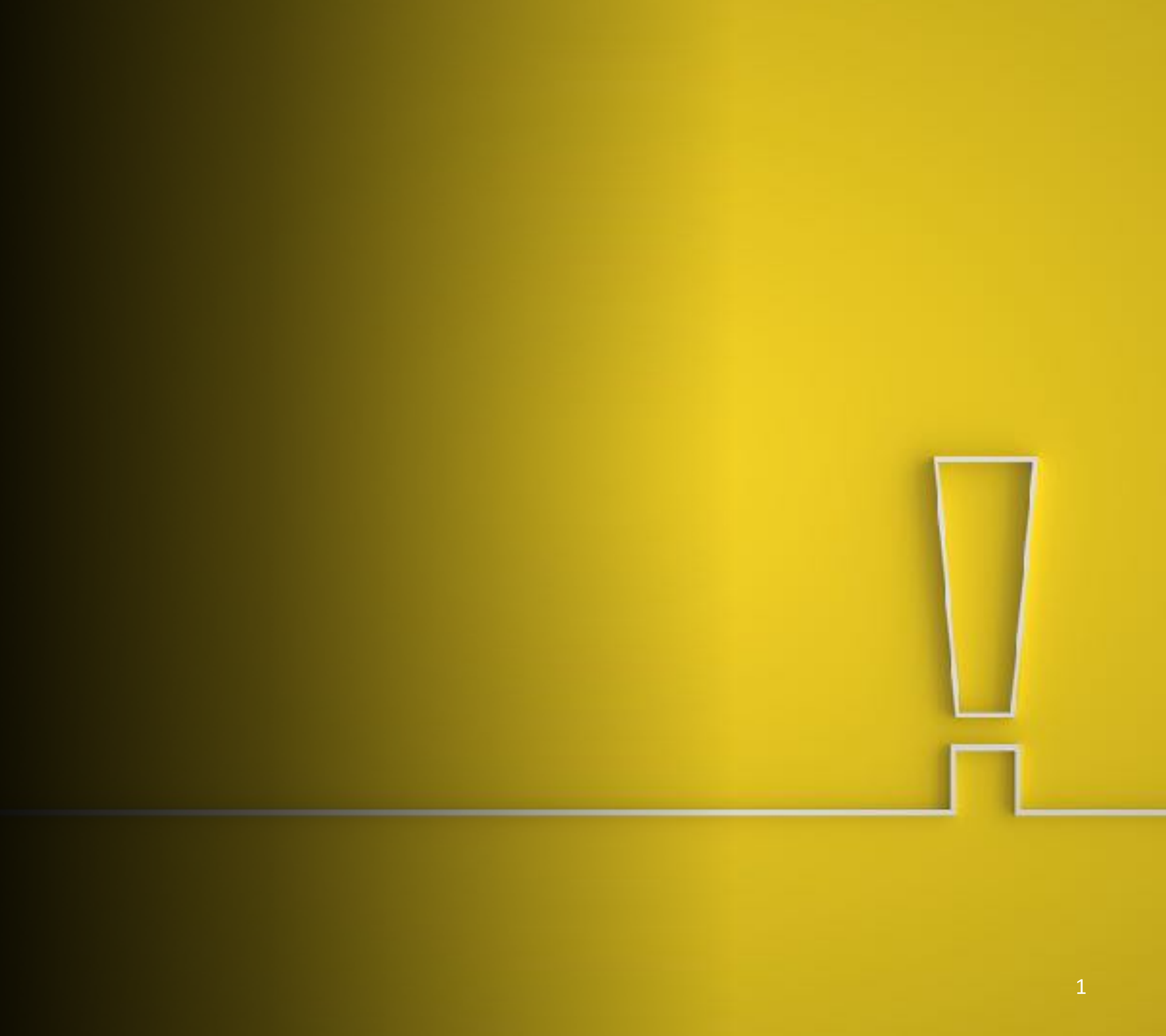
Symmetry to create classifications

Symmetry operators



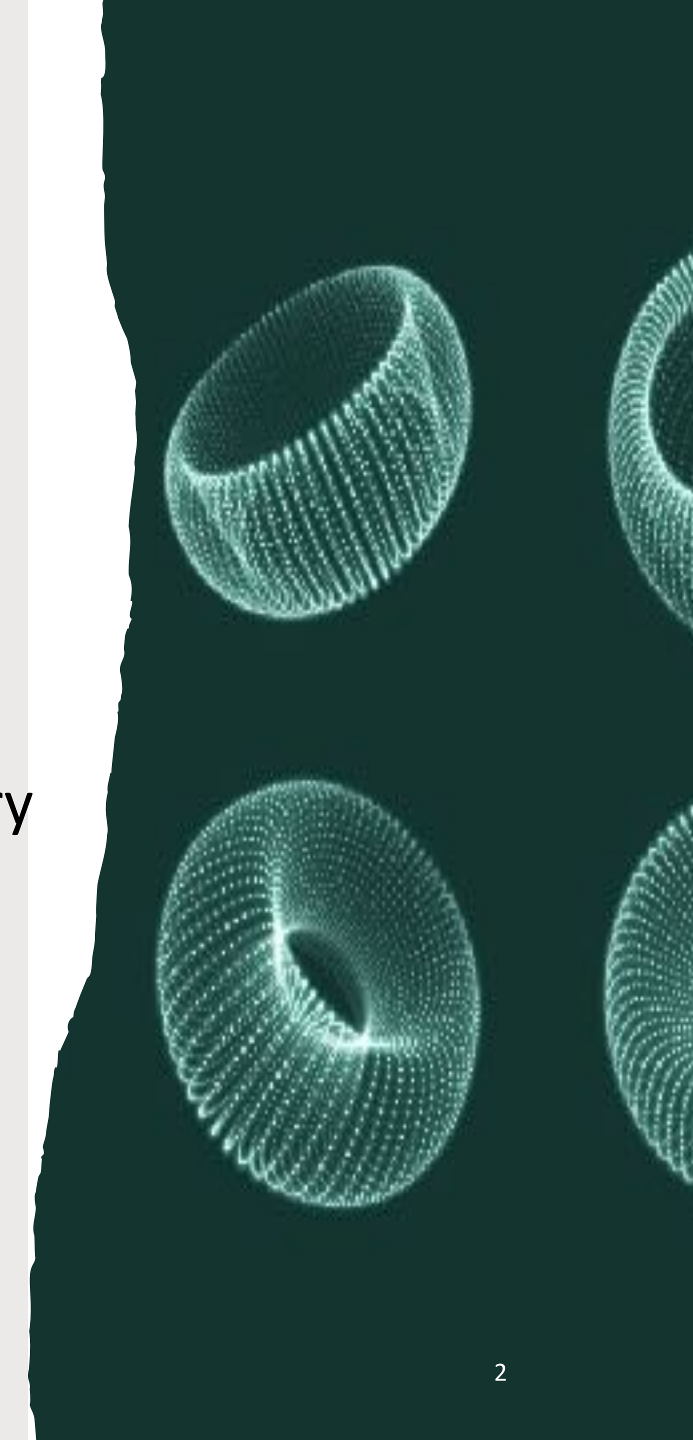
Symmetry operations/elements

- A rotation, reflection, or translation that
  - brings the lattice into self-coincidence
  - preserves distances between lattice points

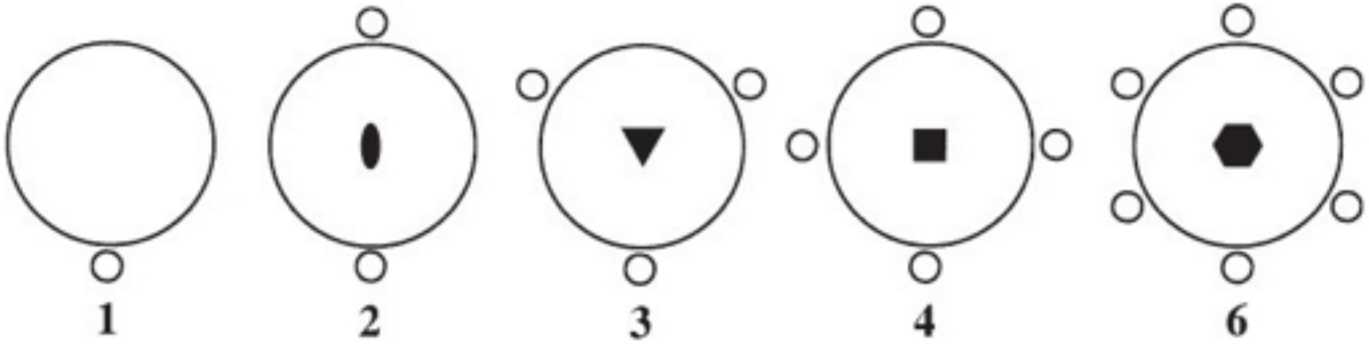
- A rotation θ about an axis is called *n*-fold, where $n = \frac{360}{\theta}$
  - Only *n* = 1, 2, 3, 4, and 6 compatible with translational symmetry
  - Diad, triad, tetrad, and hexad

- Inversion (denoted as $\bar{1}$) →(x, y, z) to ($\bar{x}$, $\bar{y}$, $\bar{z}$)

- Reflection ($\bar{2}$) is a combination of inversion and a diad



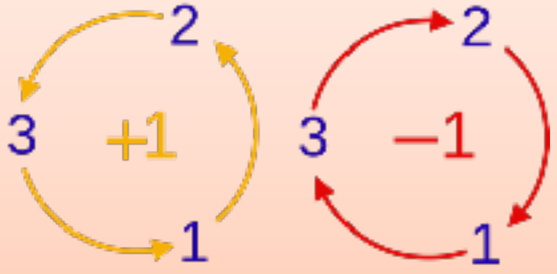
Symmetry operators as matrices



$$D_{ij} = \delta_{ij}\cos\theta - \varepsilon_{ijk} n_k \sin\theta + (1 - \cos\theta) n_i n_j$$

$$\delta_{ij} = 0,\ i \neq j$$
$$= 1,\ i = j$$

ε_{ijk}



Problem

Determine the rotation matrix for the following:

- 6-fold rotation along a_3
- 2-fold rotation along $a_1 + a_3$

Practice problem

Show that a 5-fold rotation axis is inconsistent with the definition of a lattice

