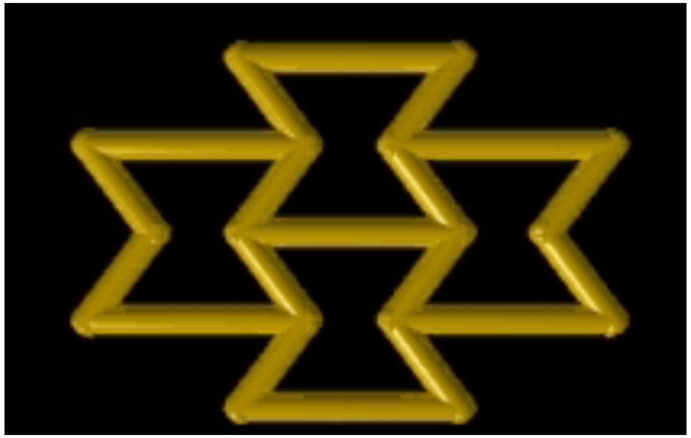

A Geometric Theory of Auxetic Deformations

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Joint work with
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Smith College

Workshop on "Geometric Structures with Symmetry and Periodicity"
Kyoto, June 8-9, 2014

Geometric Auxetics

A geometric theory of auxetic behavior in periodic bar-and-joint frameworks.

Preview of Main ideas

We identify auxetic deformation trajectories by following the variation of the Gram matrix of a basis of periods for a periodic bar-and-joint framework:

Definition: a trajectory is auxetic when all its tangent directions belong to the positive semidefinite cone.

Summary

- Auxetic behavior: a notion related to negative Poisson's ratio in elasticity theory
- Displacive phase transitions in crystalline materials
- Deformation theory of periodic frameworks

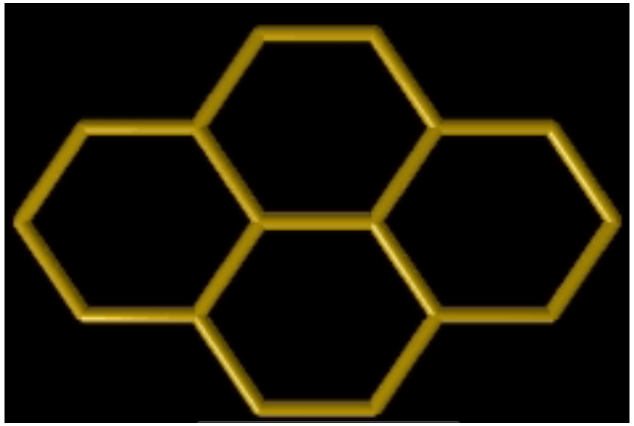
1.Auxetic behavior

Auxetic Behavior

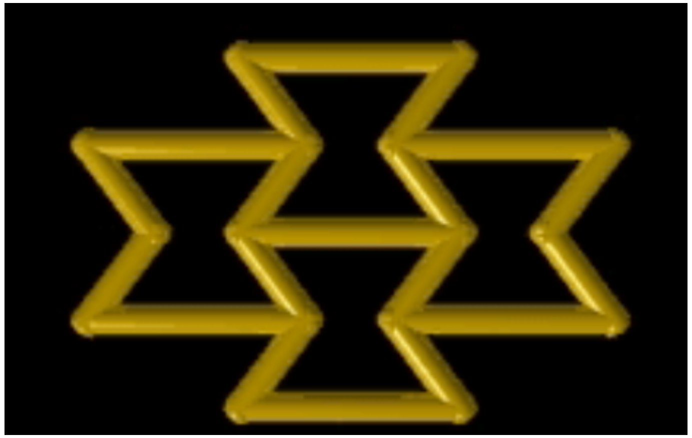
- Concept from elasticity theory.
- Auxetic behavior defined in terms of "negative Poisson's ratio"
- Intuitive "definition":

Given two orthogonal directions, a stretch in the first direction leads to a widening in the second (orthogonal) direction.

The "reentrant honeycomb"

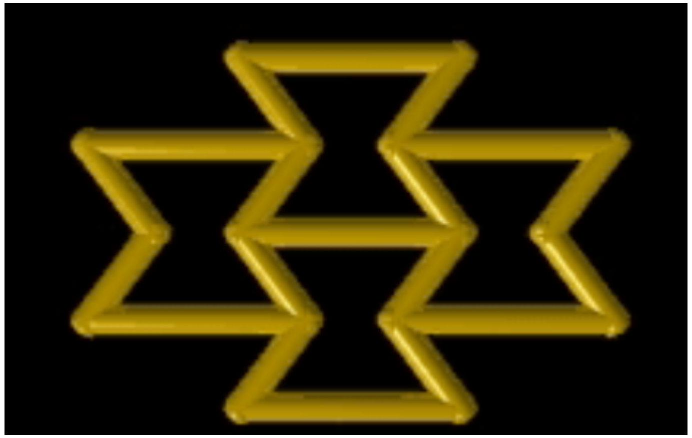


No auxetic behavior



Has auxetic behavior

A stretch in one first direction leads to a widening in a second (orthogonal) direction

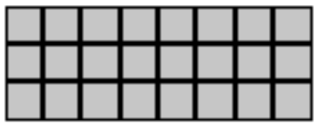


Materials with auxetic behavior…

- Have been known for over 100 years
- First reported synthetic auxetic material:

  R.S. Lakes, Science, 1987
- Term coined by K. Evans 1991:

αυξητικοζ (auxetikos) = "which tends to increase"



Selections from Materials Science literature

Kolpakov, A.G.: Determination of the average characteristics of elastic frameworks, J. Appl. Math. Mech. 49 (1985), no. 6, 739745 (1987); translated from Prikl. Mat. Mekh. 49 (1985), no. 6, 969977 (Russian).

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Baughman, R.H., Shacklette, J. M., Zakhidov, A. A. and Stafstr ▯om, S.: Negative Poisson's ratios as a common feature of cubic metals, Nature 392 (1998), 362-365.

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Grima, J.N., Alderson, A. and Evans, K.E.: Auxetic behaviour from rotating rigid units, Physica status solidi (b) 242 (2005), 561-575.

Greaves, G.N., Greer, A.I., Lakes, R.S. and Rouxel, T. : Poisson's ratio and modern materials, Nature Materials 10 (2011), 823-837.

Mathematical challenges in

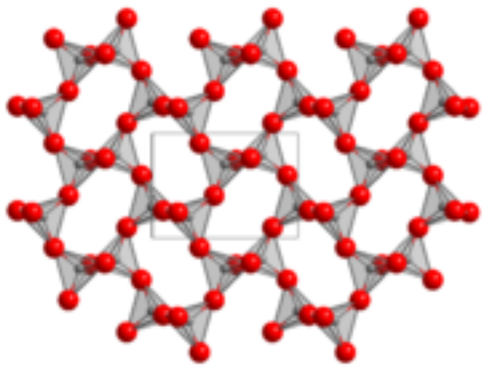
Crystallography and Materials Science

1. Explain auxetic behavior
2. Predict auxetic behavior
3. Design auxetic materials

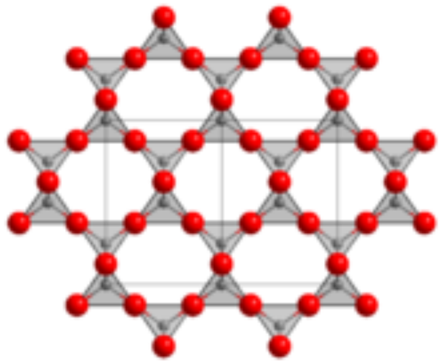
2. Displacive phase transitions in crystalline materials

To have auxetic behavior also means to be flexible...

Displacive phase transitions
in crystalline matter



α-cristobalite



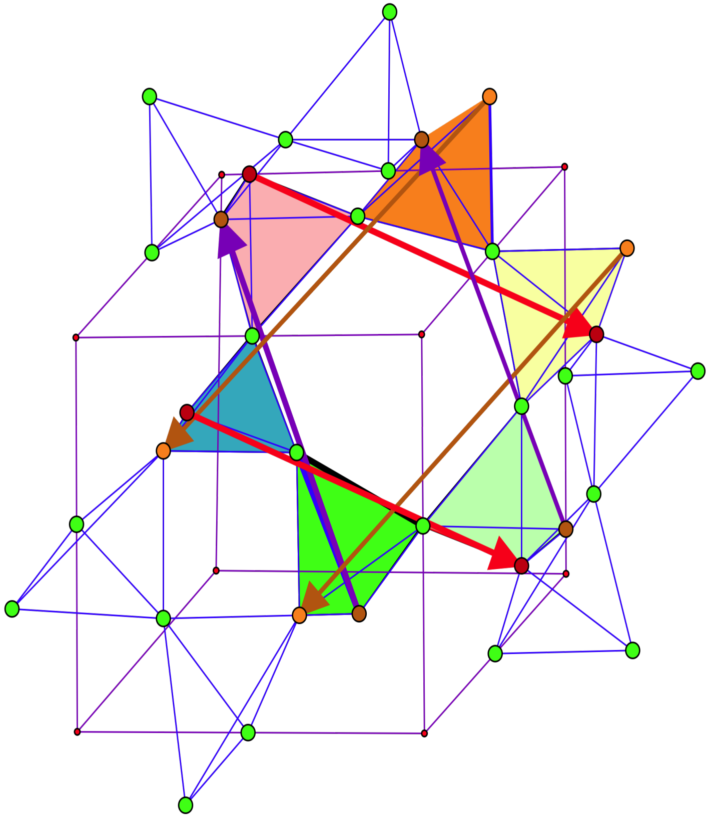
β-cristobalite

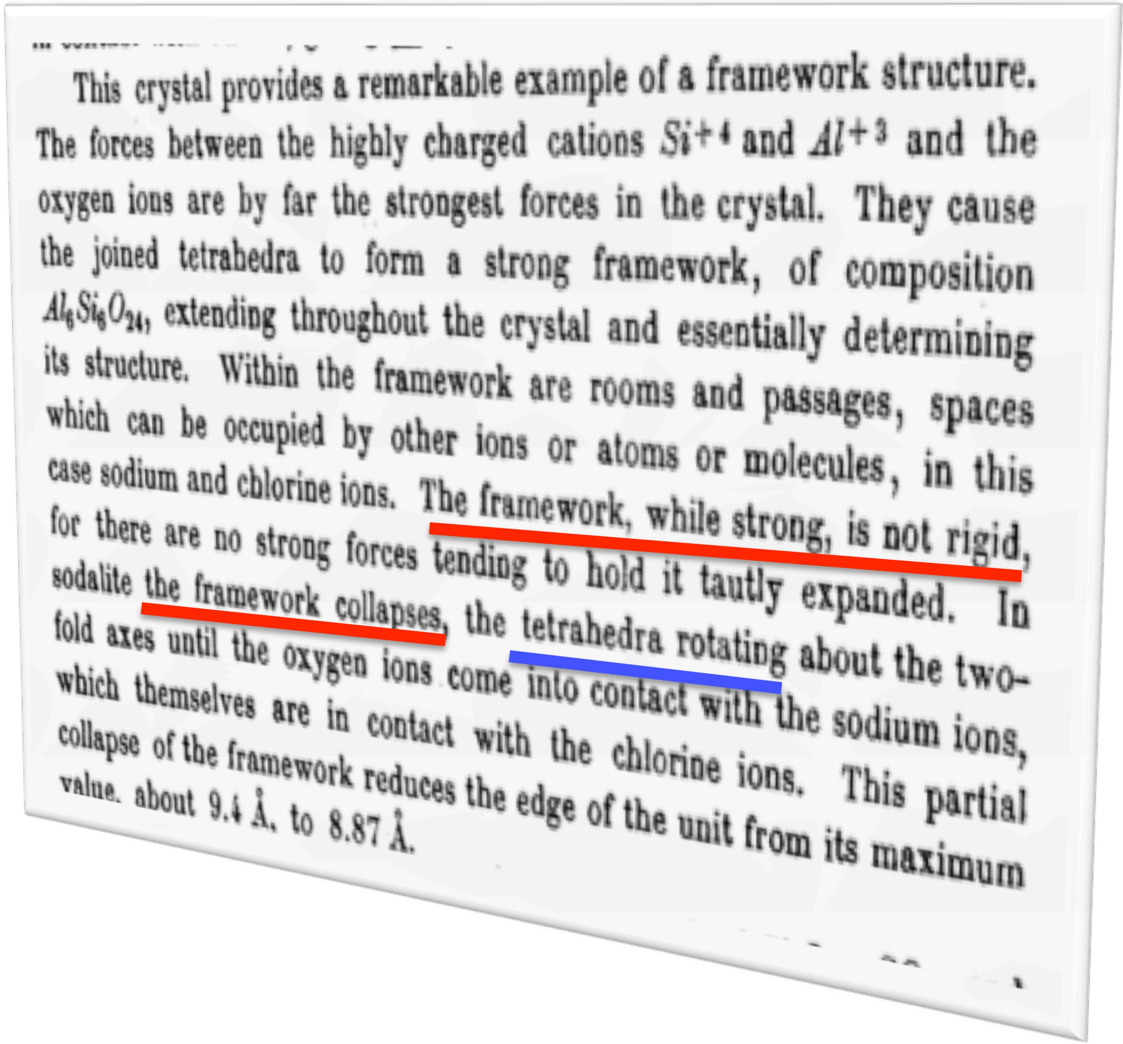
Same bond network structure – "framework"

Different positions of the atoms - "displacement"

Linus Pauling on "collapsing sodalite frameworks"

The structure of sodalite and helvite, Z. Kristallogr. 74 (1930), 213-225.





