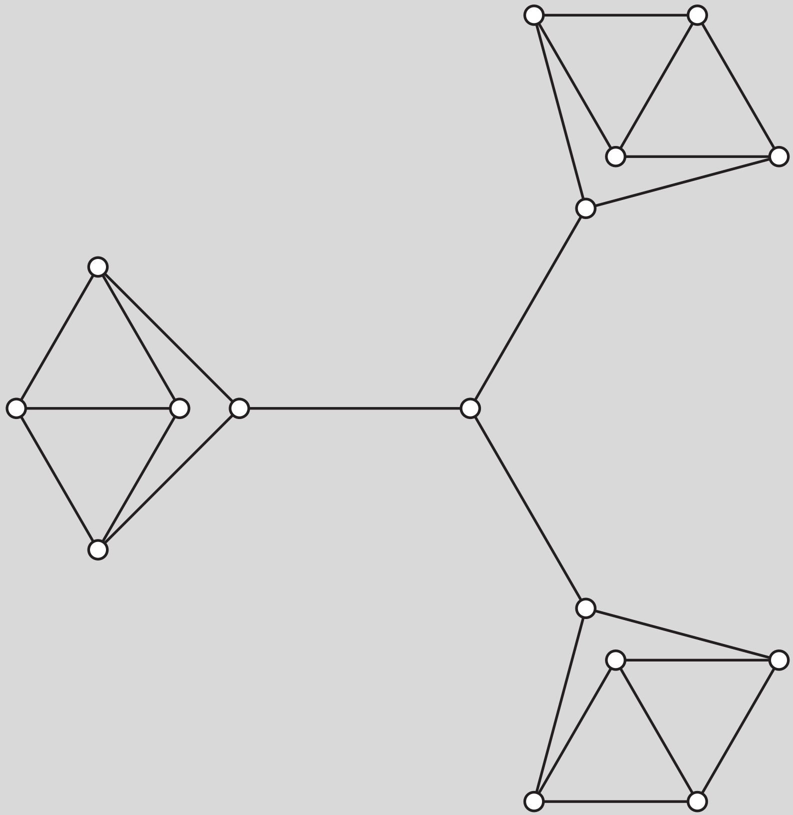


Generically globally rigid in the plane.

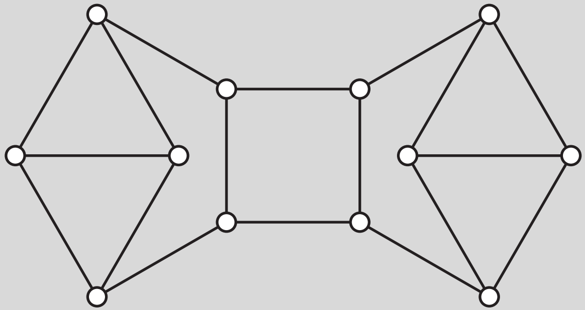
A 4-regular vertex transitive graph is globally rigid unless