Geometry of periodic structures

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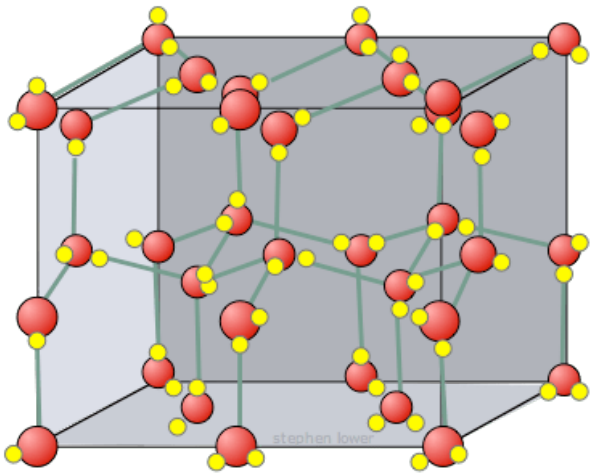
Crystal Structures

A *crystal structure* is a solid material where atoms/molecules form a periodic arrangement.

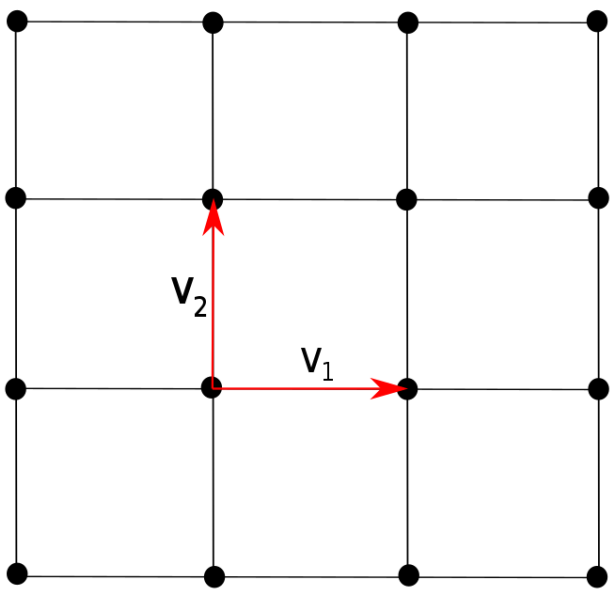


This pattern repeats infinitely in 3 independent directions, so it can be modelled by an infinite periodic graph in $\mathbb{R}^3$.

Lattices

The periodic nature of a crystal is represented by a lattice. Given a basis $\vec{v}_1, \ldots, \vec{v}_n$ in $\mathbb{R}^n$, a *lattice* is the discrete set

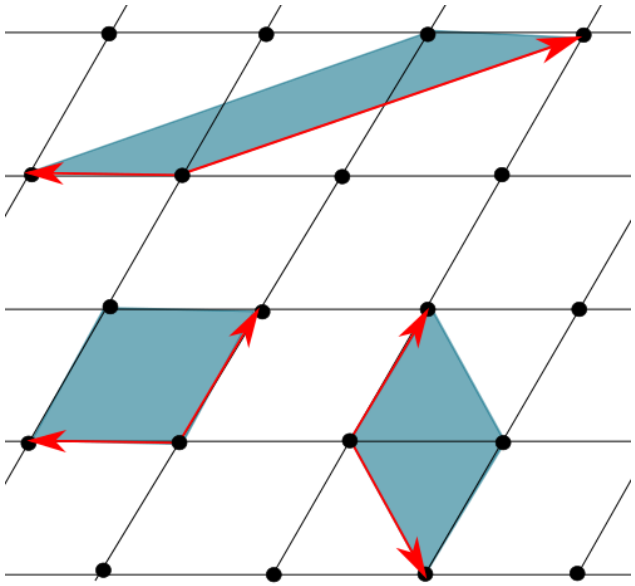
$$L = \{\sum_{i=1}^{n} m_i \vec{v}_i | m_i \in \mathbb{Z}\} \subset \mathbb{R}^n$$



The vectors $\vec{v}_1 = (1, 0)$, $\vec{v}_2 = (0, 1)$ define a square lattice in $\mathbb{R}^2$.