The Bravais Lattices

2D Bravais Nets

3D Space lattices - Development and mathematical operations

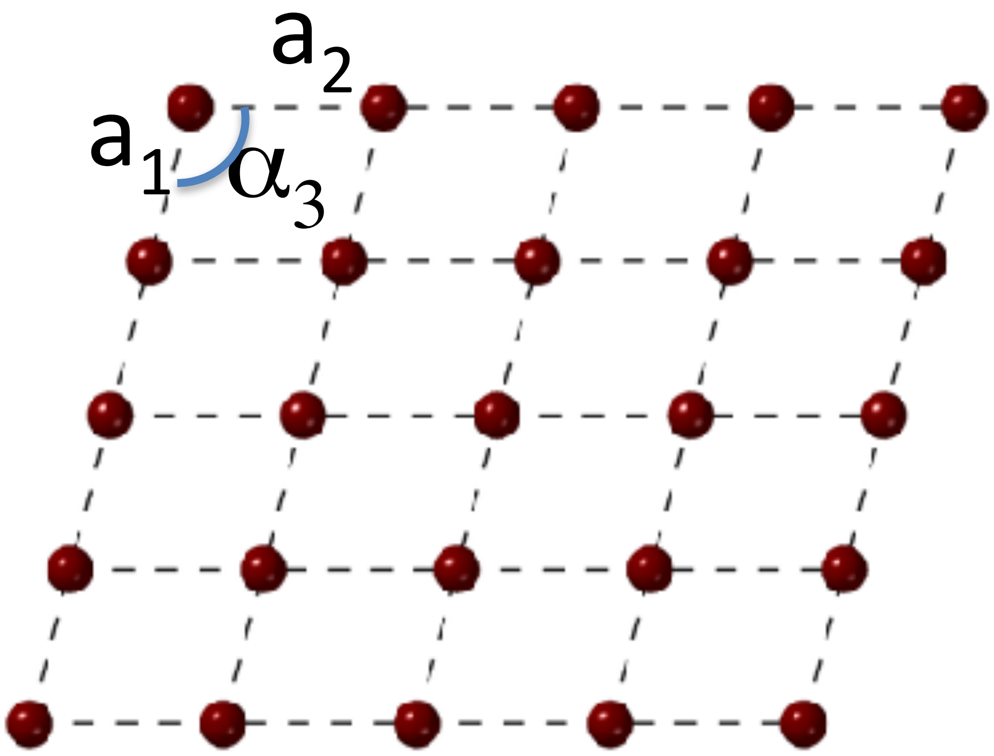
Lattice properties

- Concept of the unit cell
  - Primitive vs. Non-primitive
- Effect of adding symmetry elements
  - Distinct possibilities
  - Crystal systems
- Additional translation symmetry – centering
- Illustrate with 2-D lattice or net