it has a 3-factor consisting of s disjoint copies of K_4 with $s \geq 3$. [Jackson, S, S – 2004]



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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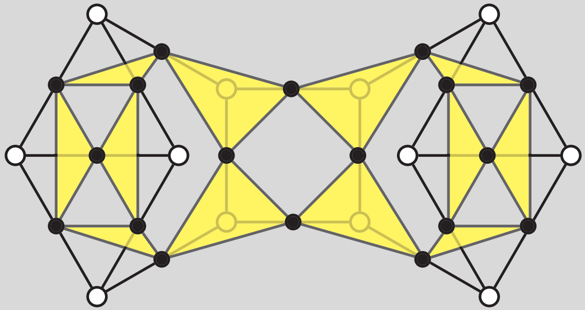
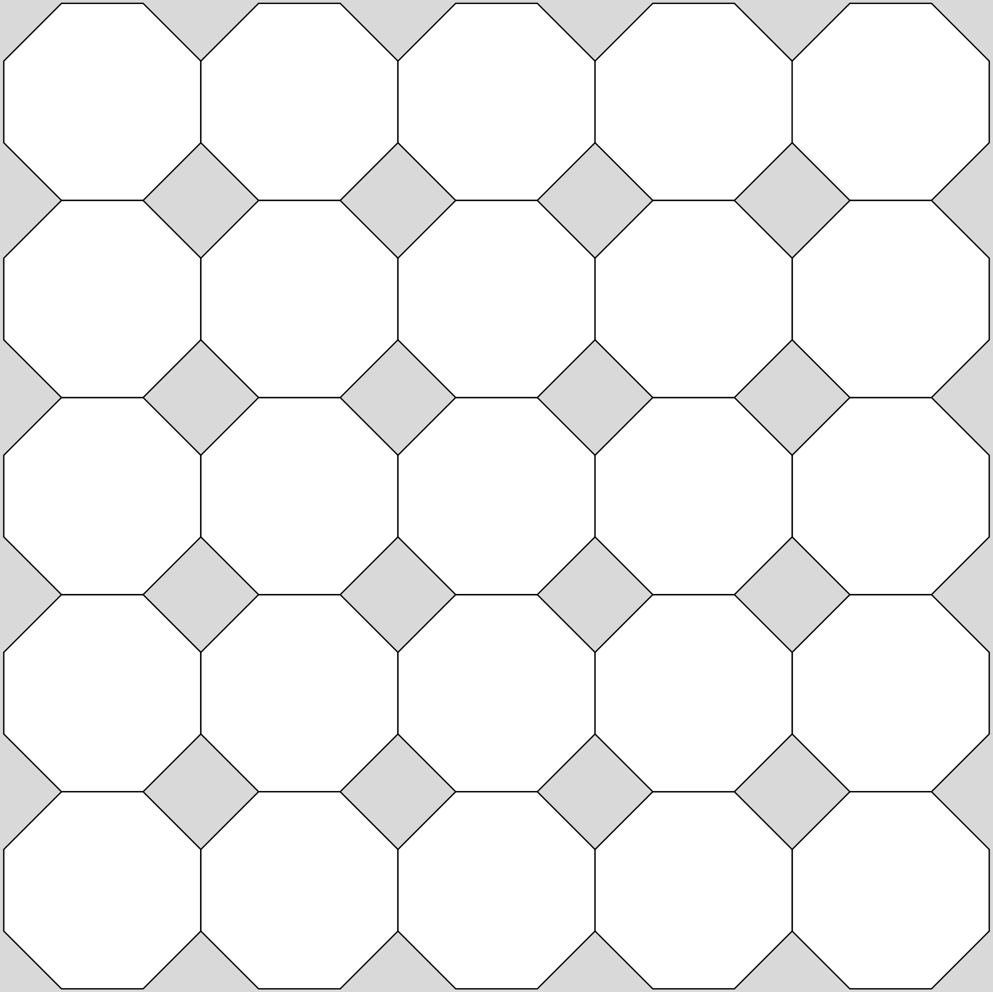
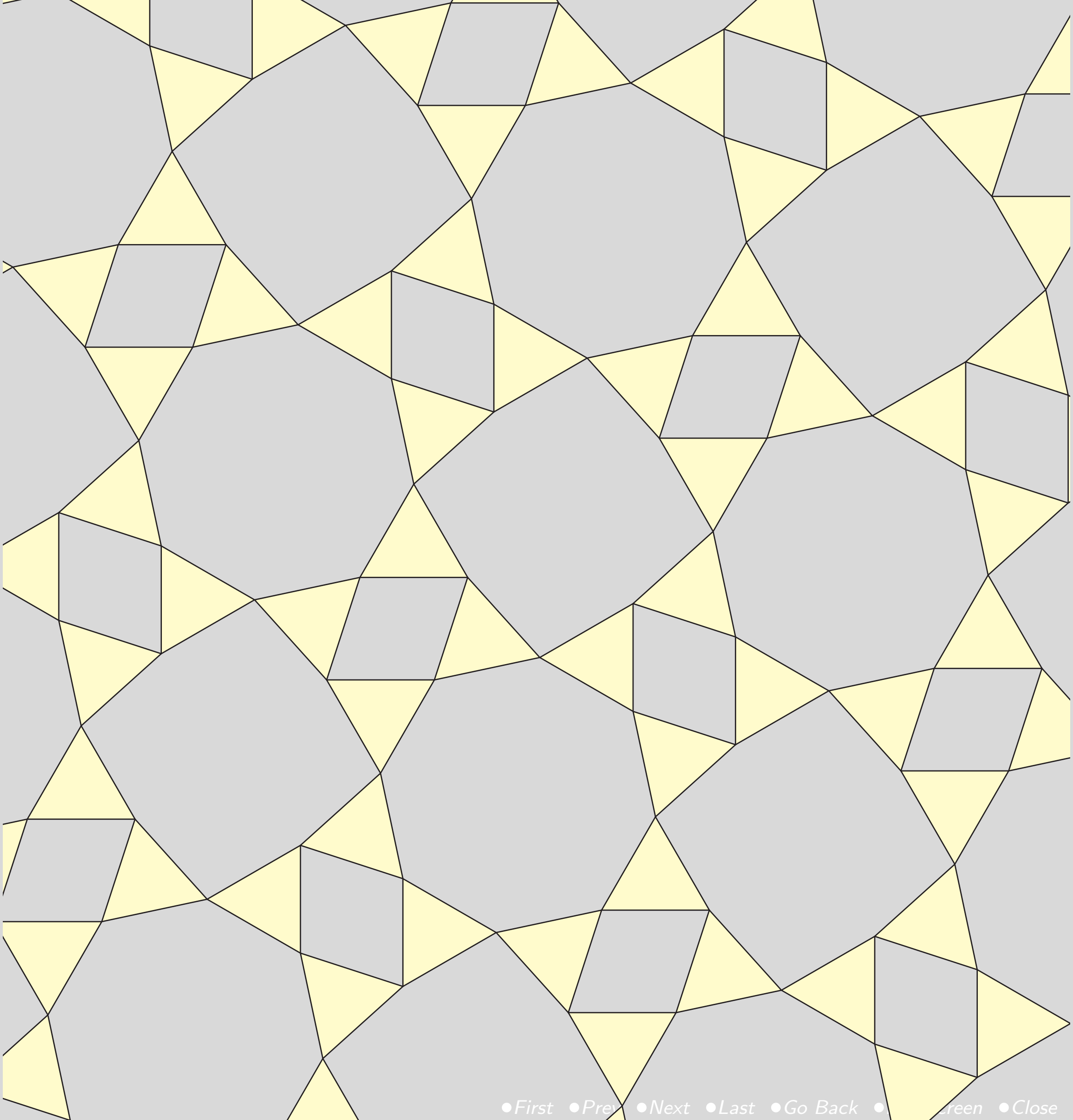
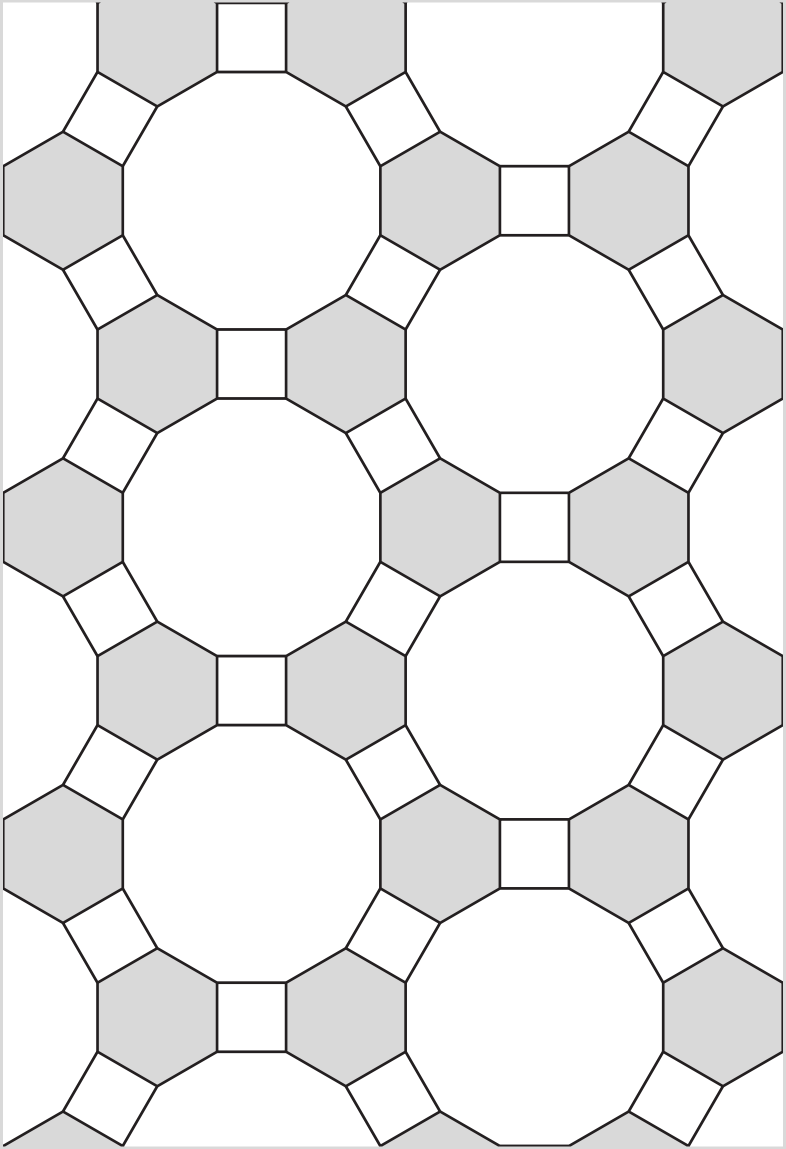