Unit cell of a lattice

A *unit cell* of a lattice L is a parallelepiped generated by any $\vec{v}_1, \ldots, \vec{v}_n \in \mathbb{R}^n$ representing L.



Infinitely many unit cells represent the same lattice.

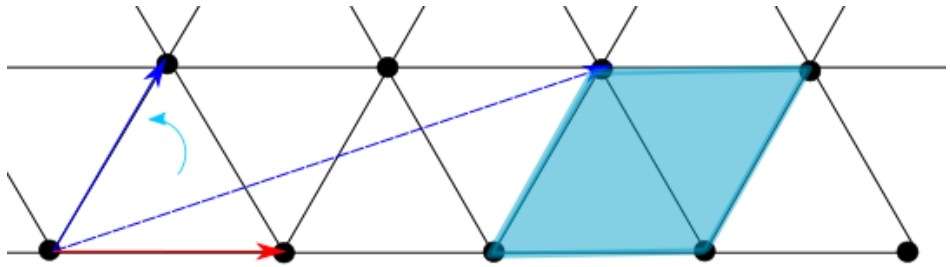
Distances between lattices

- Our goal is to give a distance between crystals to aid prediction and synthesising.
- As a first step we must compare lattices.
- Crystallographers compare two lattices by dividing the space of lattices into discrete classes depending on the symmetry of the lattices.
- The space of lattices is path-connected, so it makes more sense to compare lattices using a metric.
- An idea is to obtain a canonical unit cell and then compare them geometrically.

Niggli reduced cell

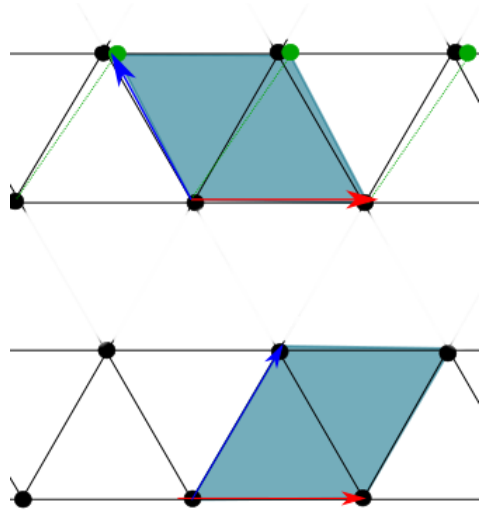
A common canonical choice is the *Niggli reduced cell*, which is defined by a basis such that

$$\| \operatorname{proj}_{\langle v_i \rangle} v_j \| \leq \frac{\| v_i \|}{2} \quad \forall i, j$$



Shortcomings of the Niggli cell

Niggli cells are not stable under perturbations.

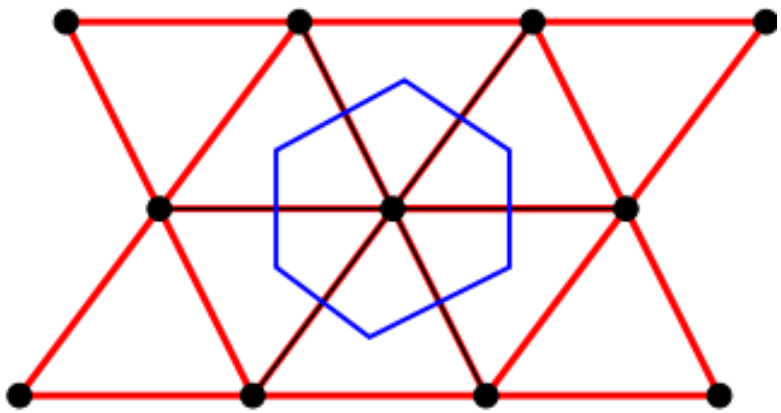


- We can construct a convergent sequence of lattices for which the Niggli cells don't converge.
- From the point of view of Chemistry, this comparison disregards the fact that atoms vibrate.