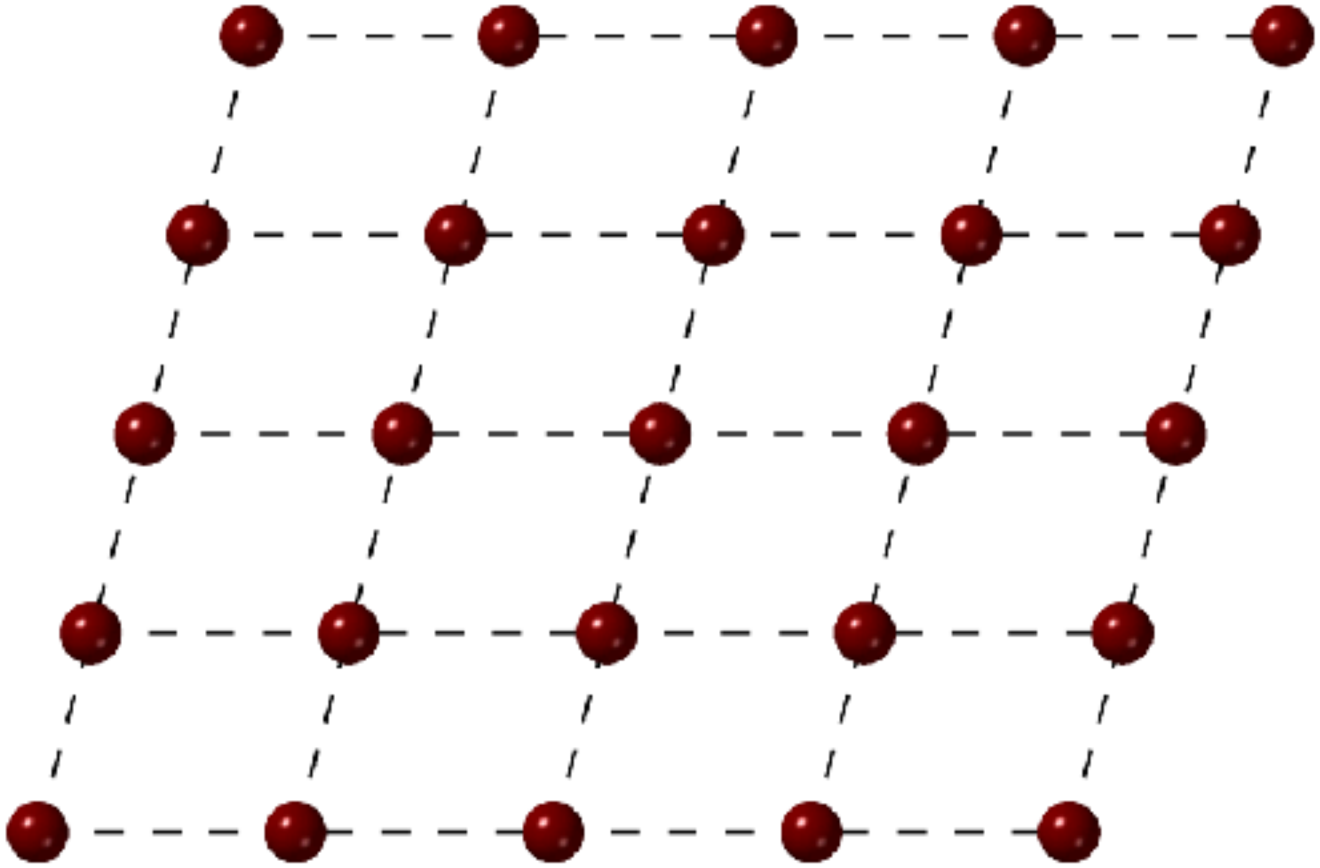
The most general net – Oblique net

$$\left(a_1, a_2, \alpha_3\right)$$

$a_1 \neq a_2, \alpha_3$ not special value



Primitive vs. Non-primitive



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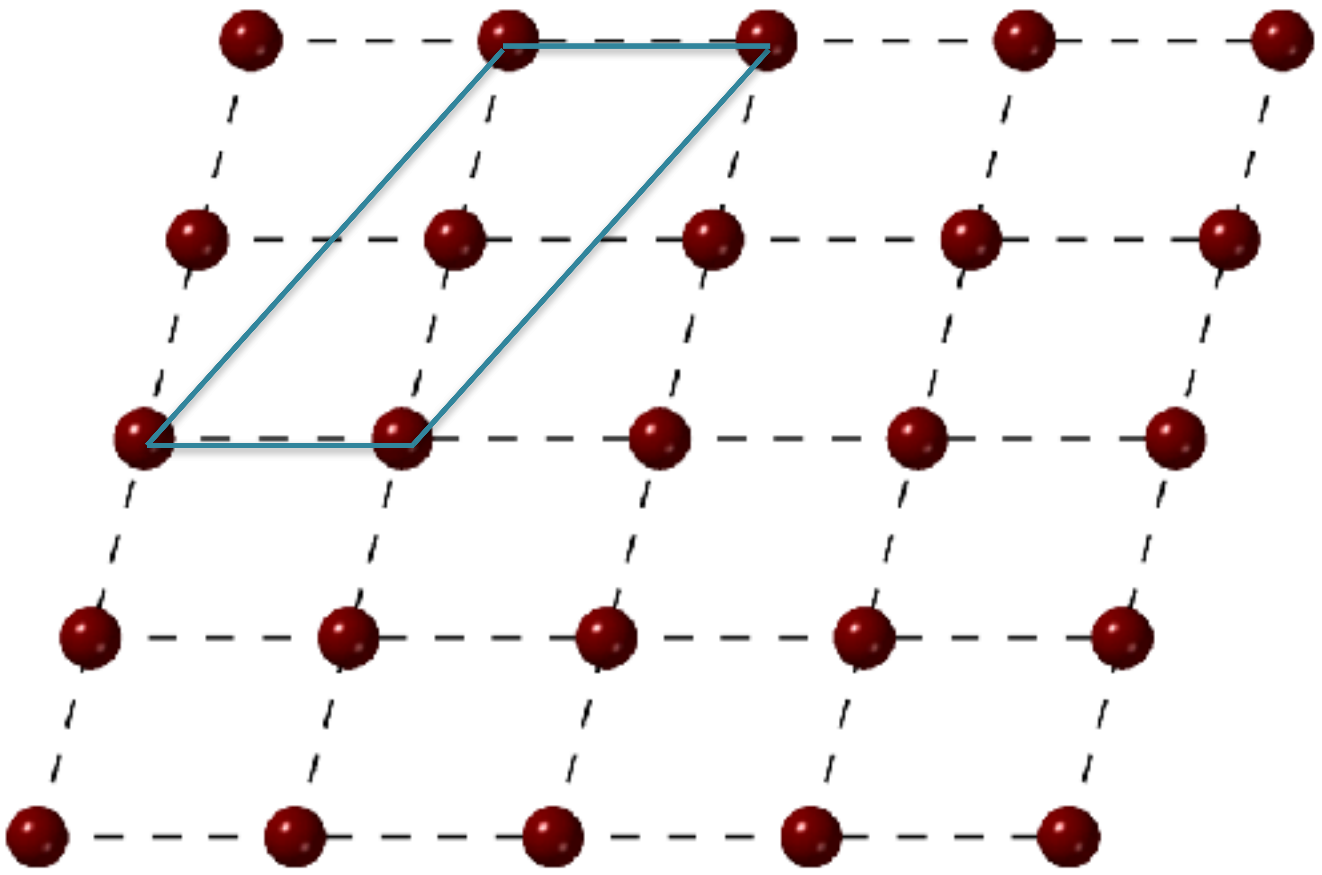
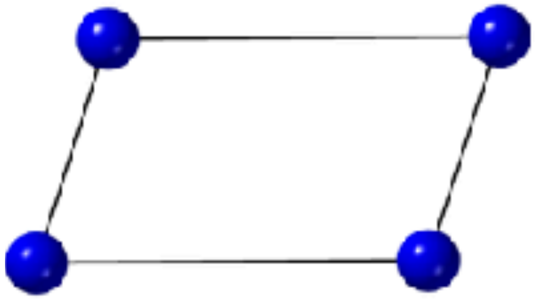