This crystal provides a remarkable example of a framework structure. The forces between the highly charged cations Si^{+4} and Al^{+3} and the oxygen ions are by far the strongest forces in the crystal. They cause the joined tetrahedra to form a strong framework, of composition $Al_6Si_6O_{24}$, extending throughout the crystal and essentially determining its structure. Within the framework are rooms and passages, spaces which can be occupied by other ions or atoms or molecules, in this case sodium and chlorine ions. The framework, while strong, is not rigid, for there are no strong forces tending to hold it tautly expanded. In sodalite the framework collapses, the tetrahedra rotating about the two-fold axes until the oxygen ions come into contact with the sodium ions, which themselves are in contact with the chlorine ions. This partial collapse of the framework reduces the edge of the unit from its maximum value, about 9.4 Å, to 8.87 Å.

The “classical tilt” for sodalite frameworks, as depicted in crystallography

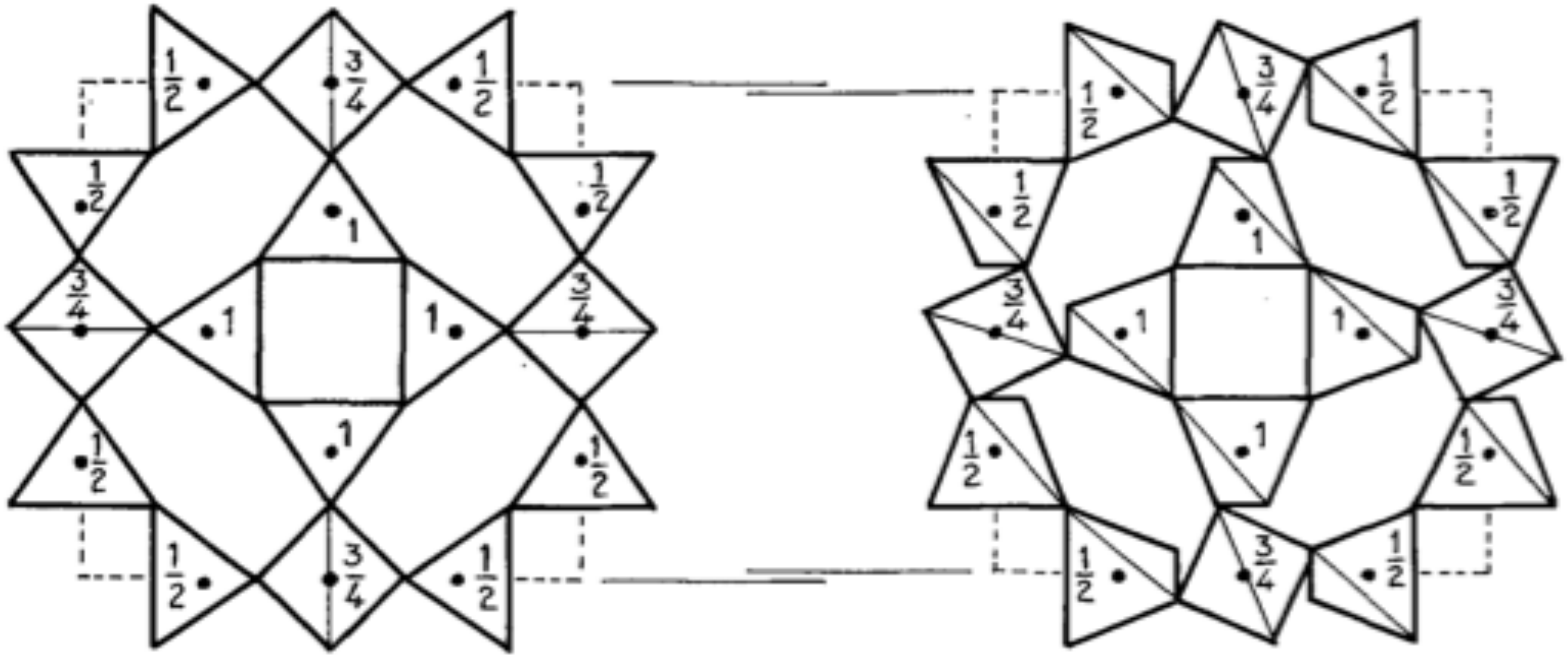
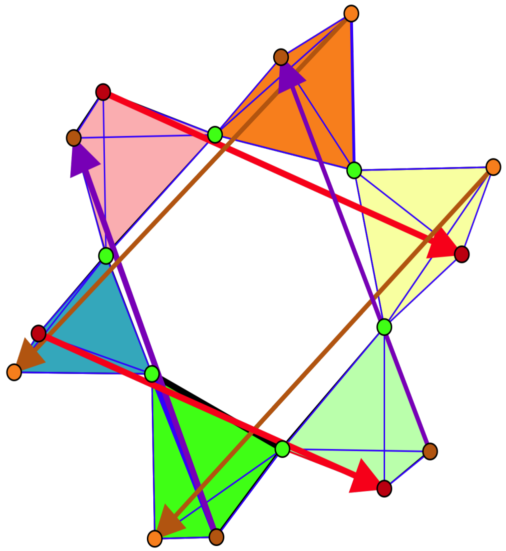


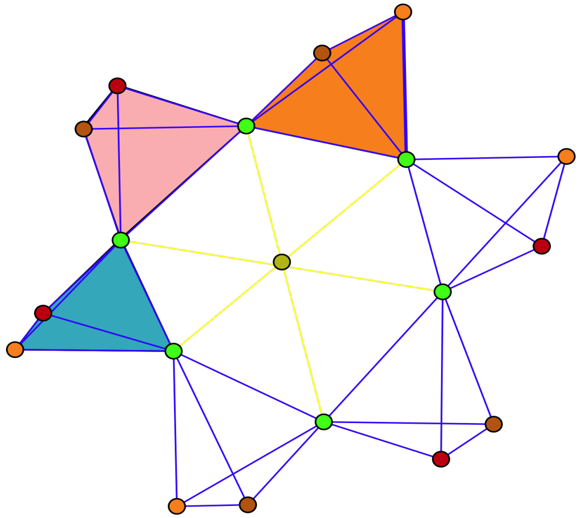
Illustration from D. Taylor:
The thermal expansion behaviour of the framework silicates,
MINERALOGICAL MAGAZINE, 38 (I972), 593-604

But in fact there is a

six-parameter deformation family

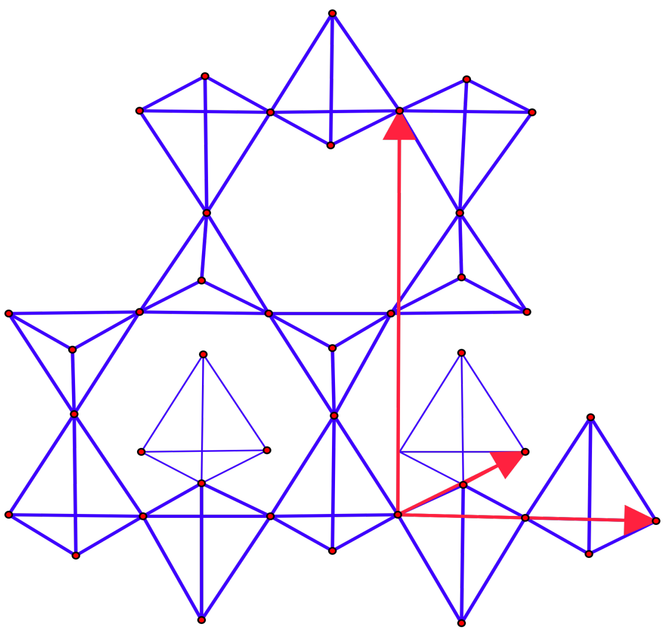
maintaining a central symmetry



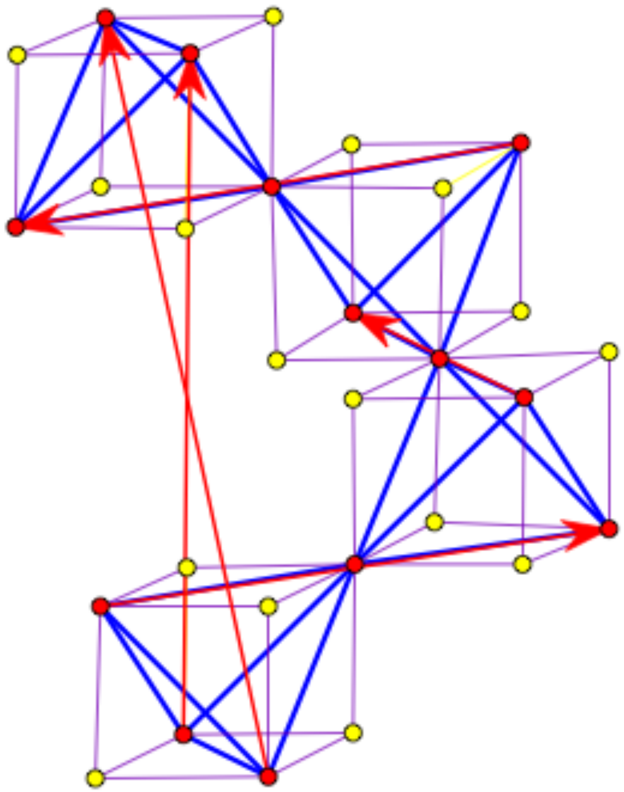


Periodic framework materials

Tridymite

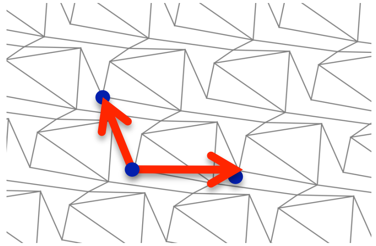


High Cristobalite



3. Deformation theory of periodic frameworks

Periodic frameworks



Definitions

A d-periodic graph is a pair (G, Γ):

$G = (V, E)$ is a simple infinite graph with vertices V , edges E and finite degree at every vertex

$\Gamma \subset Aut(G)$ is a free Abelian group of automorphisms of rank d, which acts without fixed points and has a finite number of vertex (and hence, also edge) orbits.

A periodic placement of a d-periodic graph (G, Γ) in R^d is defined by two functions:

$$p: V \rightarrow R^d \quad \text{and} \quad \pi: \Gamma \rightarrow T(R^d)$$

where:

p assigns points in R^d to the vertices of G

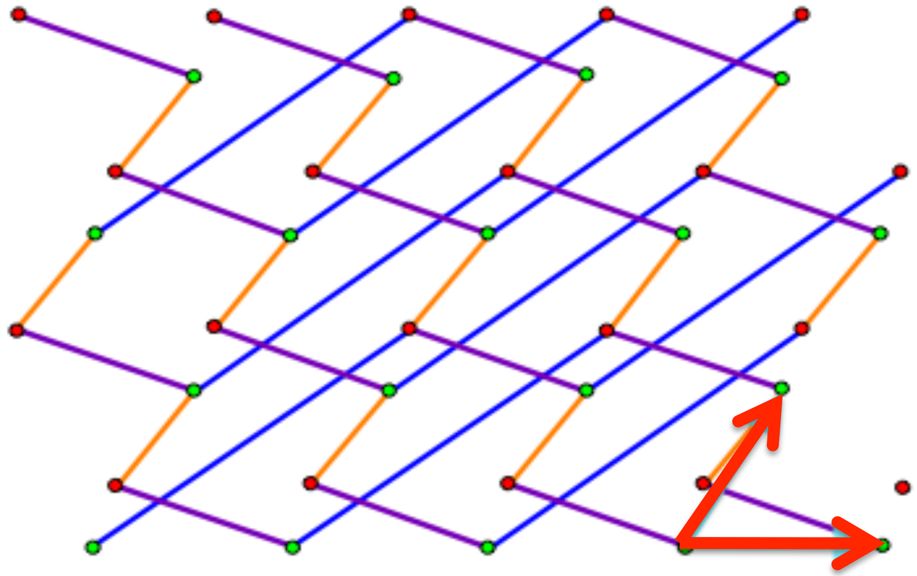
π is a faithful representation of Γ into the group of translations, with image a lattice of rank d.

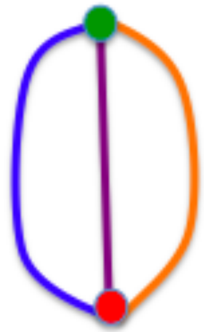
They satisfy:

$$p(gv) = \pi(g)(p(v))$$

Periodic graphs and their quotients

Important features: periodicity lattice and finite quotient





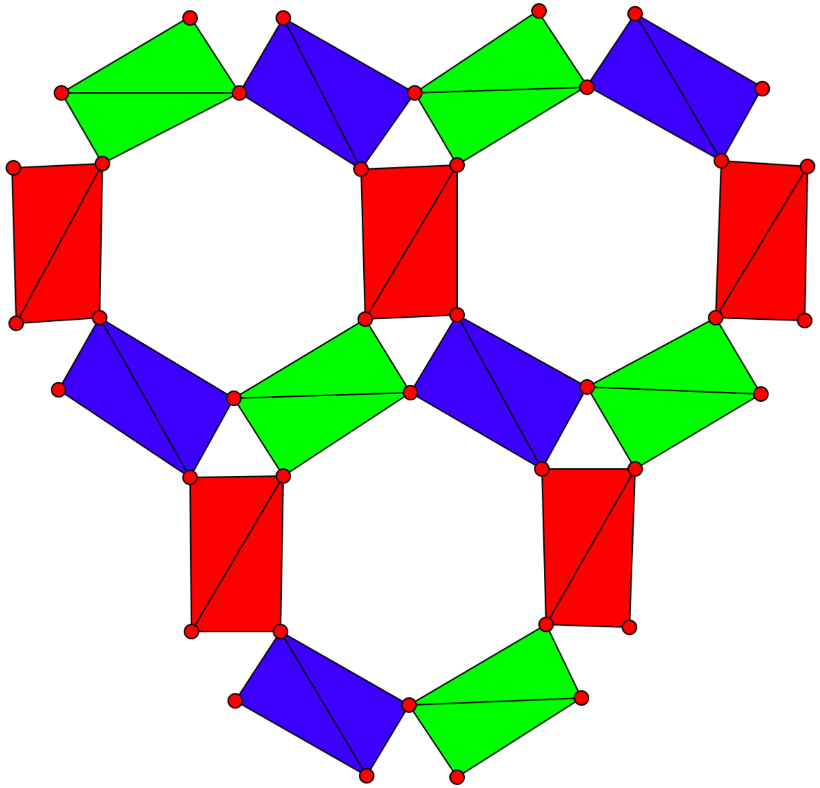
Fragment of a 2-periodic framework (d = 2), with:

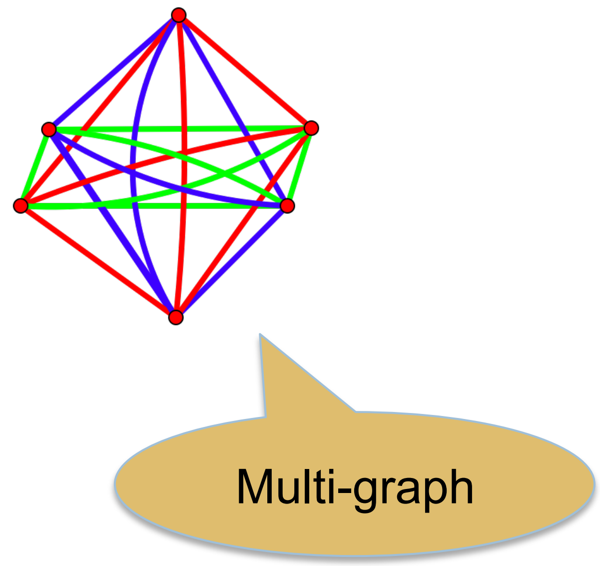
n = 2 equivalence classes of vertices, and

m = 3 equivalence classes of edges.