The Voronoi cell of a lattice L

The *Voronoi cell* of L is the neighbourhood of points $q \in \mathbb{R}^n$ that are closer to 0 than to all other points of the lattice L:

$$V(L) = \{q \in \mathbb{R}^n | \|q\| \leq \|q - l\|,\ l \in L\}.$$



For $n = 2$, the Voronoi cell $V(L)$ is a rectangle or a centrally symmetric hexagon.

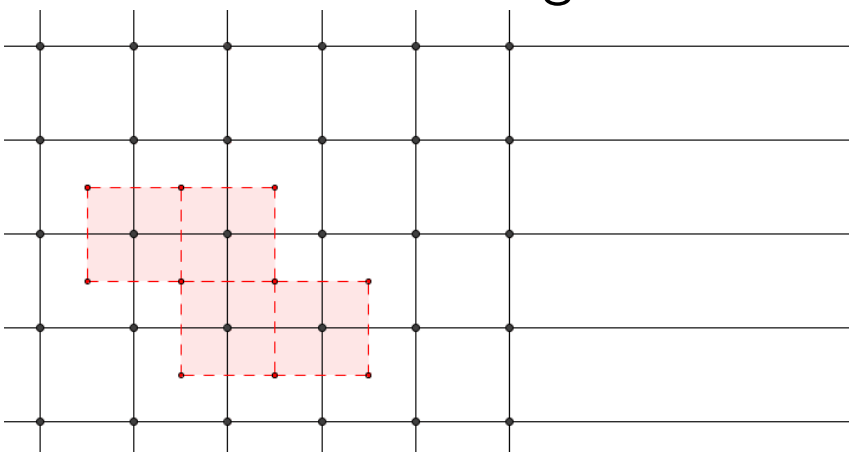
Translating $V(L)$ by points of the lattice tiles $\mathbb{R}^n$.

Distances between Voronoi cells

The *Hausdorff distance* between cells A, B (modulo rotation) is

$$d(A,B) = \min_{T \in SO(n)} \min\{\varepsilon : T(A) \subset B^{\varepsilon}, B \subset T(A)^{\varepsilon}\},$$

where B^{ε} denotes the closed ε-neighbourhood of B.
$V(L)$ changes continuously as L is continuously varied. This makes the above distance a good metric on the space of lattices.



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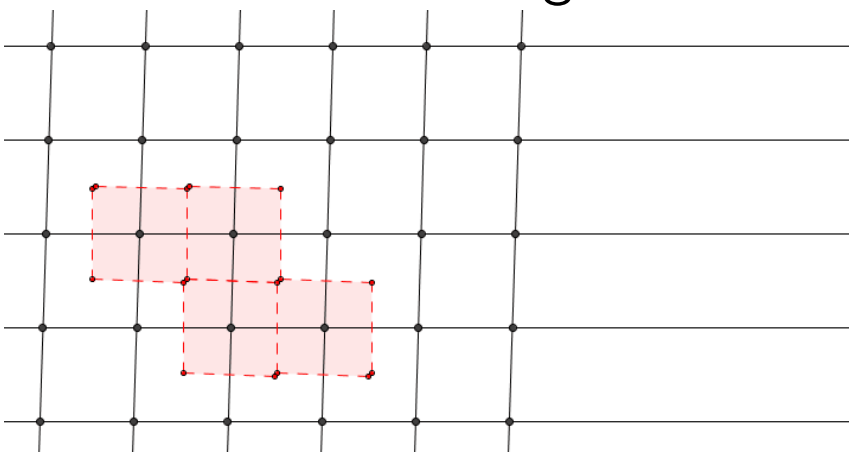