The 2D Bravais nets



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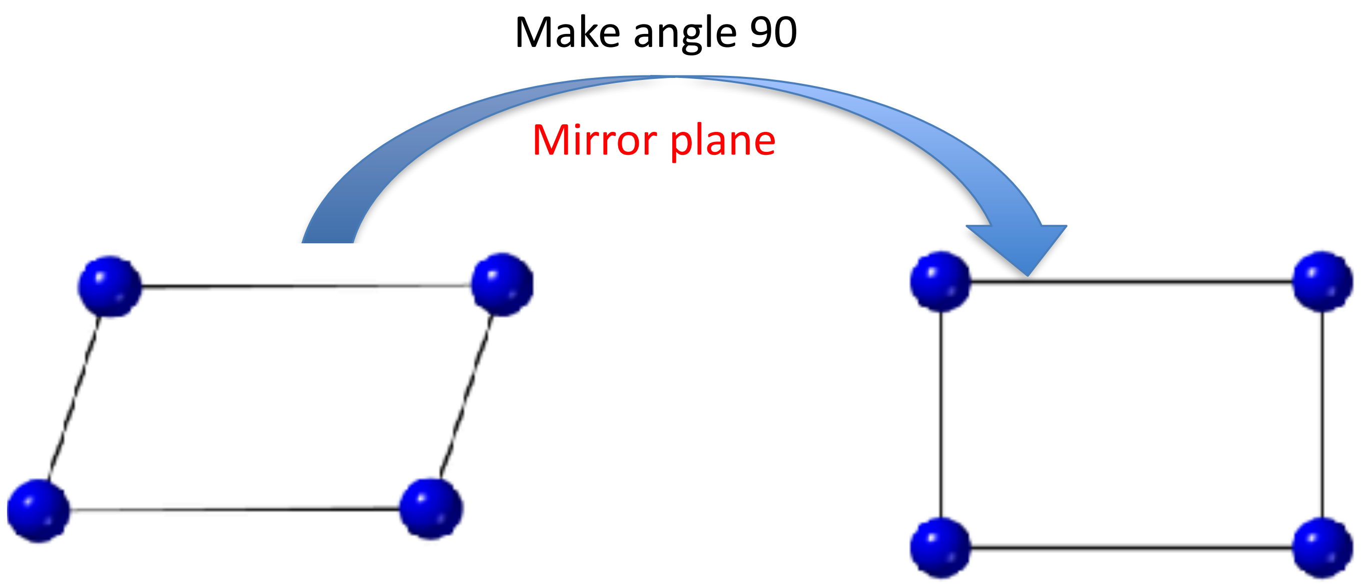
