The Combinatorics of Shape and Motion

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Worcester Polytechnic Institute, May 2018

Abstract

Molecules are often modeled as bar-and-joint frameworks in 3-space. While bar-and-joint frameworks are well understood combinatorially as well as goemetrically in the plane, there are many open problems in 3-space Some nice toy research problems accessible even to (high school) students are based on Dill's HP-model Zeolites provide yet another interesting set of examples illustrating the gap between their combinatorial and geometric properties

References

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2. P. Fazekas, O. Röschel, and B. Servatius. *The kinematics of a framework presented by H. Harborth and M. Möller.* Beitr. Algebra Geom., 54(1):201–209, 2013.
3. Jack Graver, Brigitte Servatius, and Herman Servatius. *Combinatorial rigidity*, AMS, 1993.
4. Naoki Katoh and Shin-ichi Tanigawa. *A proof of the molecular conjecture.* Discrete Comput. Geom., 45(4):647–700, 2011.
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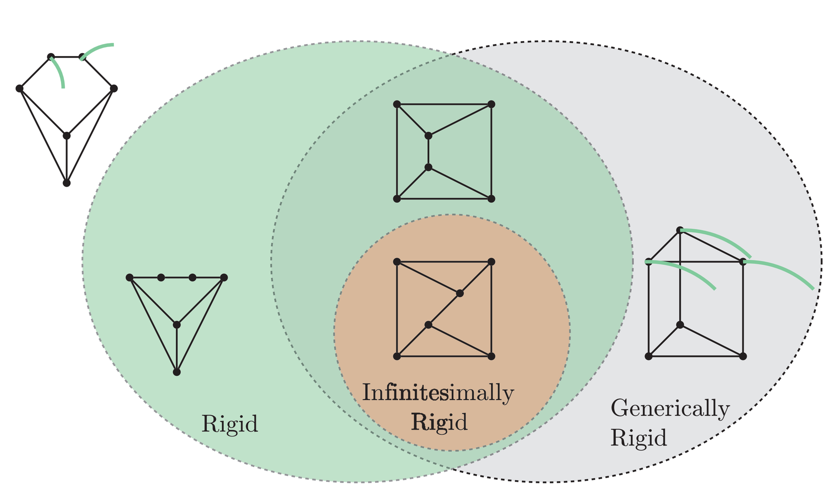
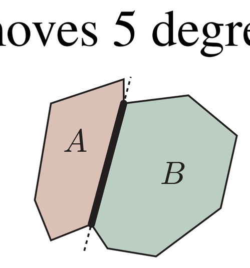
Rigidity



(Generic) Body and Hinge Frameworks in 3–Space

- Each rigid body has 6 degrees of freedom.
- If two bodies are joined along a linear hinge the resulting structure has one internal degree of freedom.
- Each hinge removes 5 degrees of freedom.



- Graph $G=(B,H)$
- B: vertices for abstract bodies,
- H: for pairs of bodies sharing a hinge.
- Necessary condition for independence:

$$5|H'| \leq 6|B'| - 6$$

- Theorem: (Tay and Whiteley – 1984) The necessary condition is also sufficient for generic independence.

Algorithms:

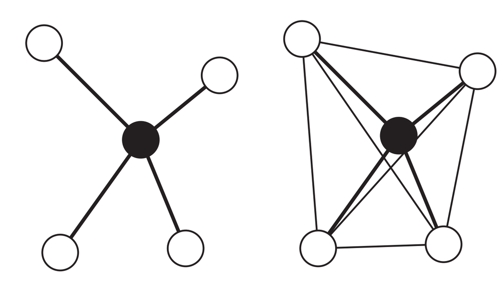
$$6|B'| - 6 = 6(|B'| - 1)$$

or

6 spanning trees in $5G(B,H)$, which is the multi-graph obtained from $G(B,H)$, by replacing each edge by a set of 5 parallel edges.

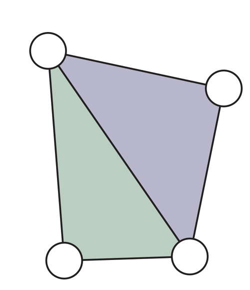
Modeling molecules

Can we predict rigidity for special graphs?
Single atom and associated bonds:



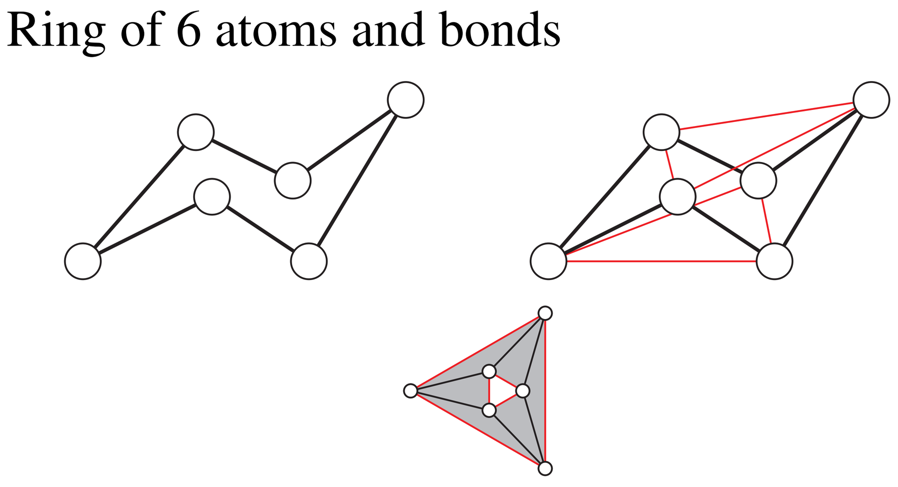
$|V| = 5$ $|E| = 10$
$|E| = 3|V| - 5$ overbraced

Adjacent atom clusters
When are they Flexible?



$|B| = 2, |H| = 1,$ $5|H| = 6|B| - 7,$
$|V| = 4, |E| = 5,$ $|E| = 3|V| - 7$

Ring of 6 atoms and bonds



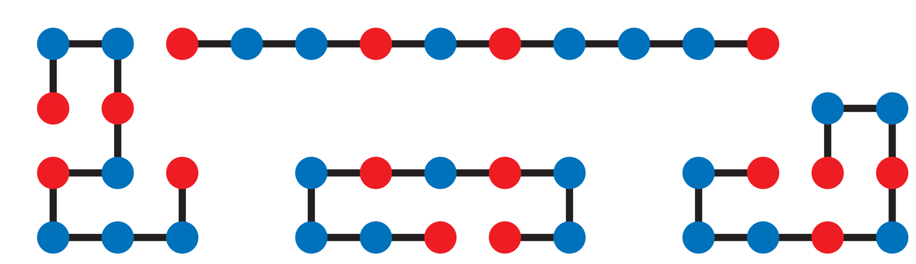
Bar and Joint: $|V| = 6, |E| = 12,$
$|E| = 3|V| - 6$

Body and hinge: $|B| = 6, |H| = 6,$
$5|H| = 6|B| - 6$
Just the right number to be rigid - generically.

Molecular Theorem

The geometric and combinatorial rigidity community focuses on multiple approaches for detecting whether an input set of polynomial equations representing a geometric constraint system (a) has a solution (independence), (b) has continuous paths of solutions (flexibility), (c) has locally isolated solutions (rigidity), or (d) has exactly one solution up to a space of "trivial" transformations in the chosen geometry (global rigidity).

The Molecular conjecture was formulated in 1984 Molecular Theorem (Katoh & Tanigawa 2011) A graph G can be realized as an infinitesimally rigid body-hinge framework in $\mathbb{R}^d$ if and only if it can be realized as an infinitesimally rigid panel-hinge framework in $\mathbb{R}^d$.

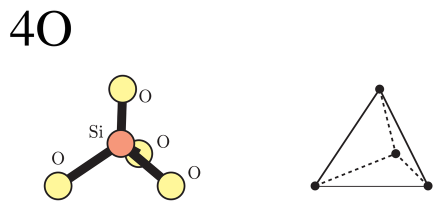


Dill's HP Model of Protein Folding

Zeolites

Chemical Zeolites • crystalline solid

- units: Si + 4O



- two covalent bonds per oxygen

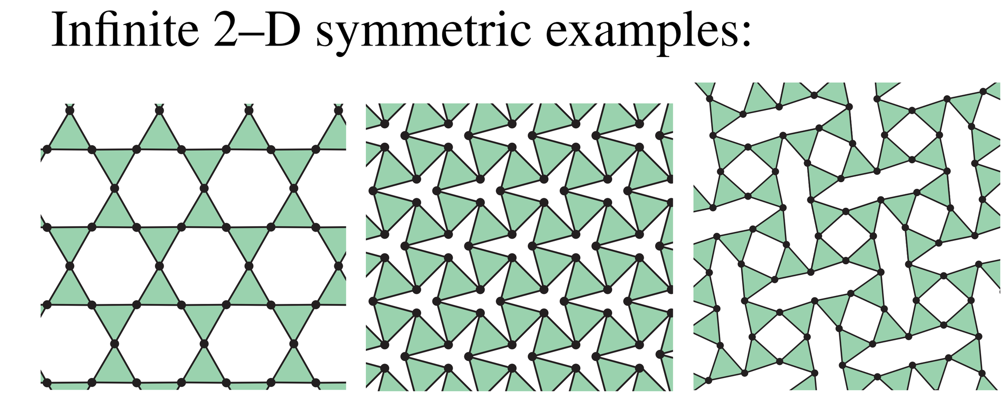
Combinatorial Zeolites • A connected complex of corner sharing d-dimensional simplices

- At each corner there are exactly two distinct simplices
- Two corner sharing simplices intersect in exactly one vertex.