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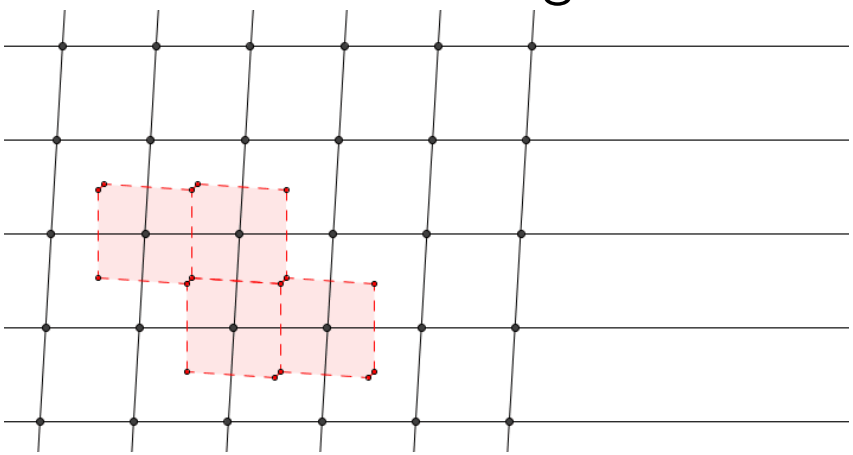

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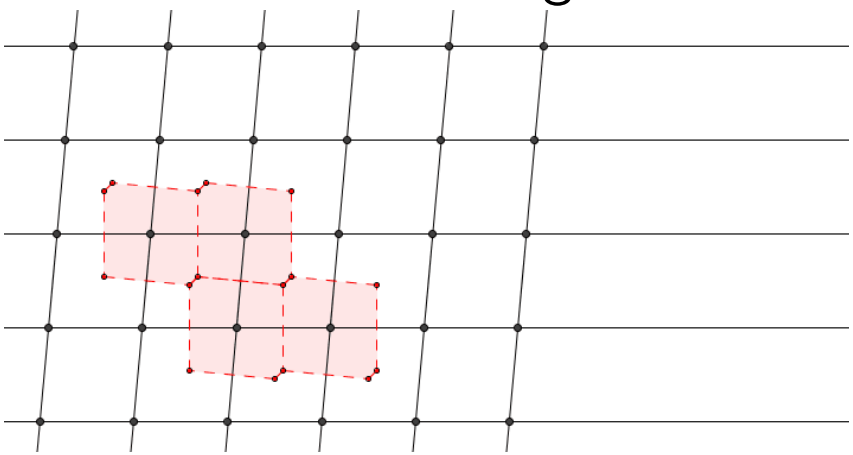

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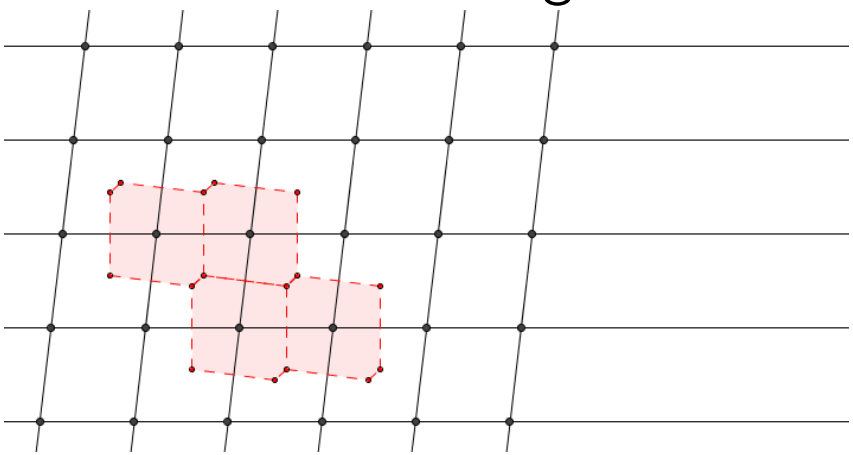