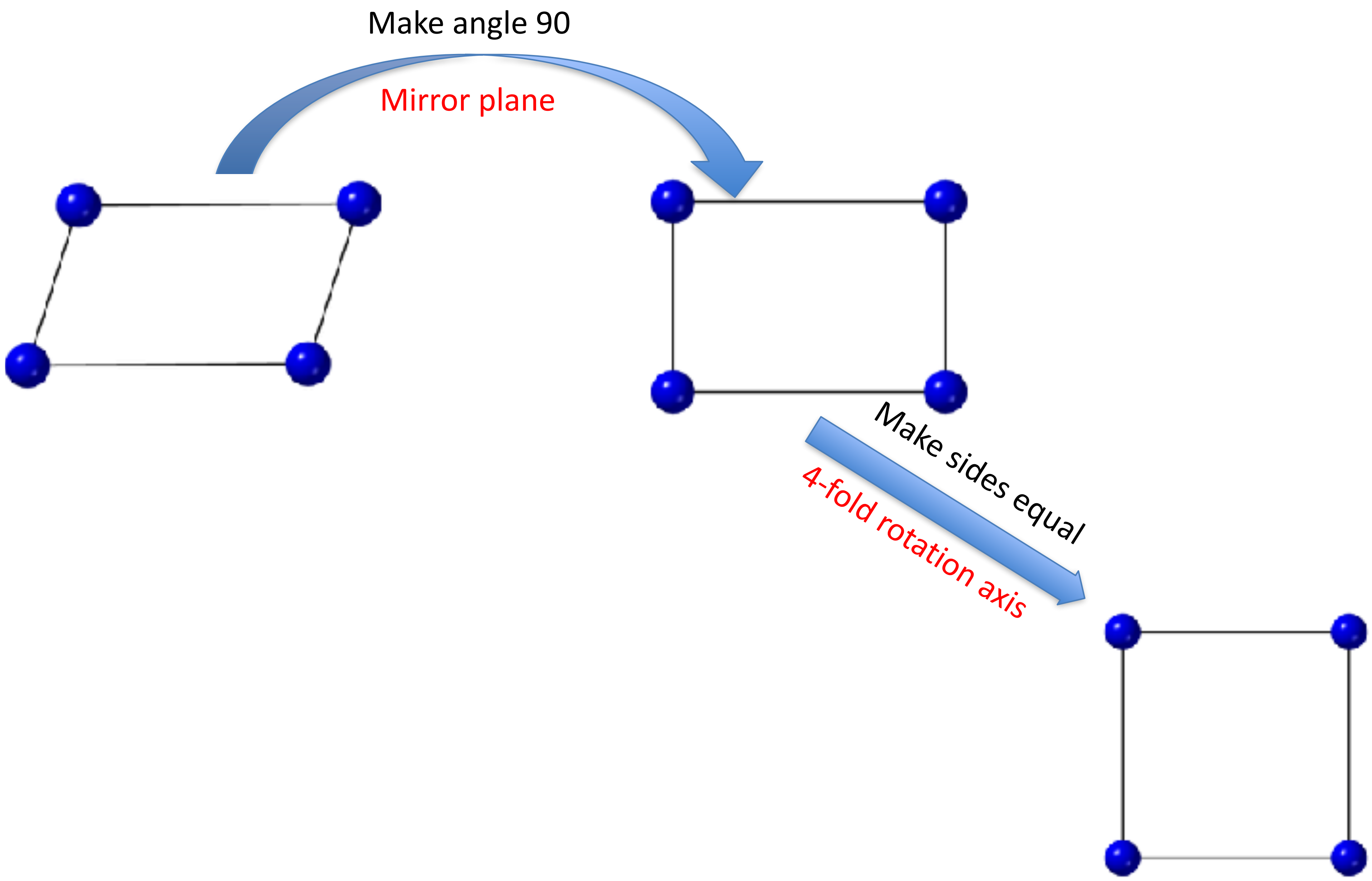
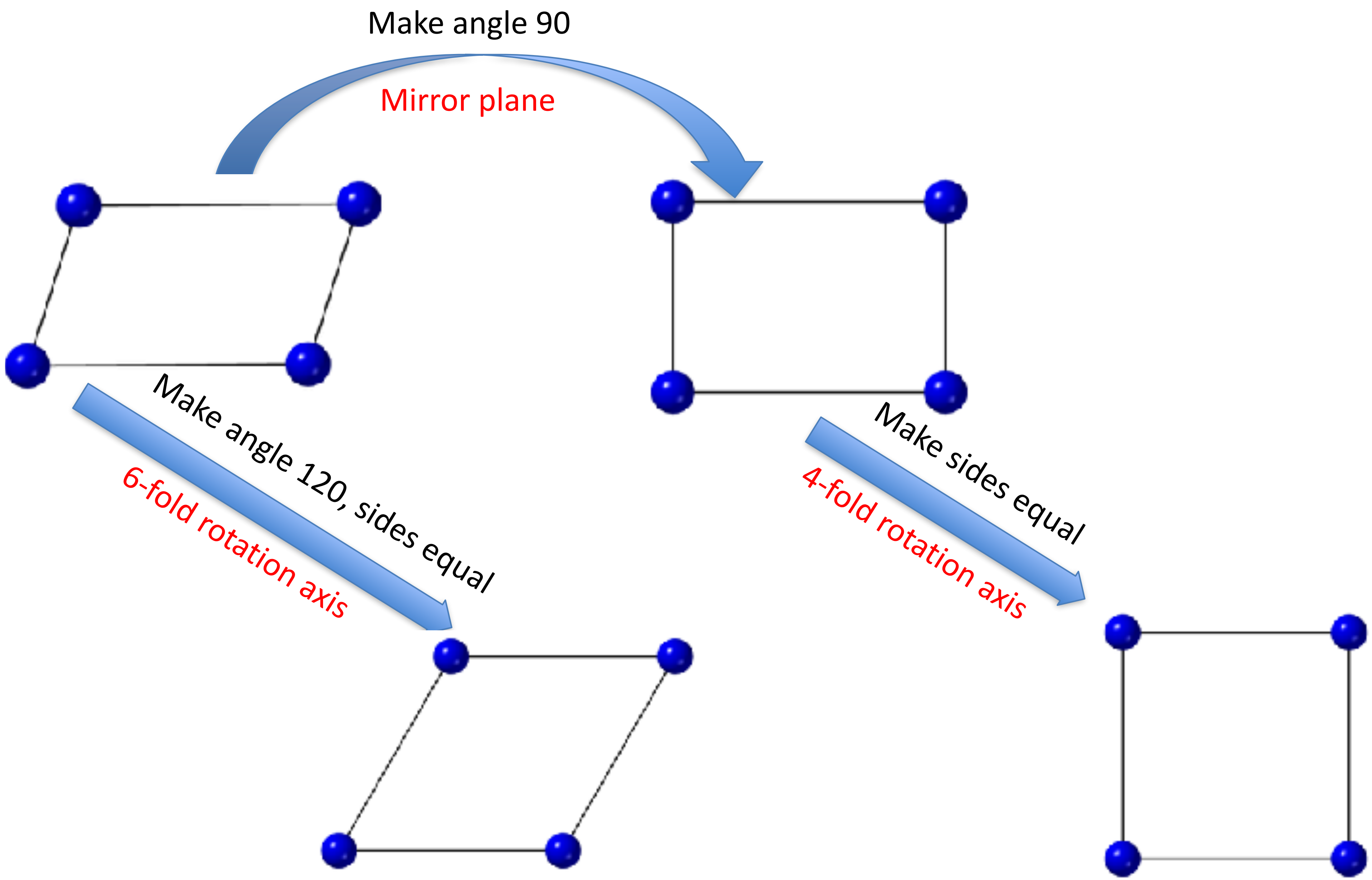