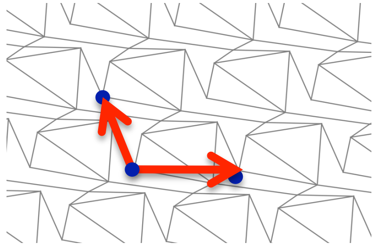
The generators of the periodicity lattice are marked by arrows.

The quotient map for quartz





Realizations of fixed edge-length periodic frameworks



Given:

A *periodic framework* (G, Γ, p, π)

Fix all edge lengths $\ell(u,v) = |p(v) - p(u)|$: *weighted periodic graph* (G, Γ, ℓ).

A realization of the weighted d-periodic graph (G, Γ, ℓ) in R^d is a periodic placement that induces the given weights.

The configuration space of (G, Γ, ℓ) is the quotient space of all realizations by the group $E(d)$ of isometries of R^d.

The *deformation space* of a periodic framework (G, Γ, p, π) is the connected component of the corresponding configuration.

Infinitesimal deformations of a periodic framework (G, Γ, p, π): given by the real tangent space to the realization space.

Infinitesimal flexes: quotient space by the $\binom{d+1}{2}$-dimensional subspace of trivial infinitesimal motions.

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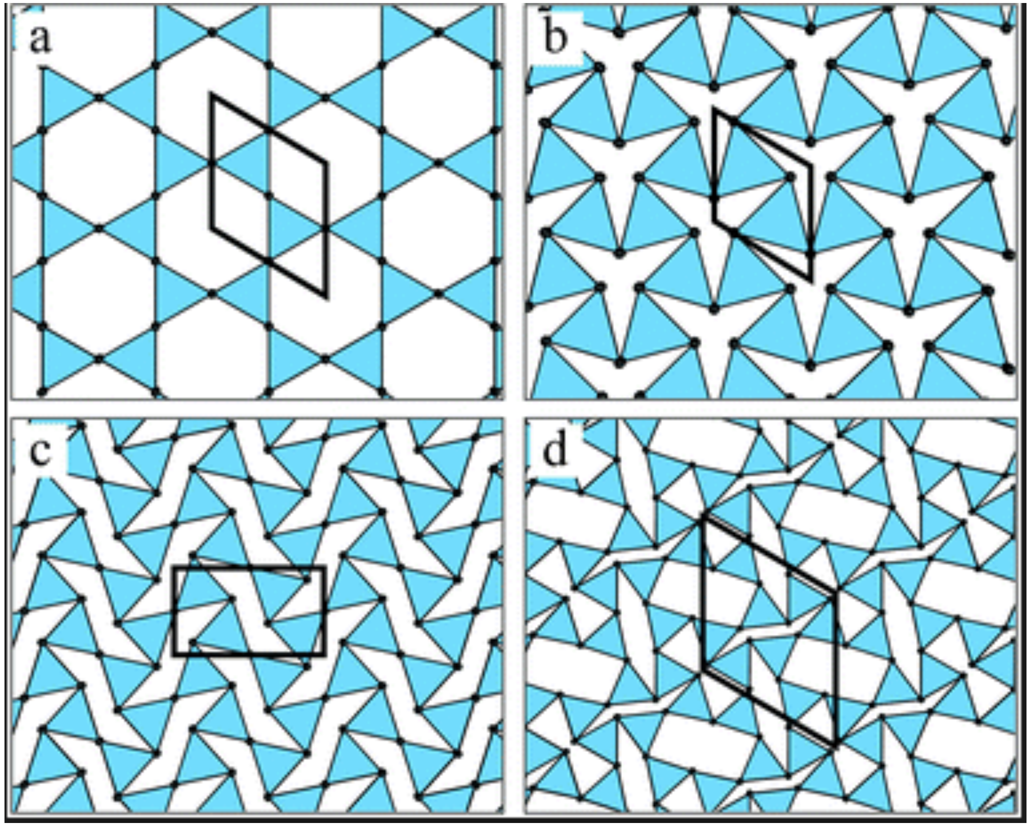
Borcea and Streinu: Periodic frameworks and flexibility, Proc. Roy. Soc. A 466 (2010), 2633-2649.

Borcea and Streinu: Minimally rigid periodic graphs, Bulletin London Math. Soc. 43 (2011), 1093-1103.

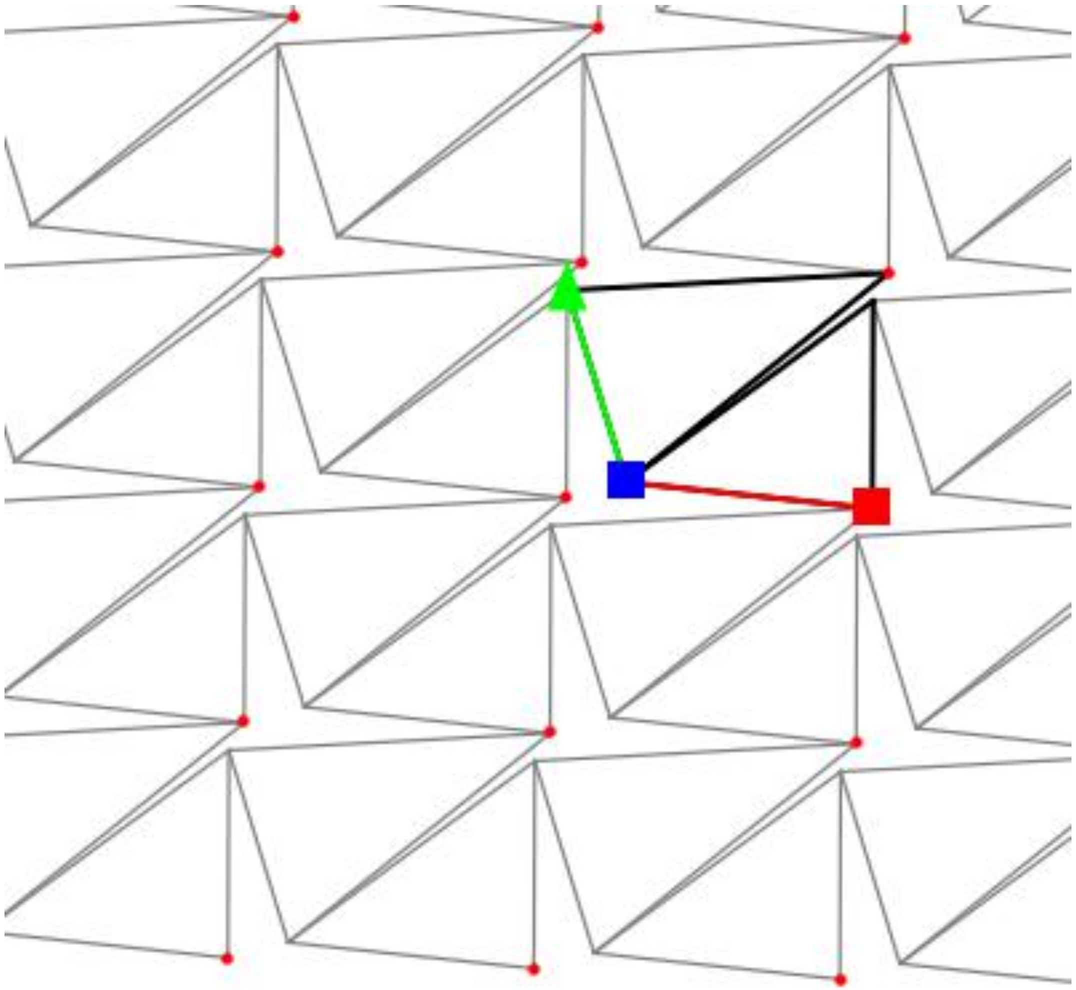
Borcea and Streinu: Frameworks with crystallographic symmetry, Phil. Trans. Roy. Soc. A 372 (2014), 20120143.

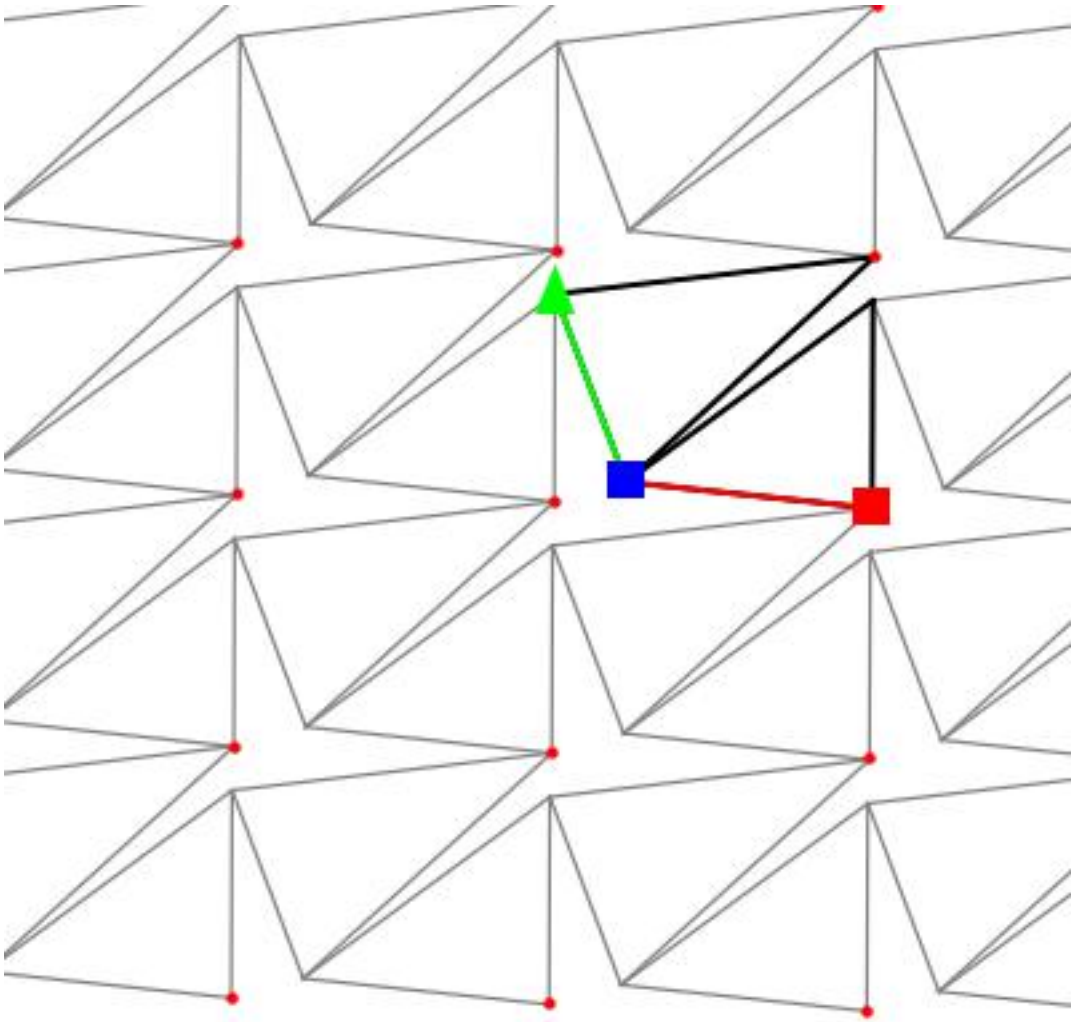
Example:

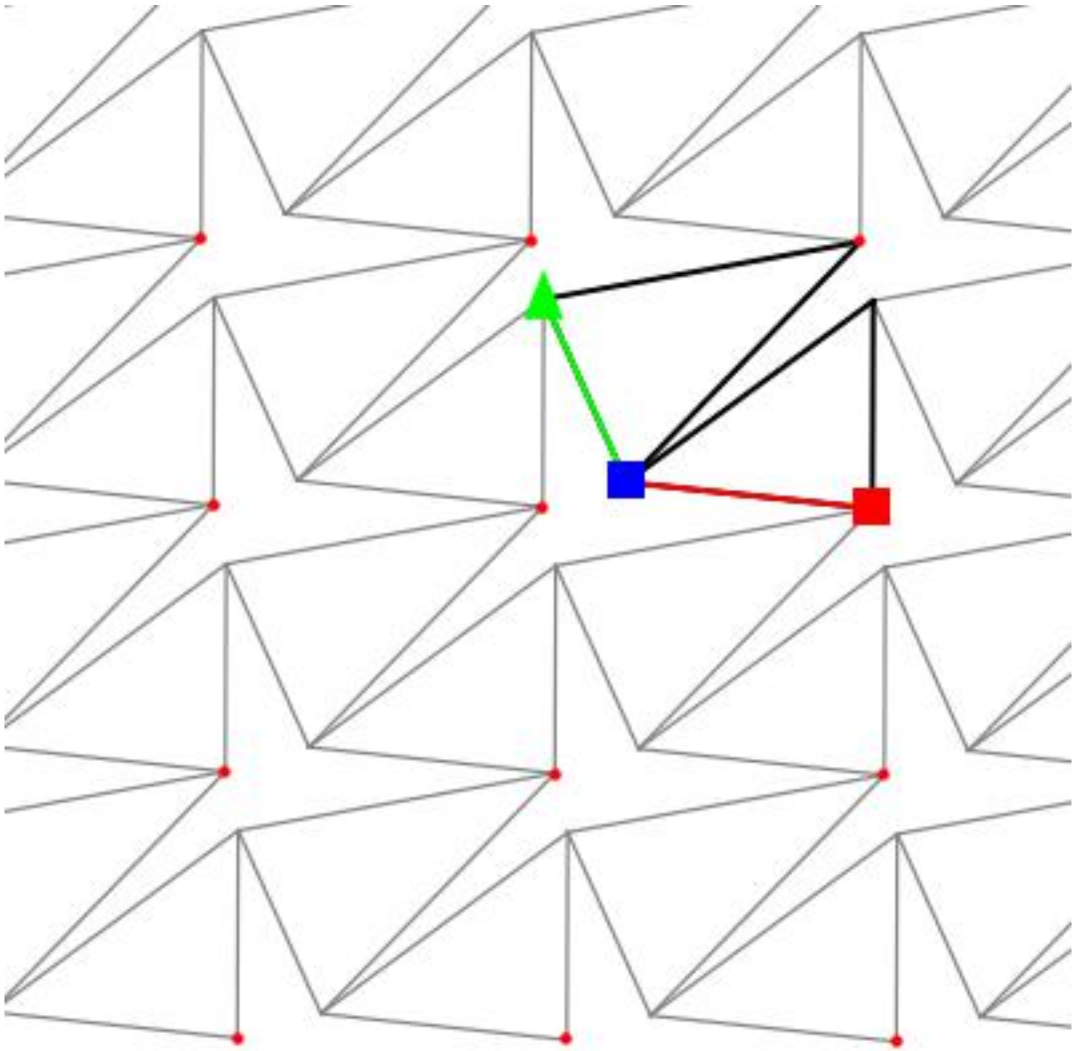
The (one-parameter) deformation of the Kagome framework

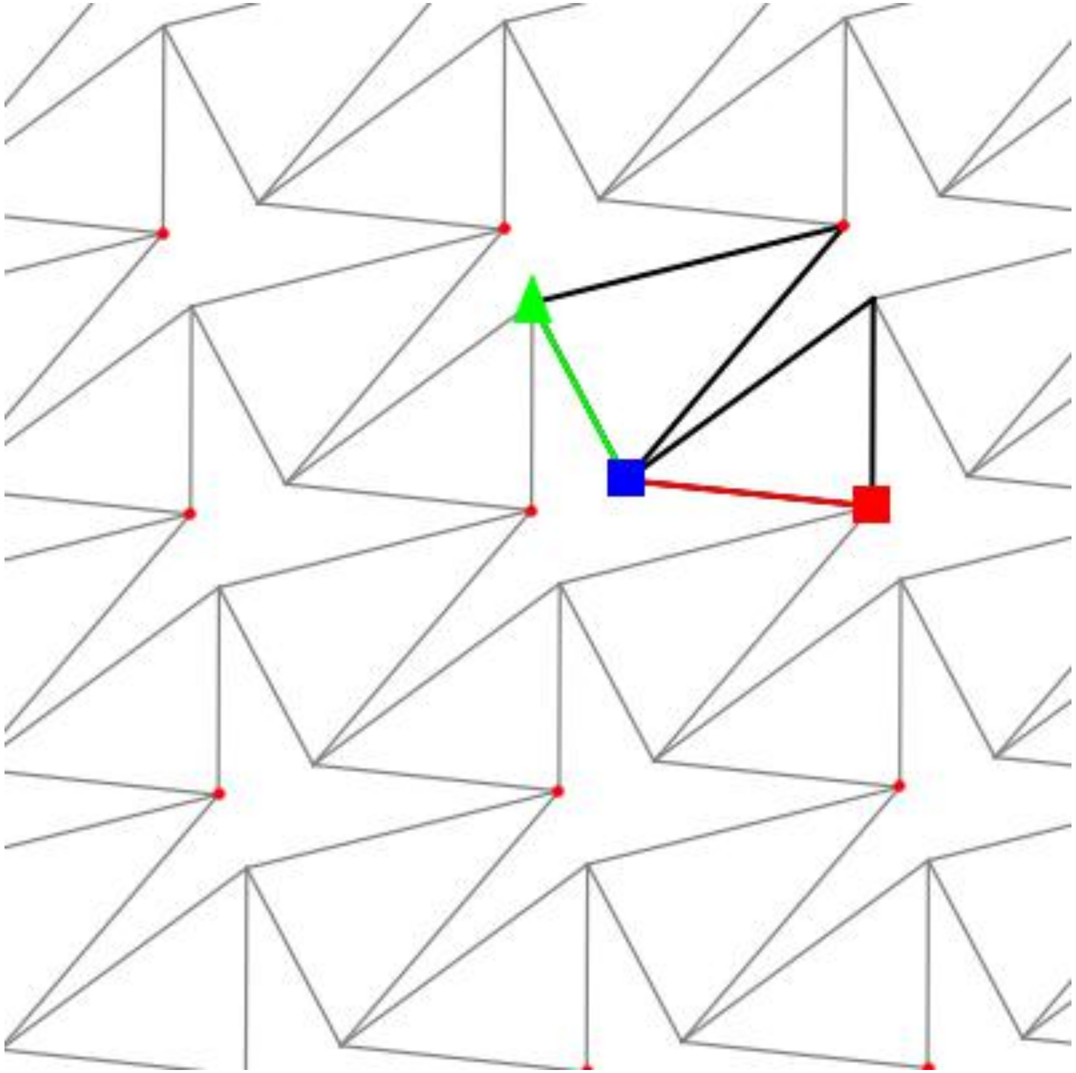


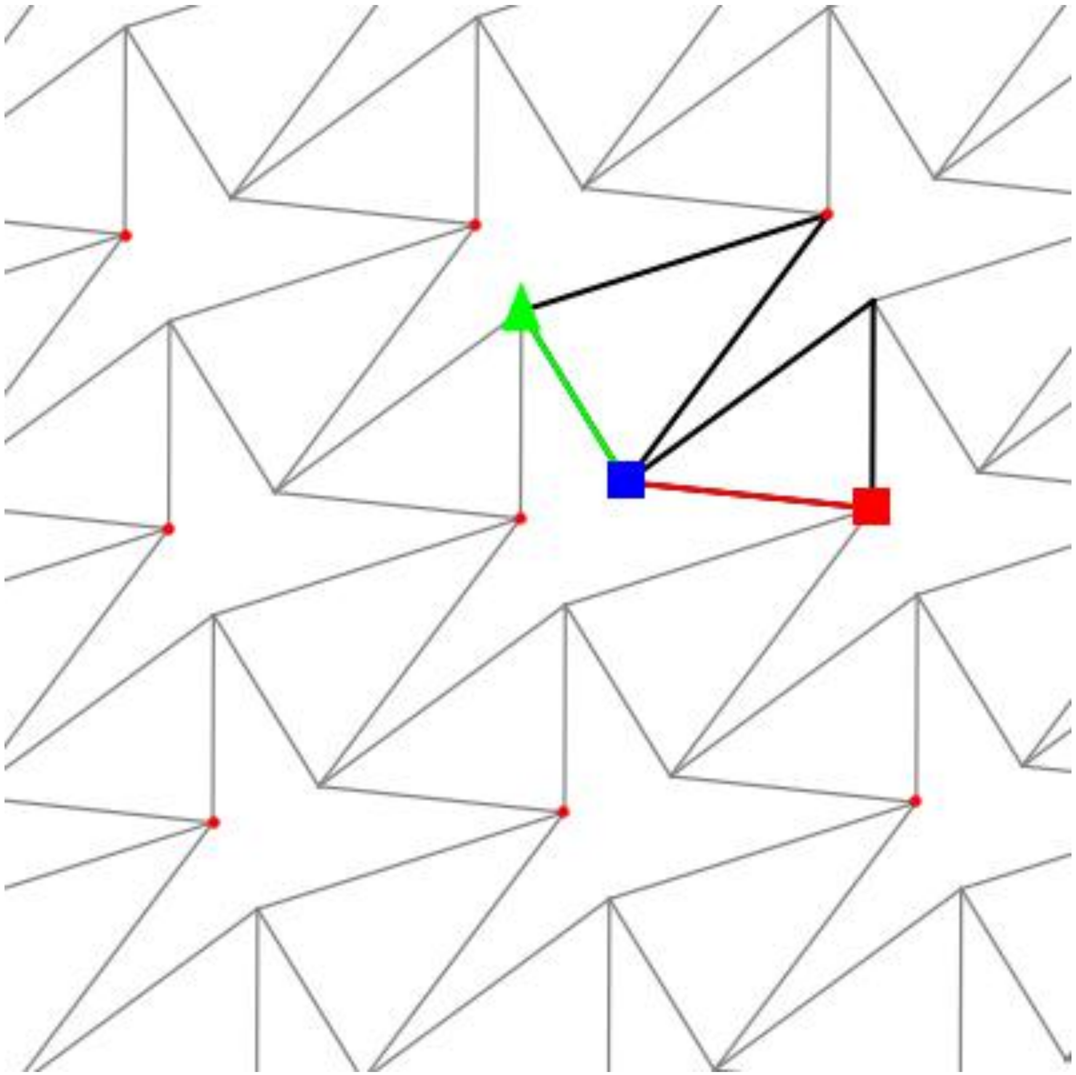
Kapko, Dawson et al. Flexibility of ideal zeolite frameworks, Phys. Chem. Chem. Reviews, 2010