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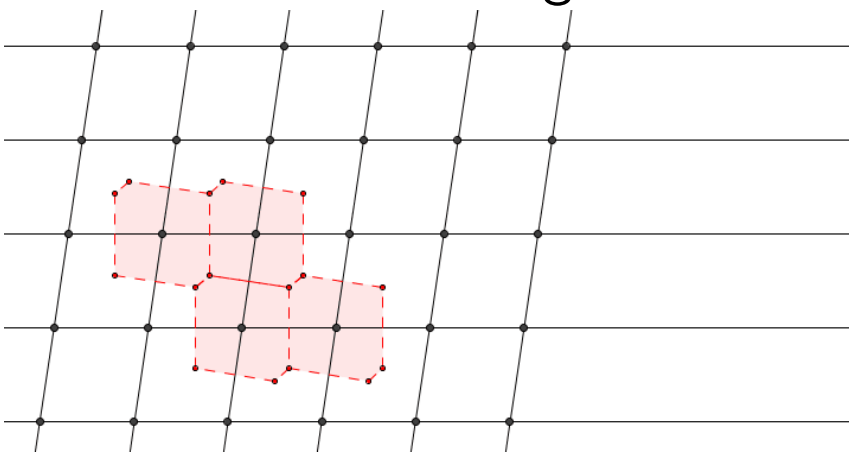

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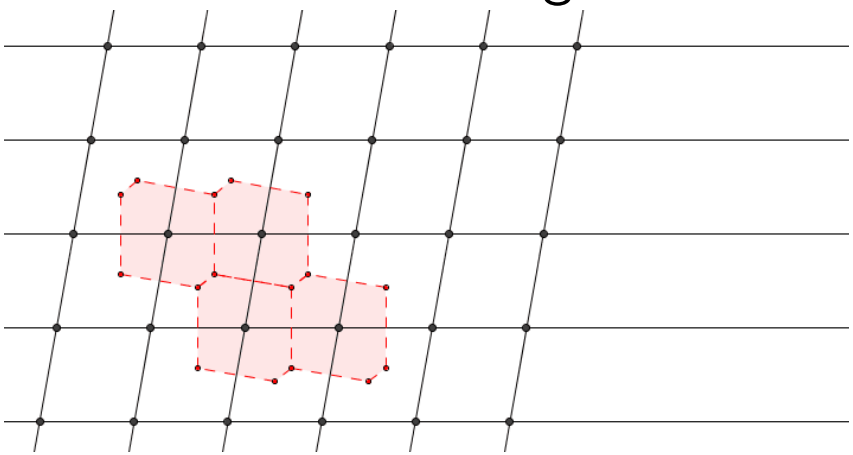

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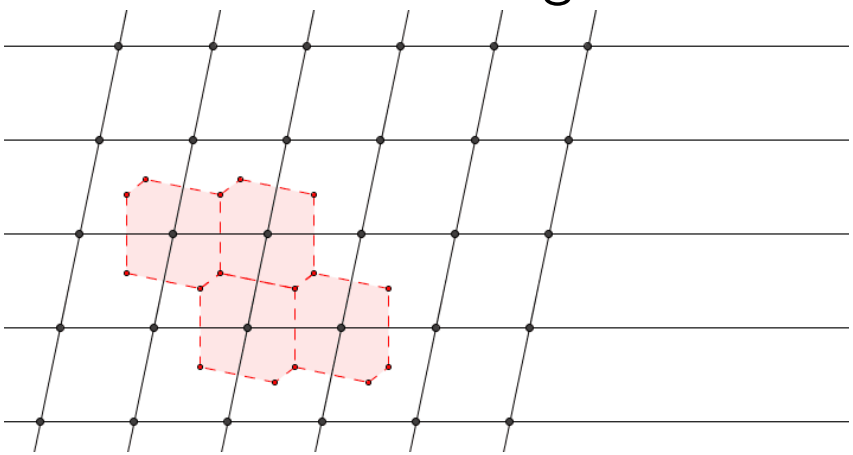

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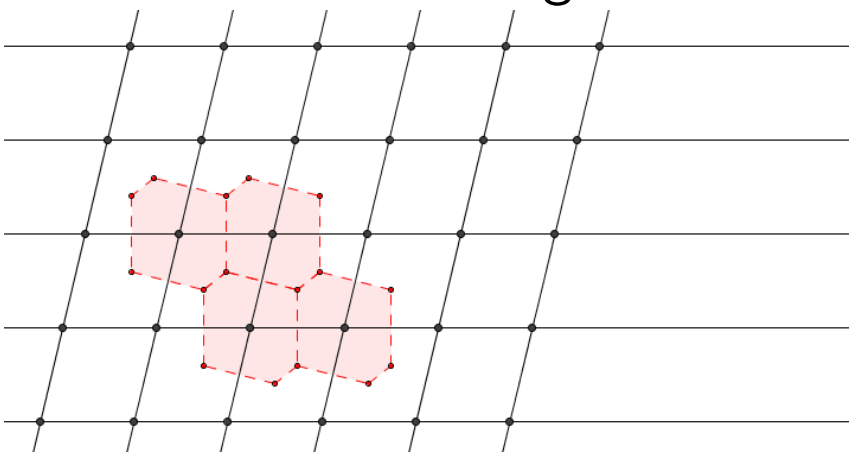