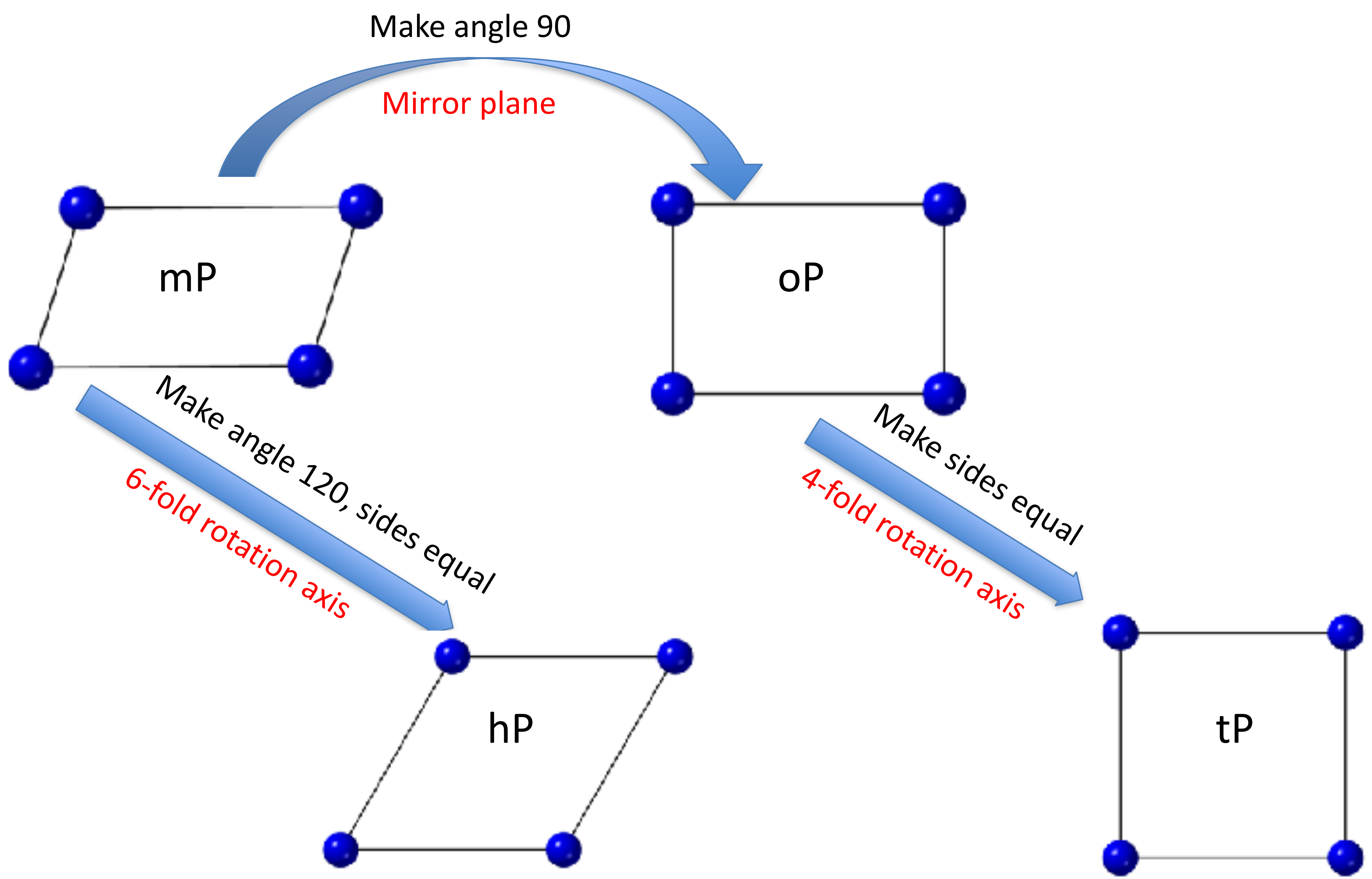
The 2D Bravais nets



The 2D Bravais nets

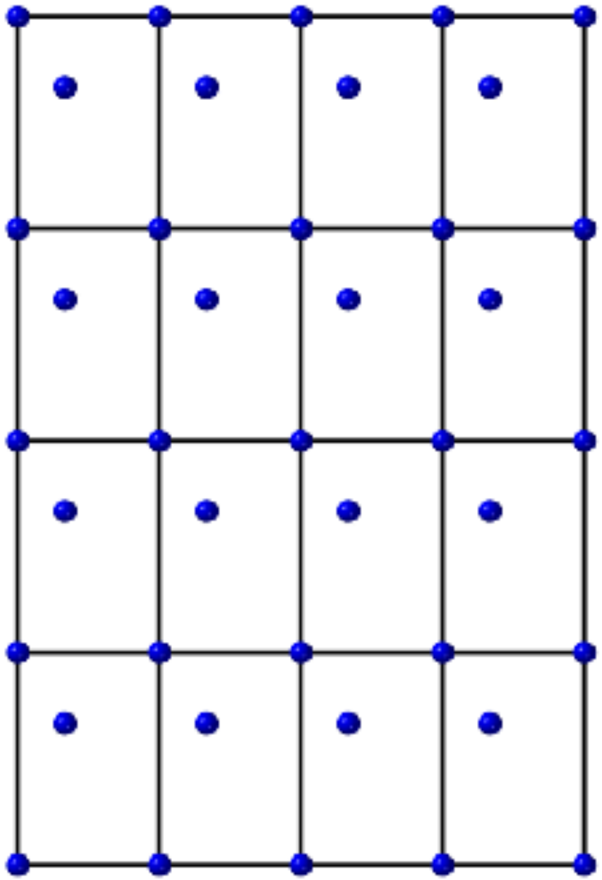


The 2D Bravais nets



Additional Lattice points

Where can we put additional lattice points ?



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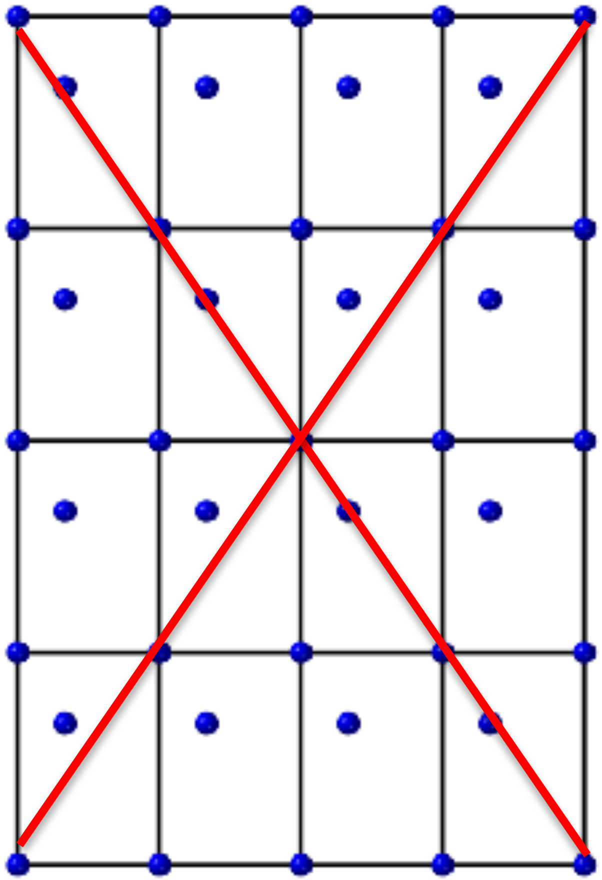