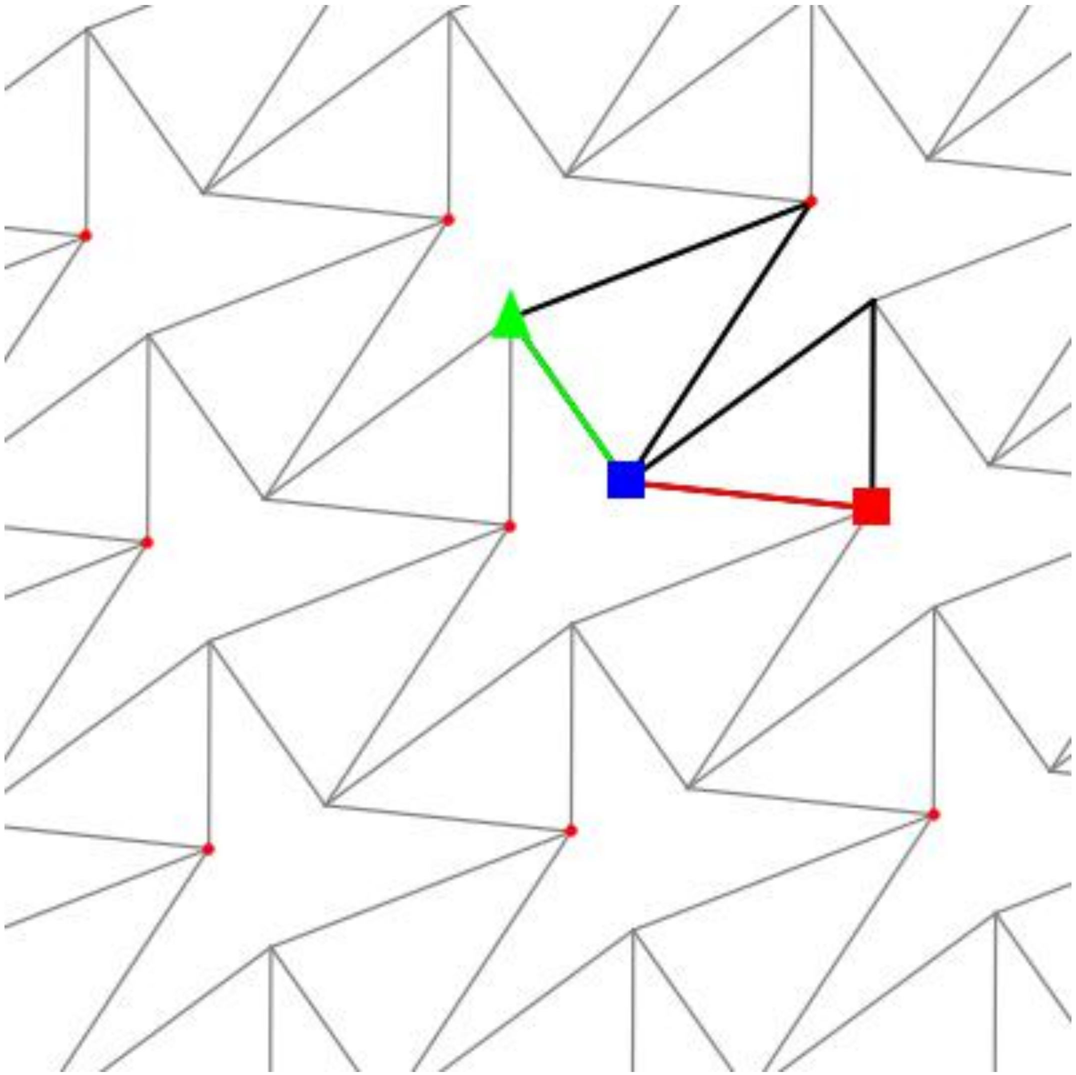












Mathematical challenges in
Crystallography and Materials Science

1. Explain auxetic behavior
2. Predict auxetic behavior
3. Design auxetic materials

Geometric Auxetics

Geometric auxetics

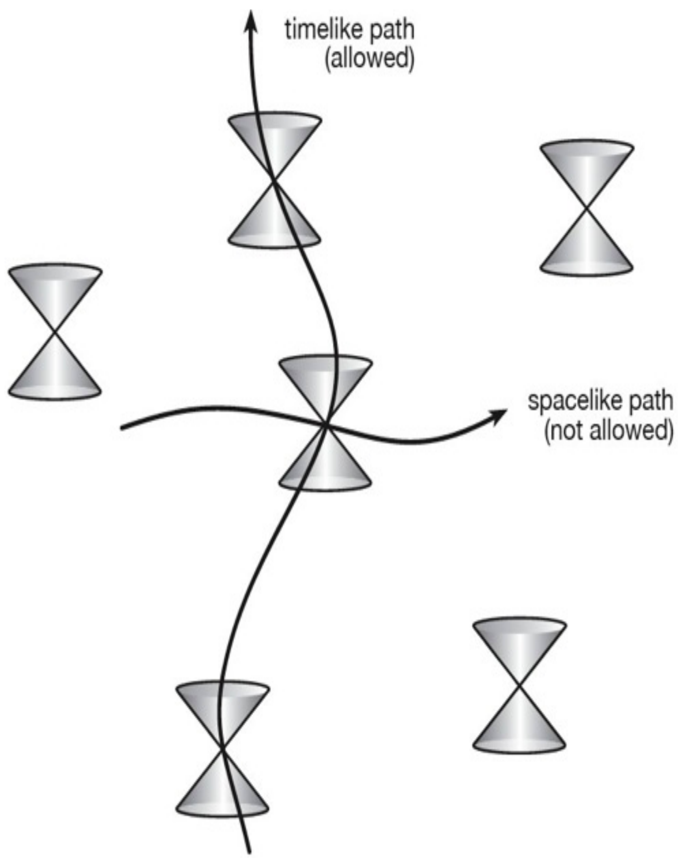
A purely geometric approach to defining auxetic behavior for periodic frameworks.

Definition. A one-parameter deformation of a periodic framework is an auxetic path when for any $t_1 < t_2$, the linear operator taking the period lattice Λ_{t2} to Λ_{t1} is a contraction i.e. has operator norm at most 1.

Theorem: A one-parameter deformation of a periodic framework is an auxetic path when the curve given by the Gram matrices of a basis of periods has all velocity vectors (tangents) in the positive semidefinite cone.

This is analogous to `causal-lines' in special relativity i.e. curves with all their tangents in the `light cone'.

Causal trajectories in Special Relativity



A causal line (world line)
in Minkowski space
must have all its tangent
directions in the light cone.

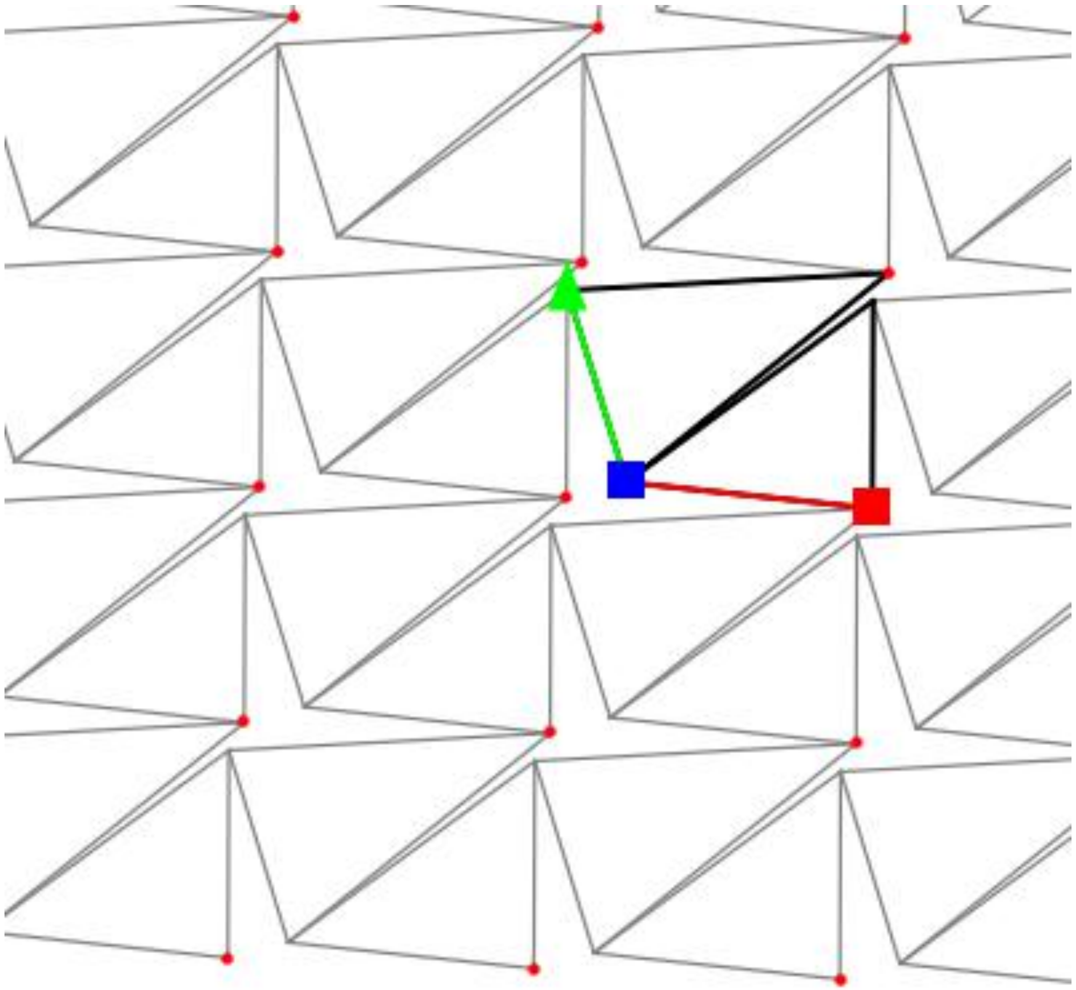
Illustration uses three dimensional
Minkowski space.

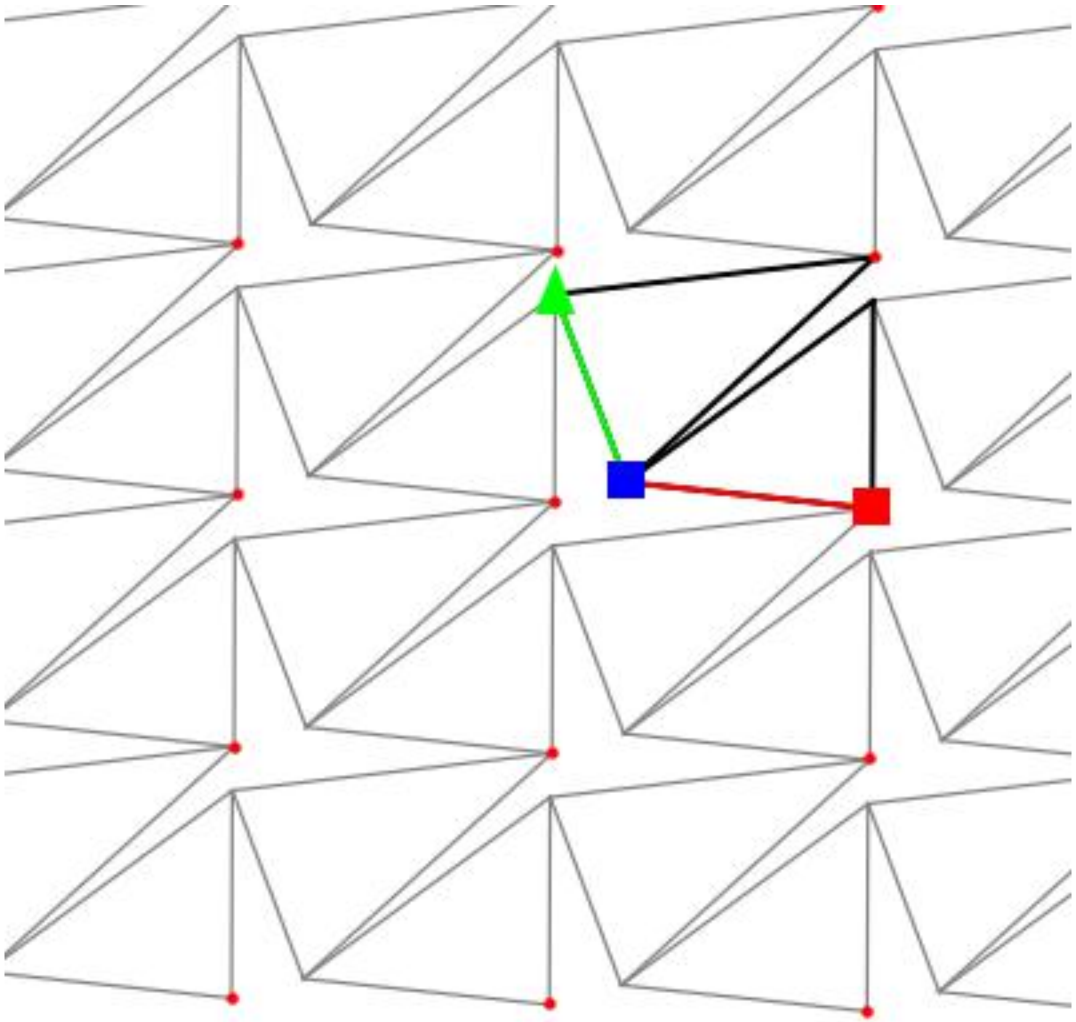
Auxetic vs. Expansive

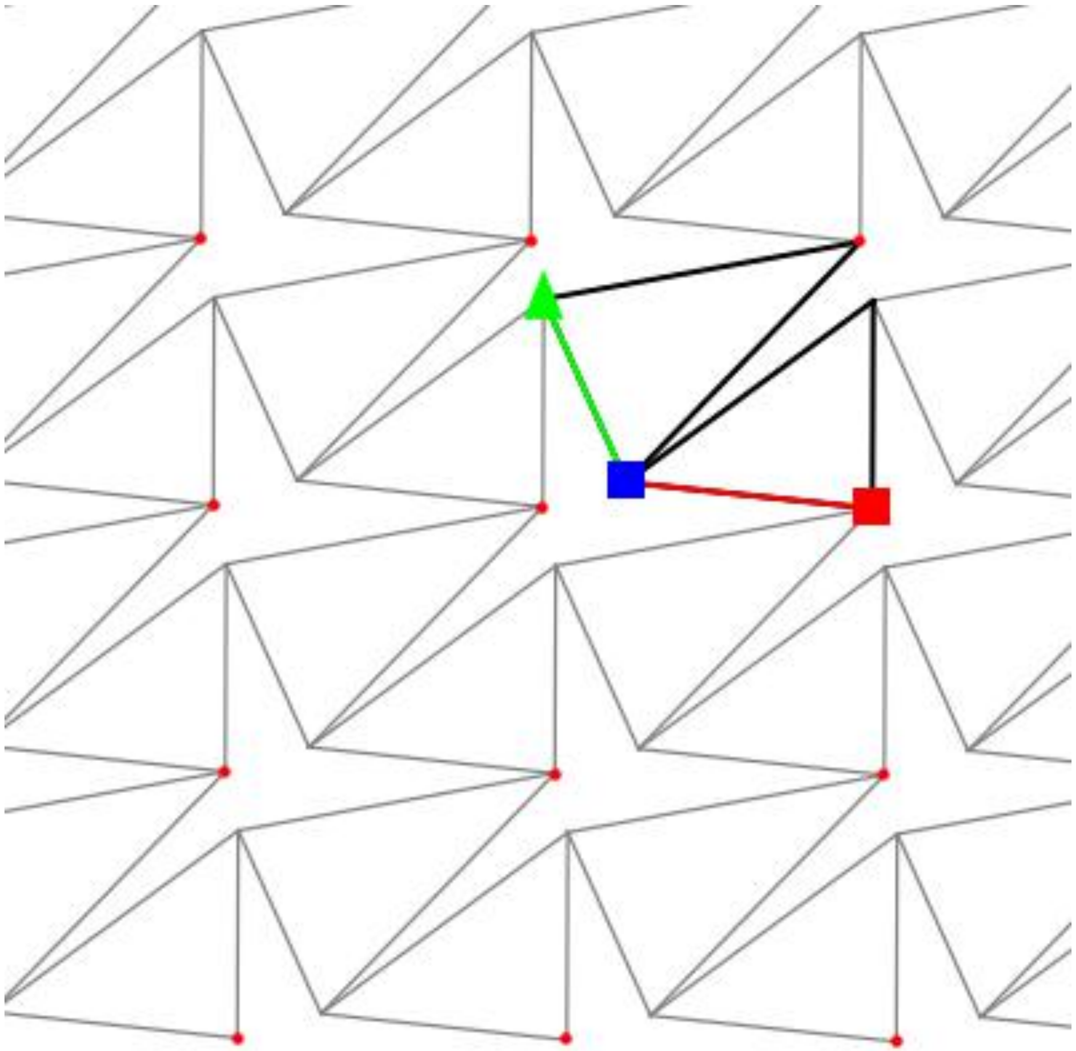
Definition.
A one-parameter deformation of a periodic framework is expansive when the distance between any pair of vertices increases or stays the same.