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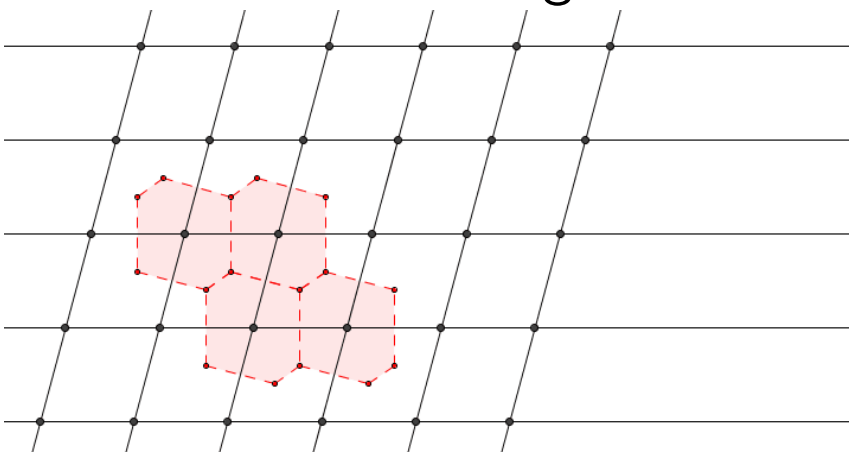

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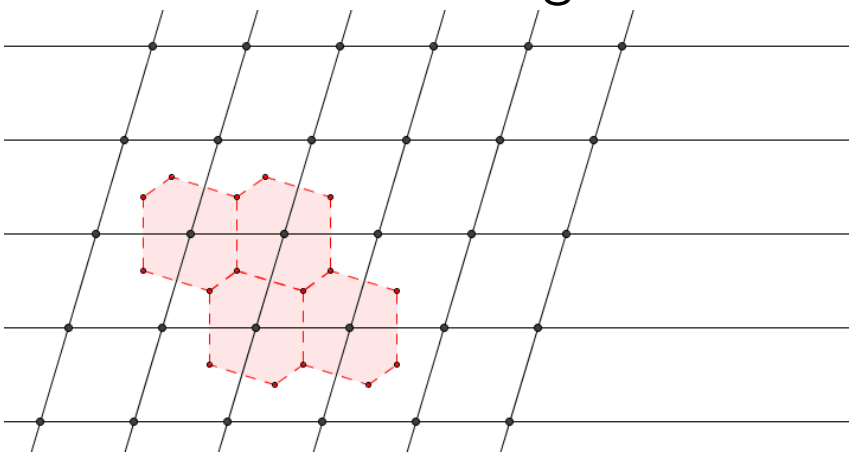

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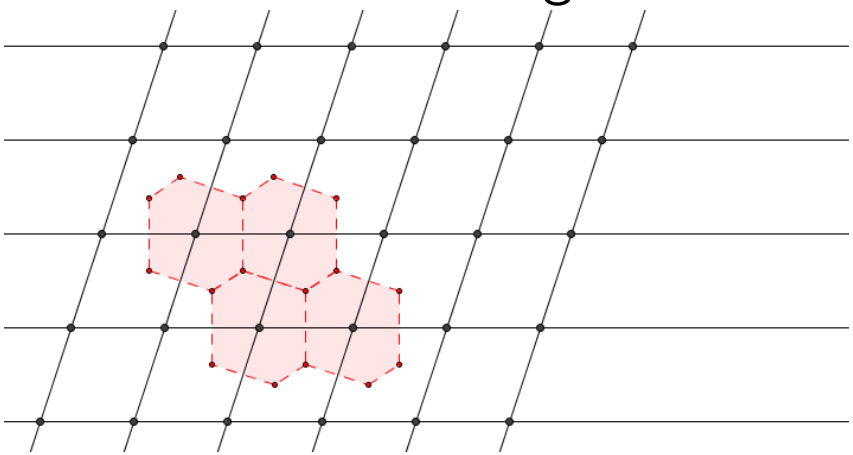