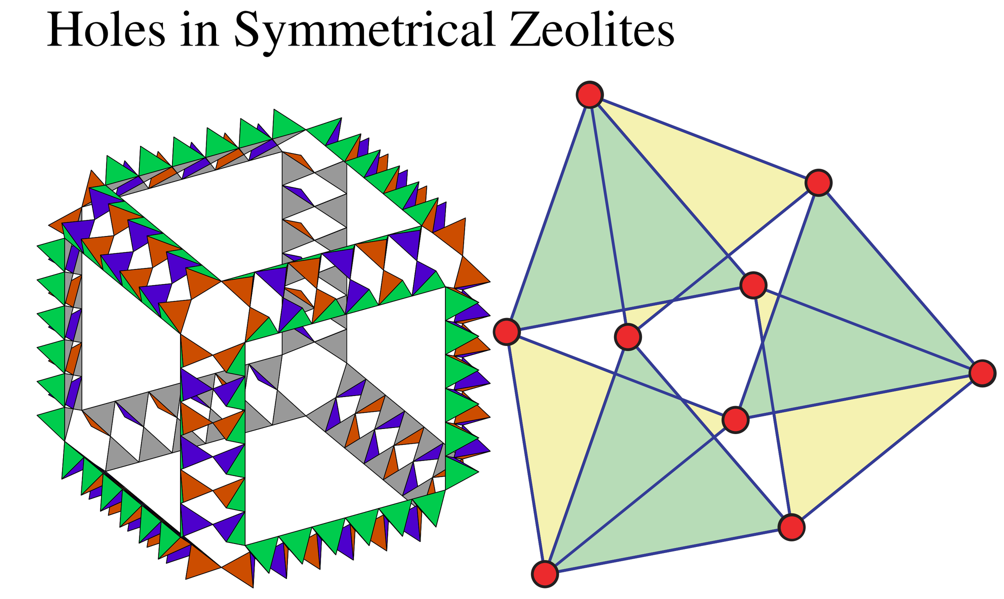
body-pin graph Vertices: simplices (silicon)
Edges: bonds (oxygen)

There is a one-to-one correspondence between combinatorial d-dimensional zeolites and d-regular body-pin graphs.

Infinite 2–D symmetric examples:



Holes in Symmetrical Zeolites



Analyzed Harborth-Möller example (with Peter Fazekas and Otto Röschel)

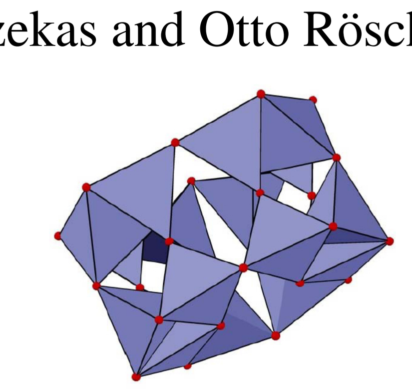


Figure 1: Saturated Packing of 16 tetrahedra

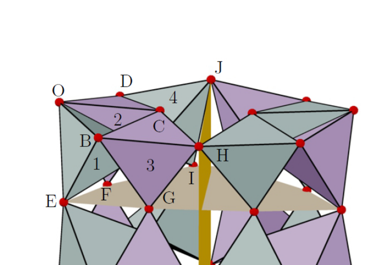


Figure 3: Model with its two planes of symmetry

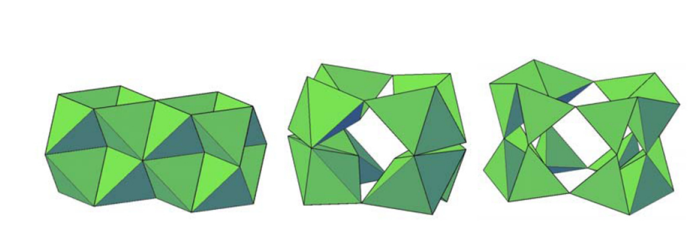


Figure 7: Positions of the model where the channel reaches the minimal and the maximal cross section