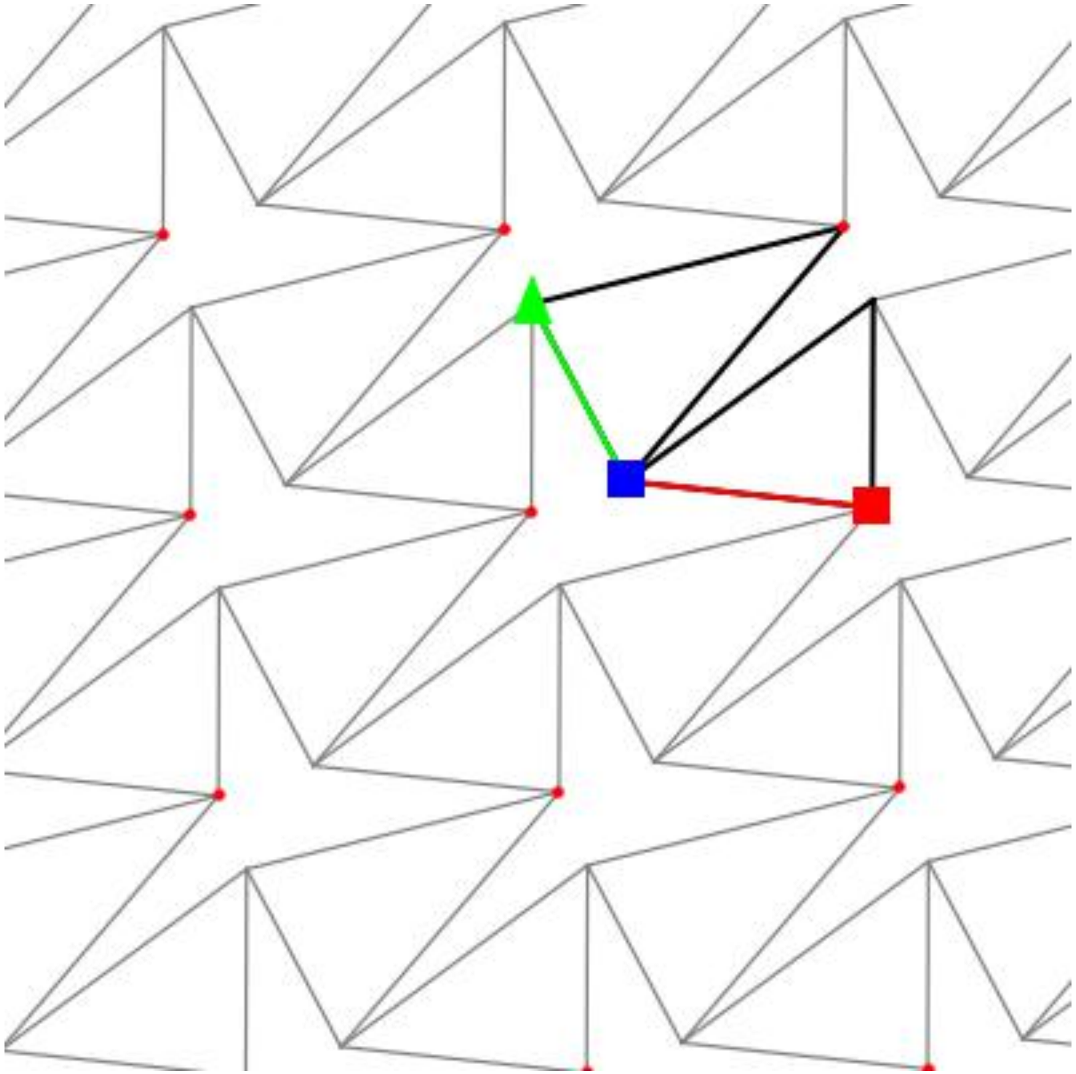
Theorem.
An expansive path is auxetic.
But an auxetic path need not be expansive.