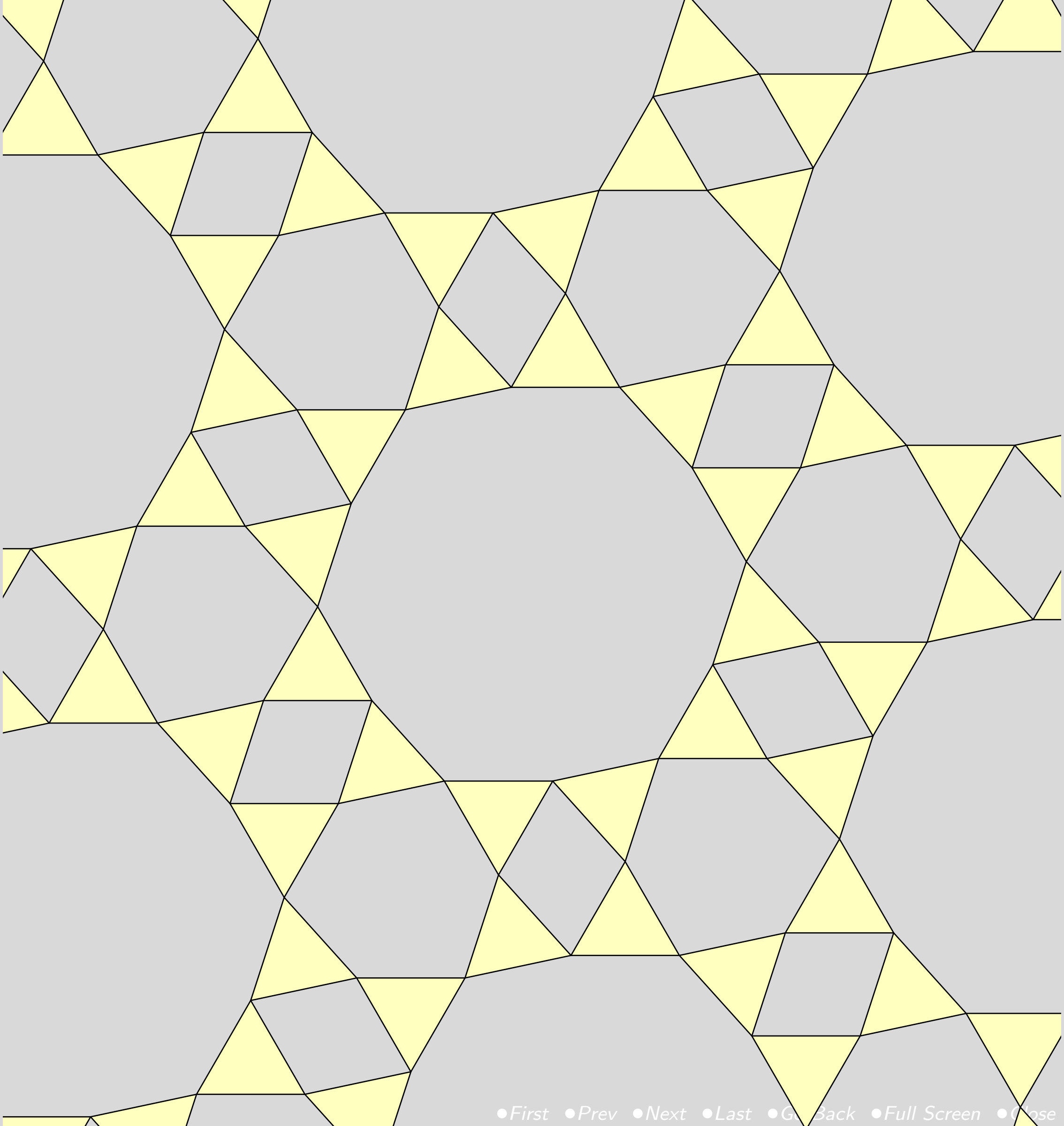
See [5]

8. Vertex transitive 3-regular

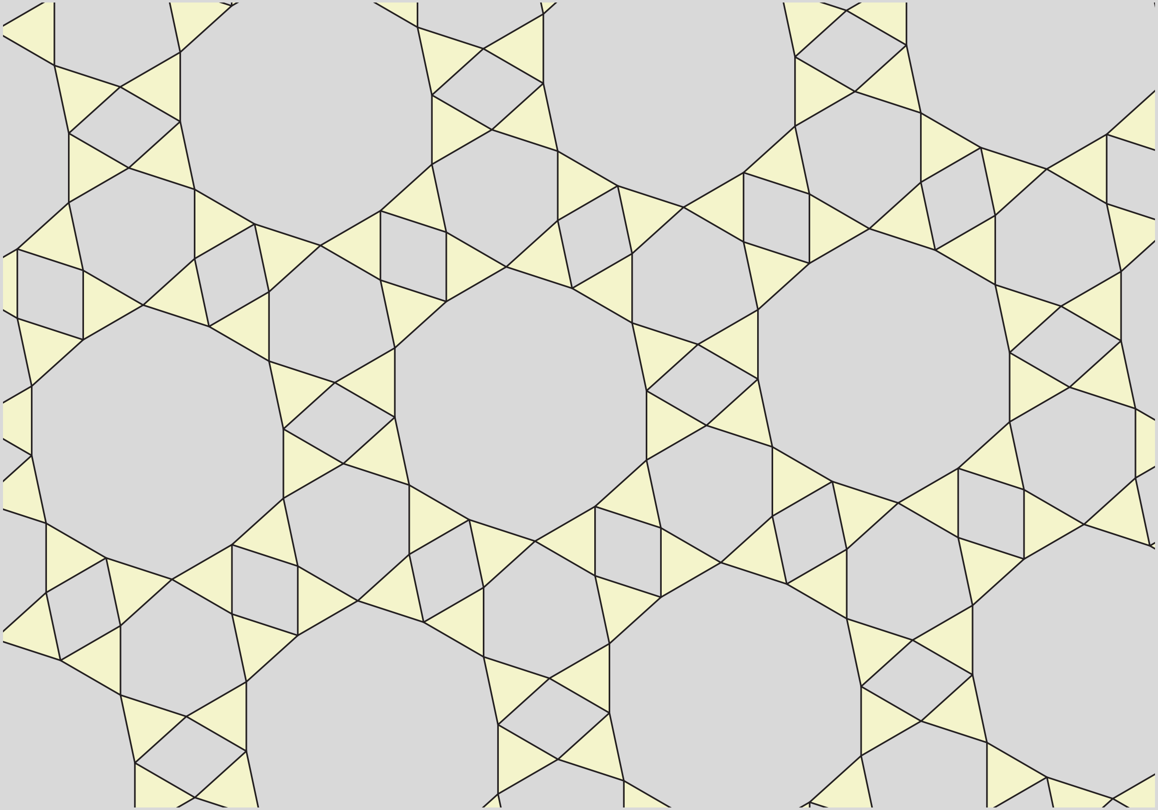








Design nano lentils and prove their realization