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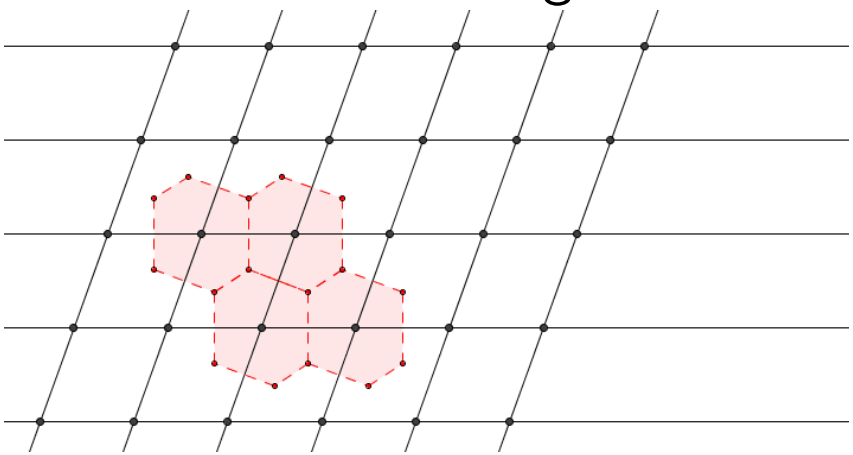

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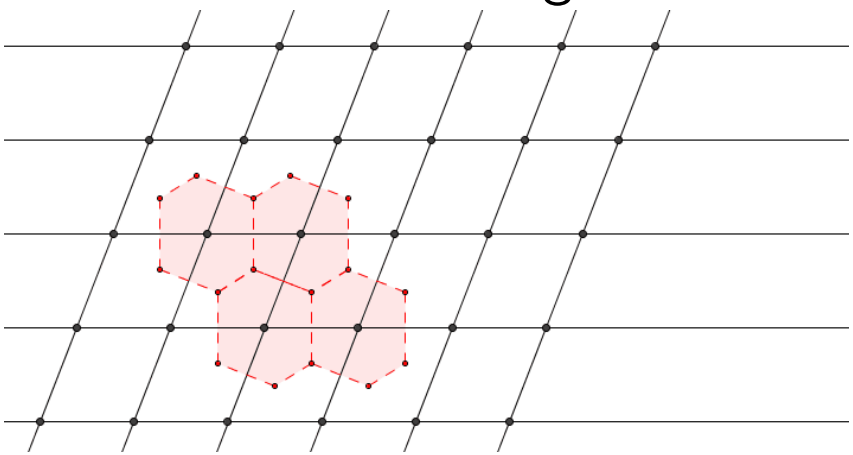

Computing $V(L)$

A typical way to obtain $V(L)$ is to first fix a unit cell, extend it k times in all directions, and search for the boundary of $V(L)$ in this extended cell $C(k)$.

Theorem (G-P–Kurlin)

Given any lattice L and any $k \in \mathbb{N}$ there is a unit cell such that $C(k)$ does not contain $V(L)$.

Theorem (G-P–Kurlin)

In $\mathbb{R}^2$, the extended cell $C(2)$ of a Niggli cell contains $V(L)$. Higher dimensions are work in progress.

Future work

- We are now working on incorporating all the information of a crystal: how can we encode in a unique way a configuration of points (atoms) inside a unit cell.
- A usual technique in Chemistry is to take the distances to the closest neighbours of each atom.
- I constructed a family of counterexamples of different crystals, all with the same list of distances to the closest, 2nd closest,..., k-closest neighbours.

Thank you!