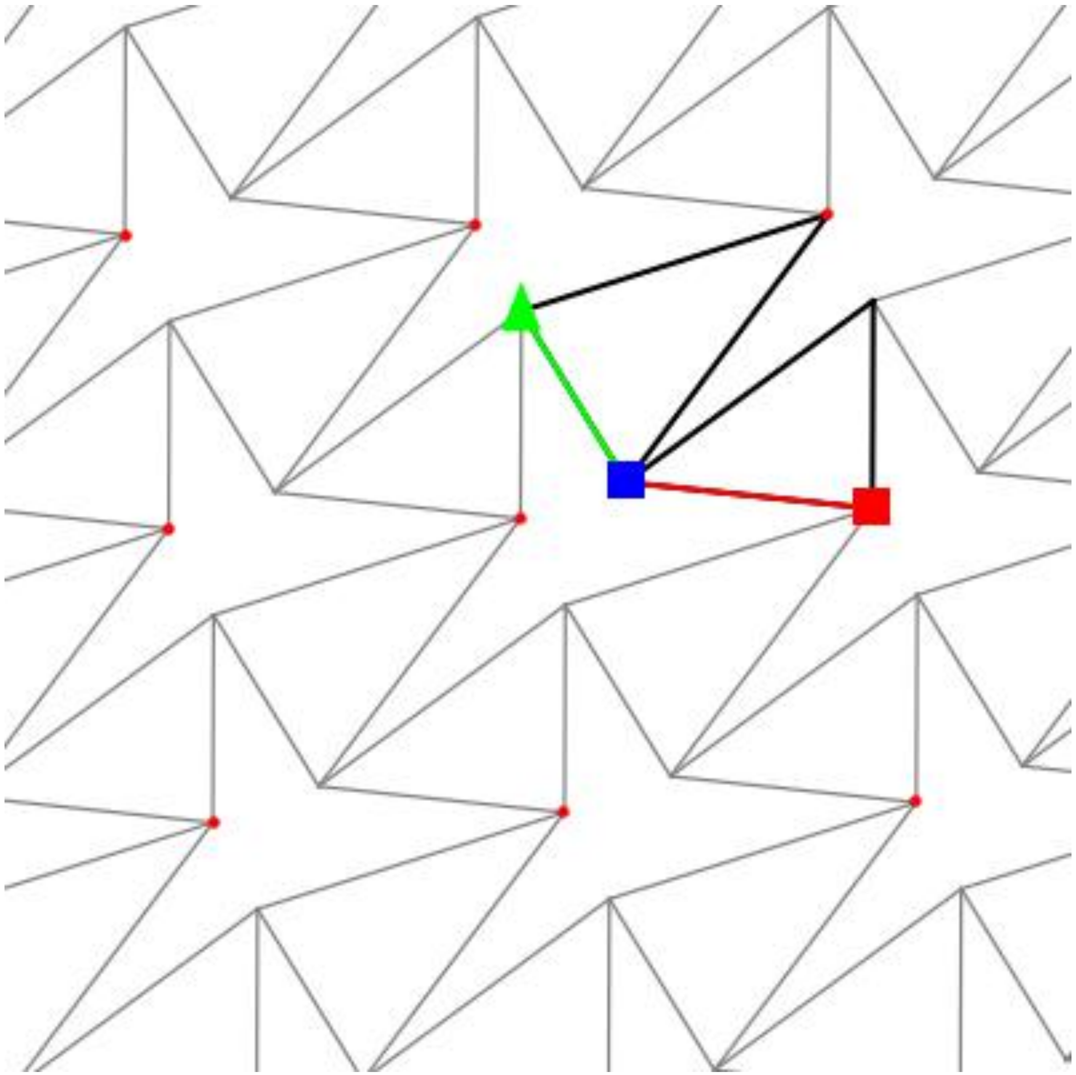
Spot the difference …

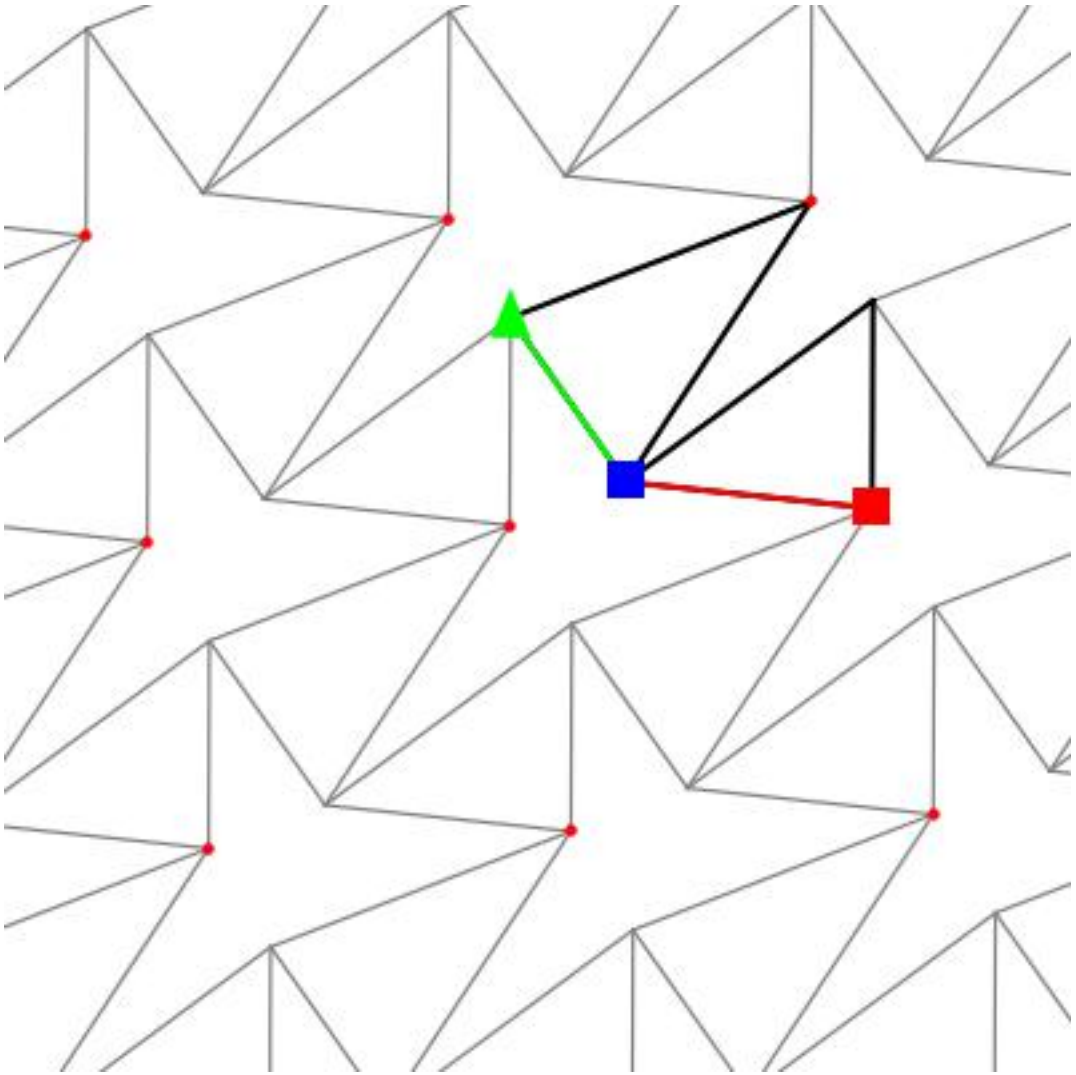


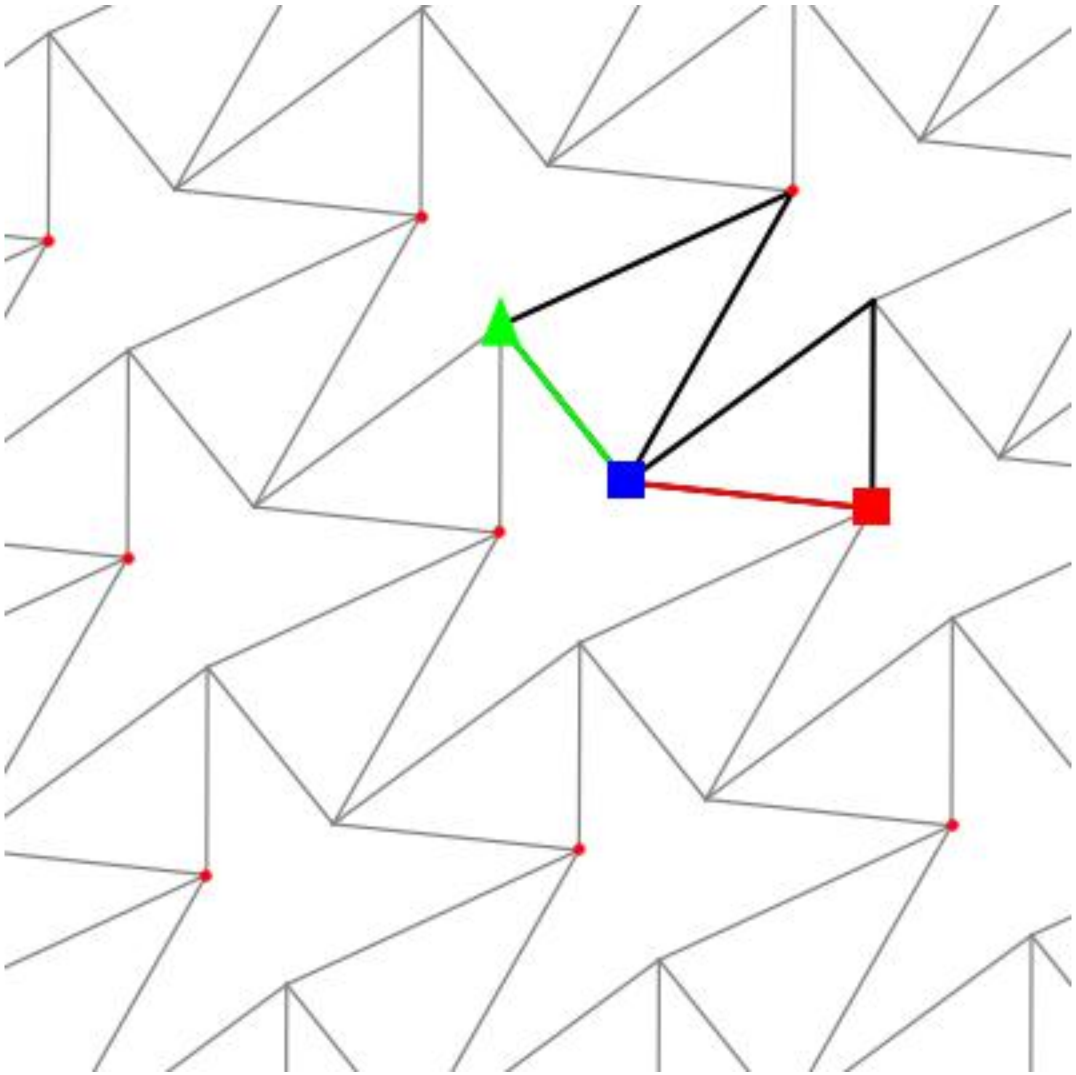


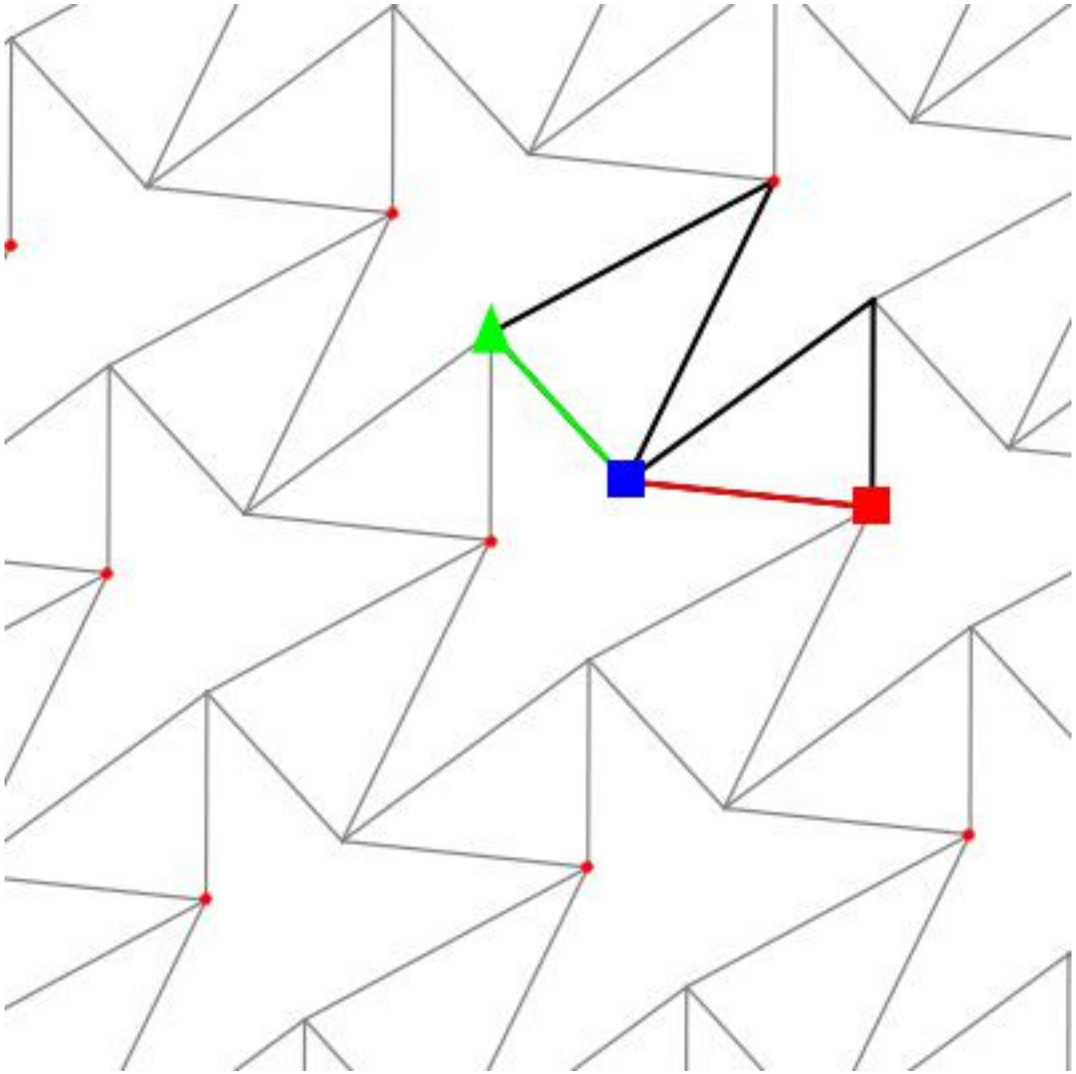


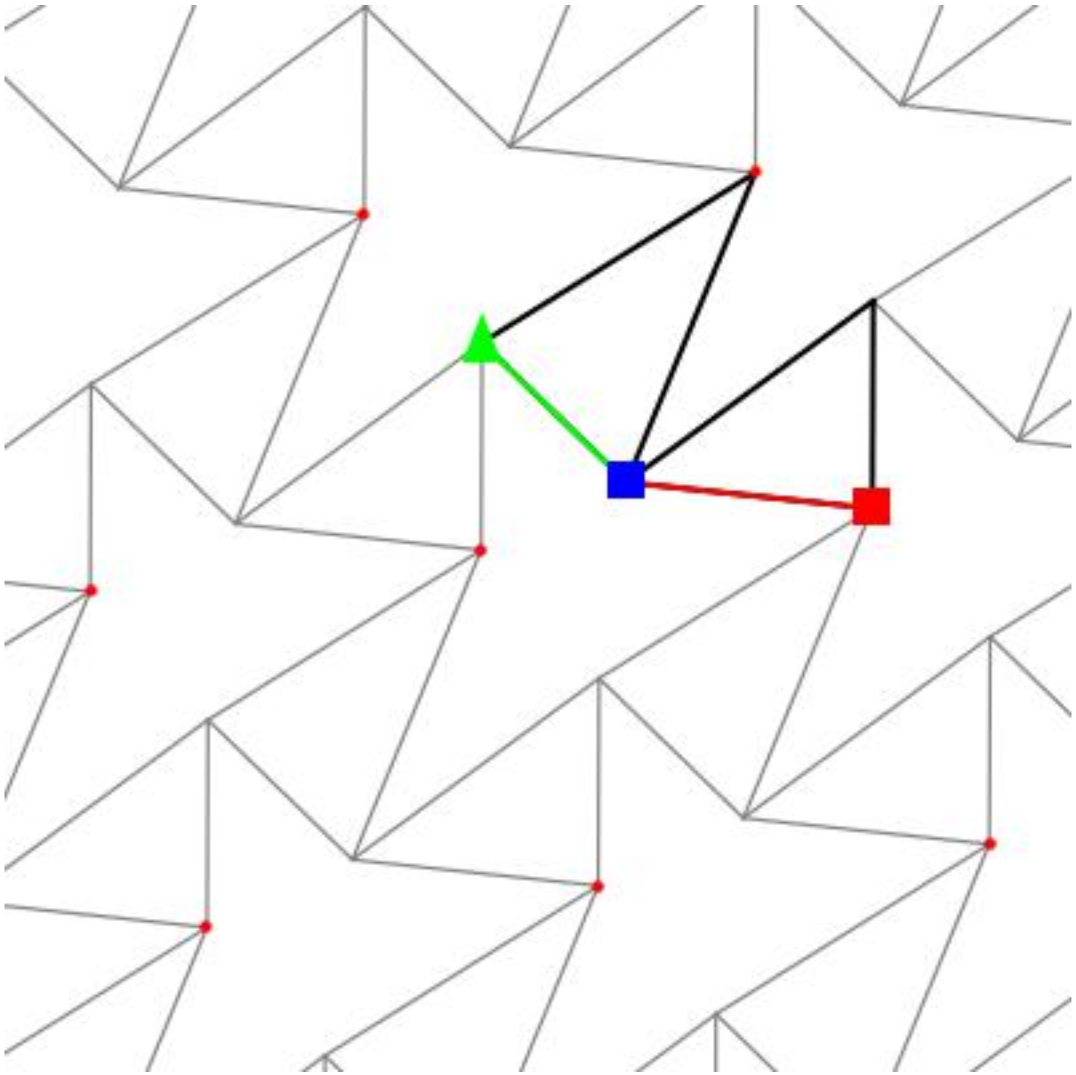


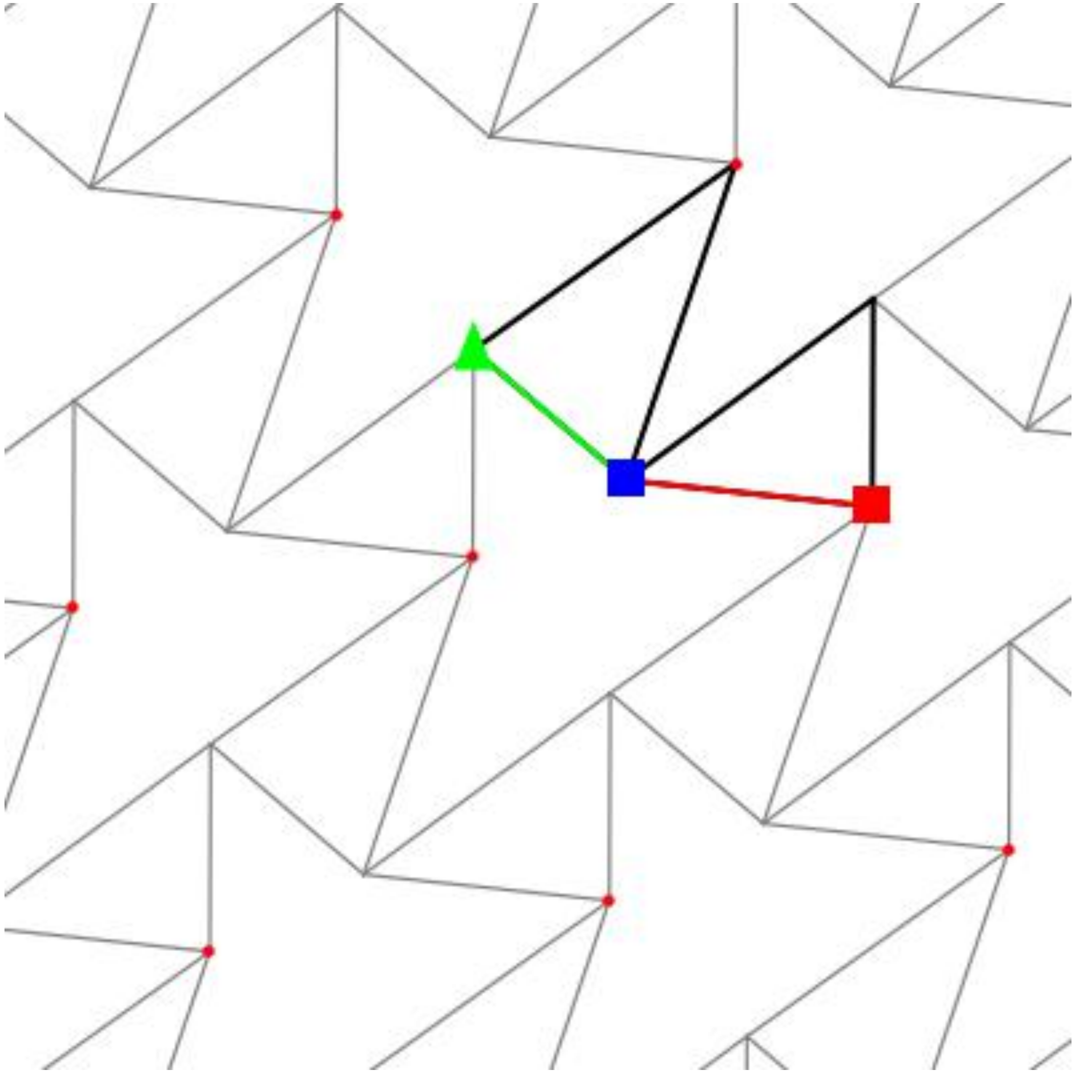


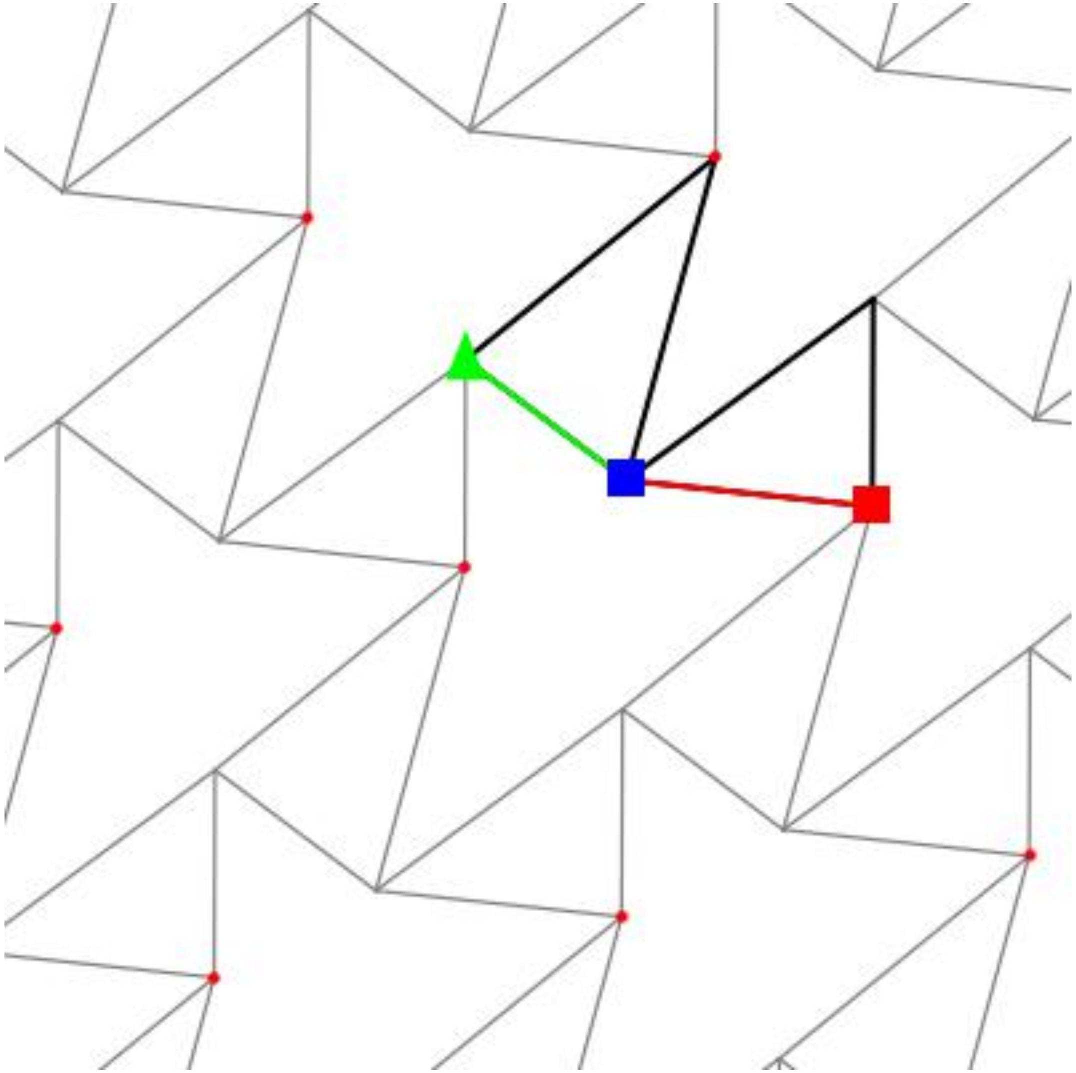


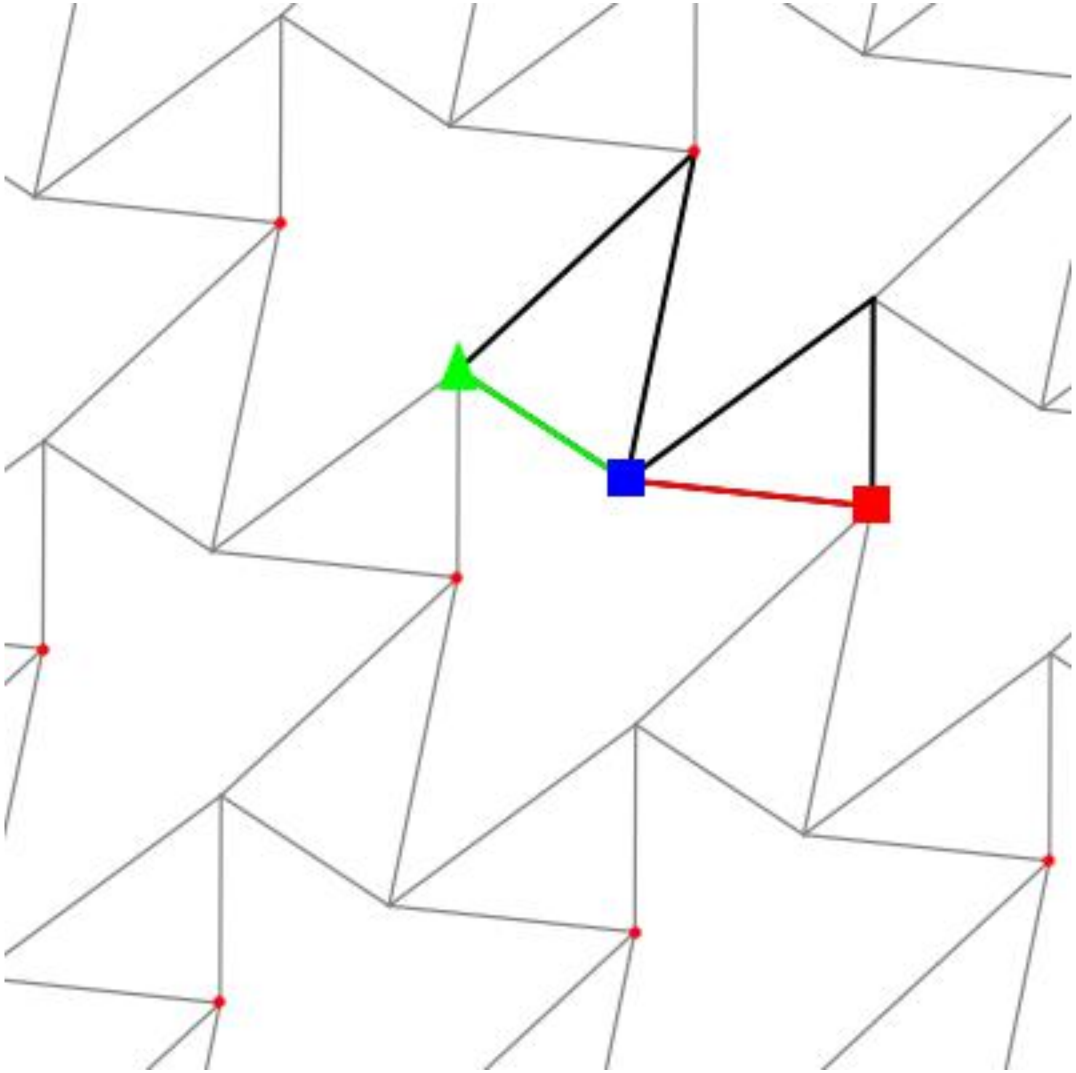


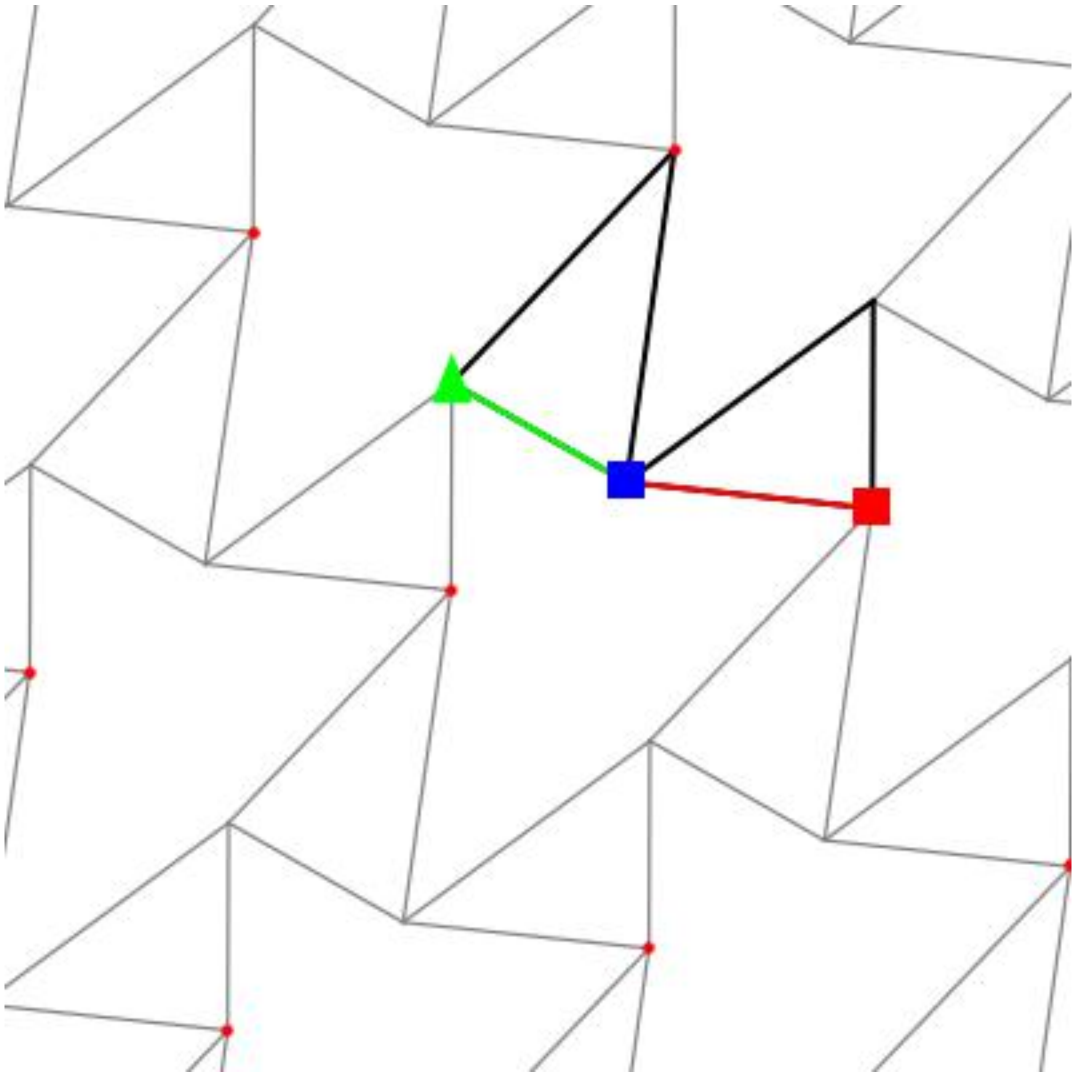


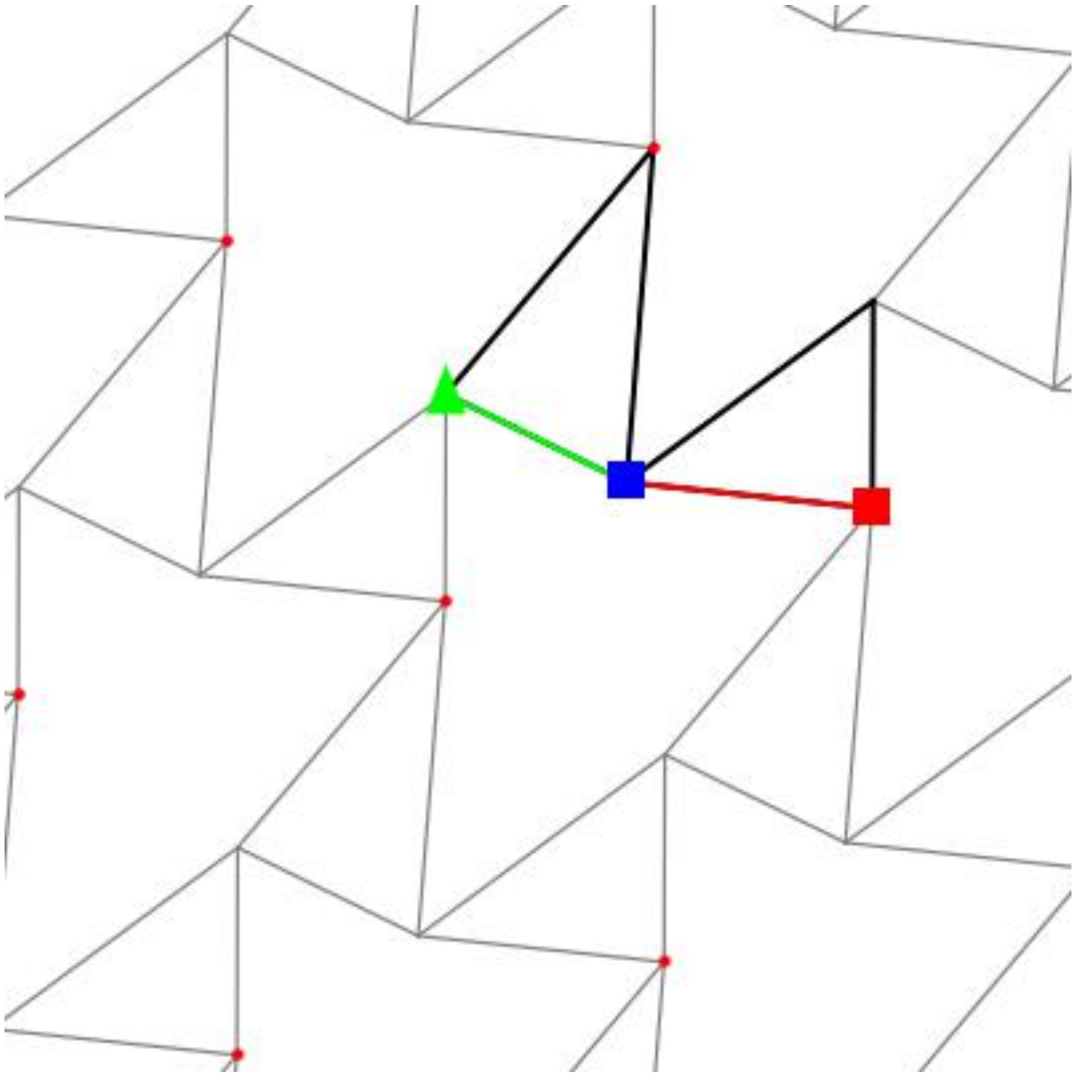












Summary

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- Displacive phase transitions in crystalline materials
- Deformation theory of periodic frameworks

Summary

- **Auxetic behavior**: a notion related to negative Poisson's ratio in elasticity theory
- **Displacive phase transitions** in crystalline materials
- **Deformation theory** of periodic frameworks

See our SoCG talk on Wednesday for full characterization of expansive periodic frameworks in dim 2.

Hence: we have an infinite supply of examples of frameworks with auxetic behavior

References

C.S.Borcea and I. Streinu: Liftings and stresses for planar periodic frameworks, SoCG'14

C.S. Borcea and I. Streinu: Kinematics of expansive planar periodic mechanisms, ARK'14

C.S. Borcea and I.Streinu: Geometric auxetics, 2014

Thank you