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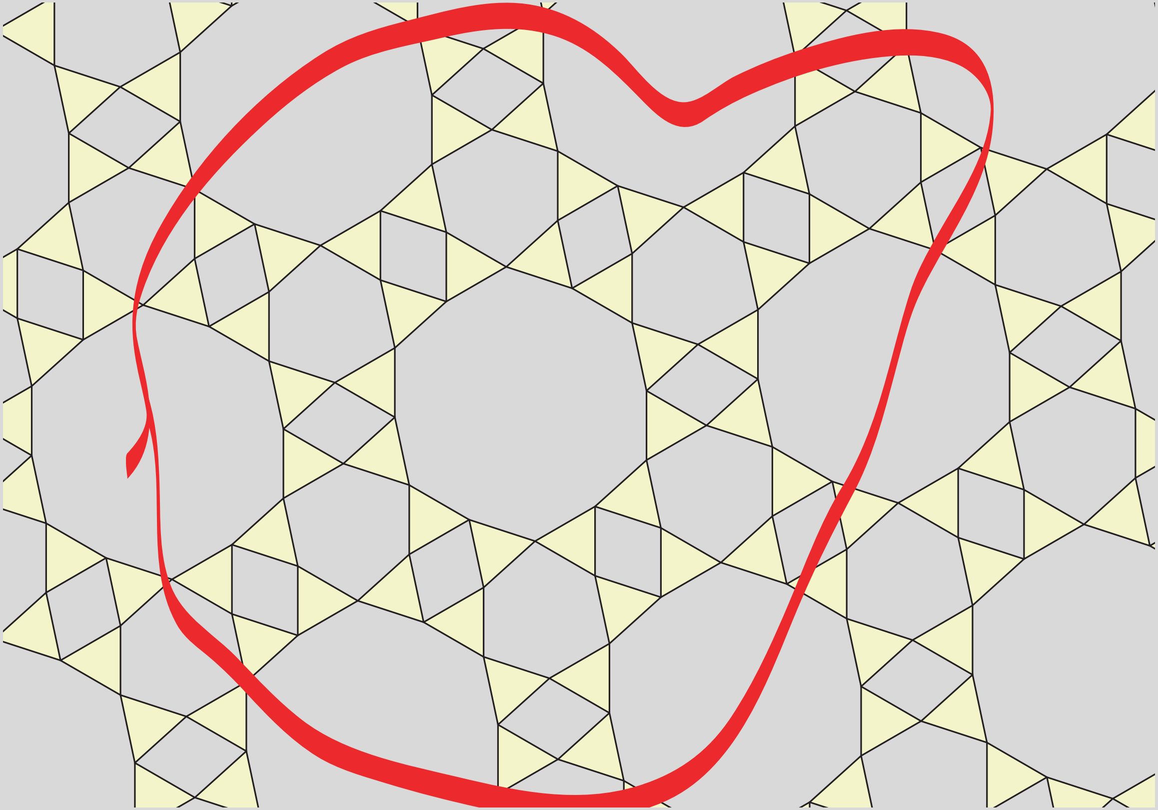

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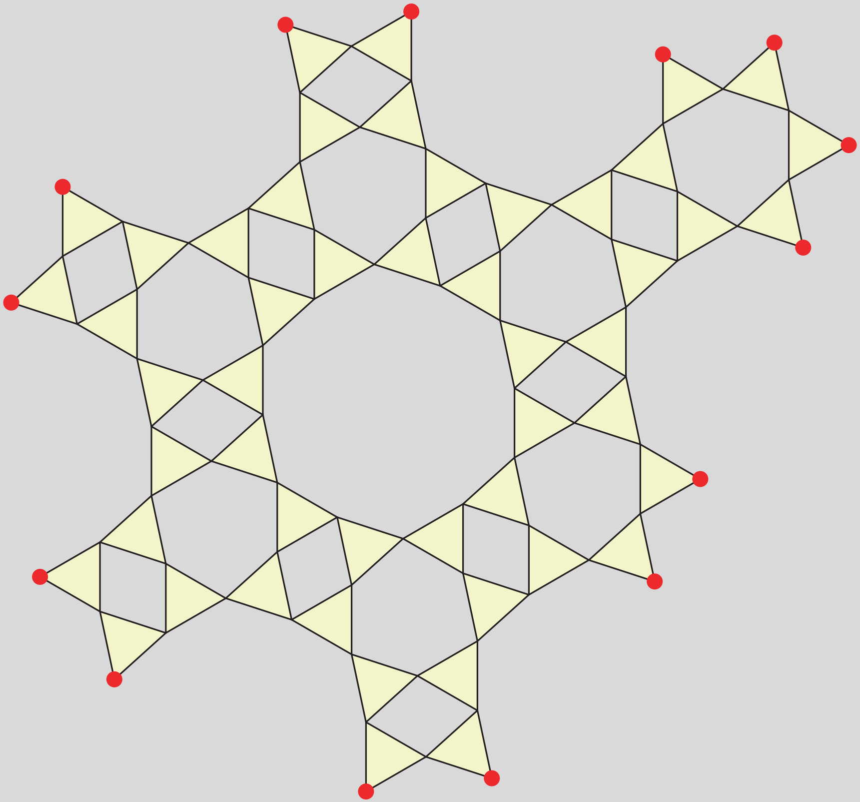

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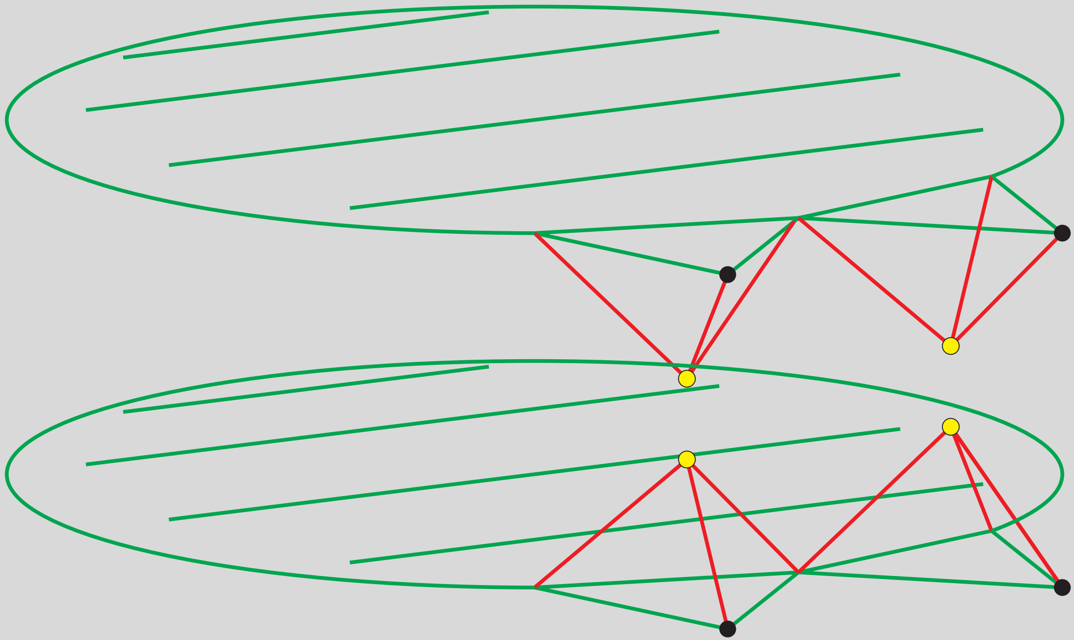

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[6] Y. Kiyozumi, T. Nagase, Y. Hasegawa, and F. Mizukami, *A process for synthesizing bilayer zeolite membranes*, Materials Letters - MATER LETT, 62 (2008), pp. 436–439.

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