Additional Lattice points

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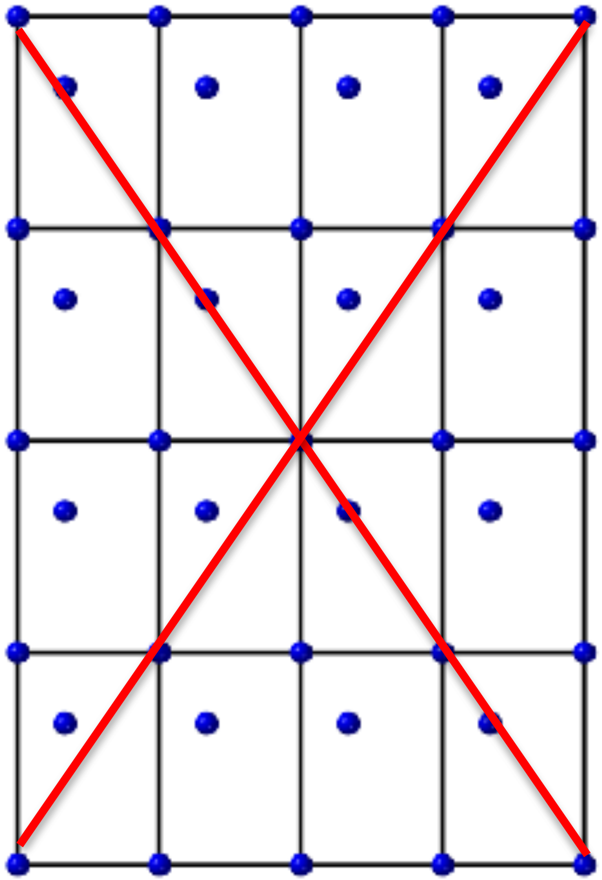
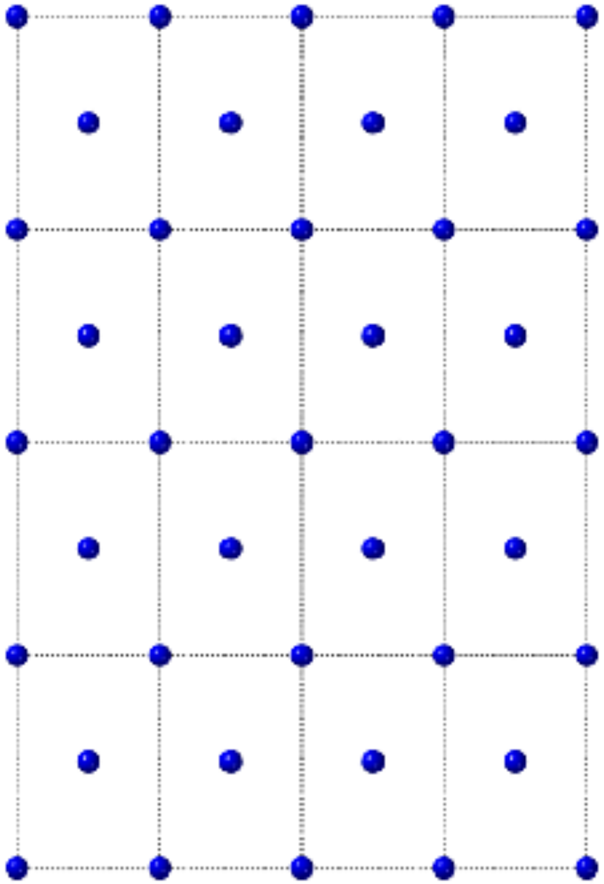
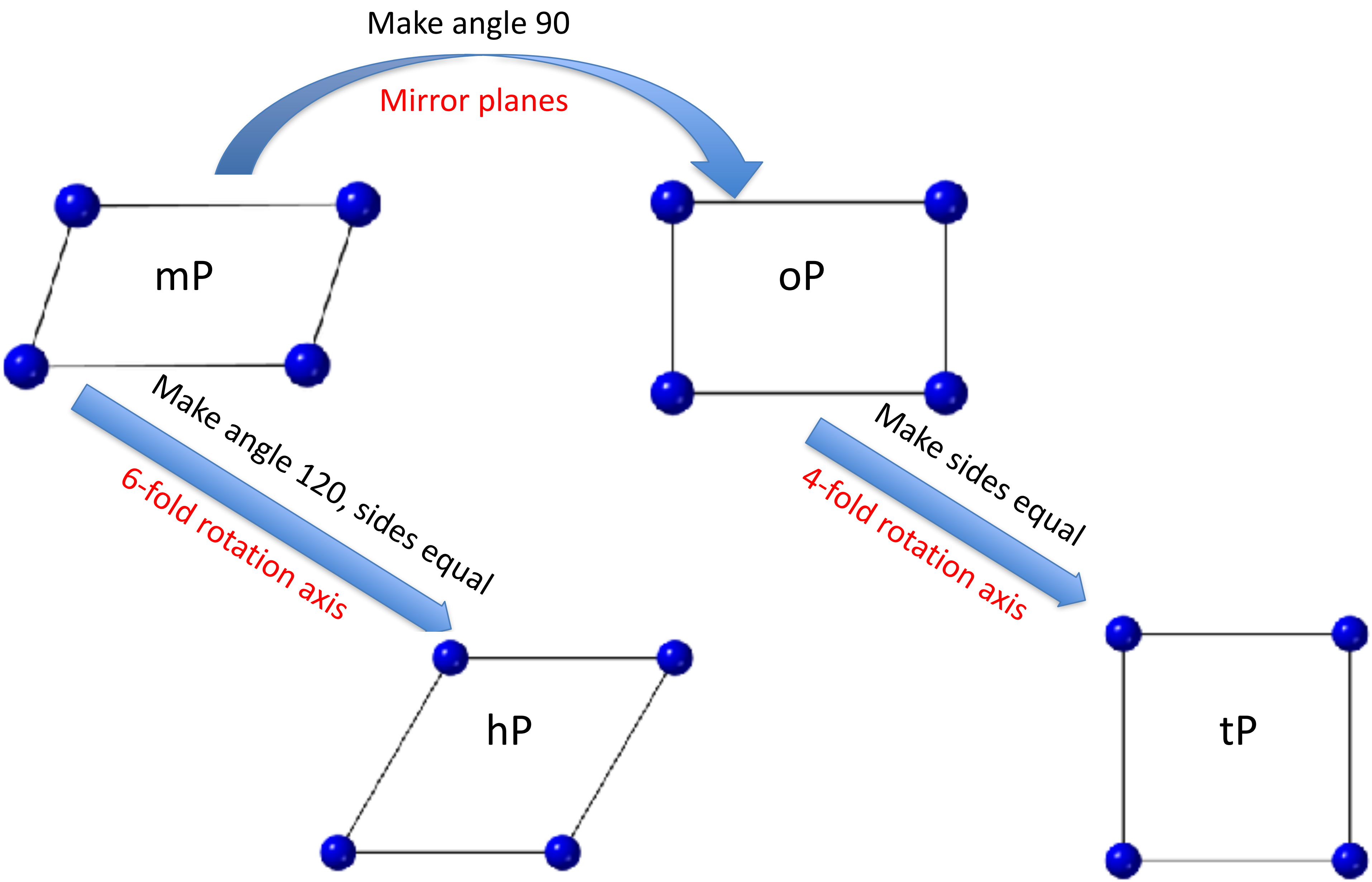
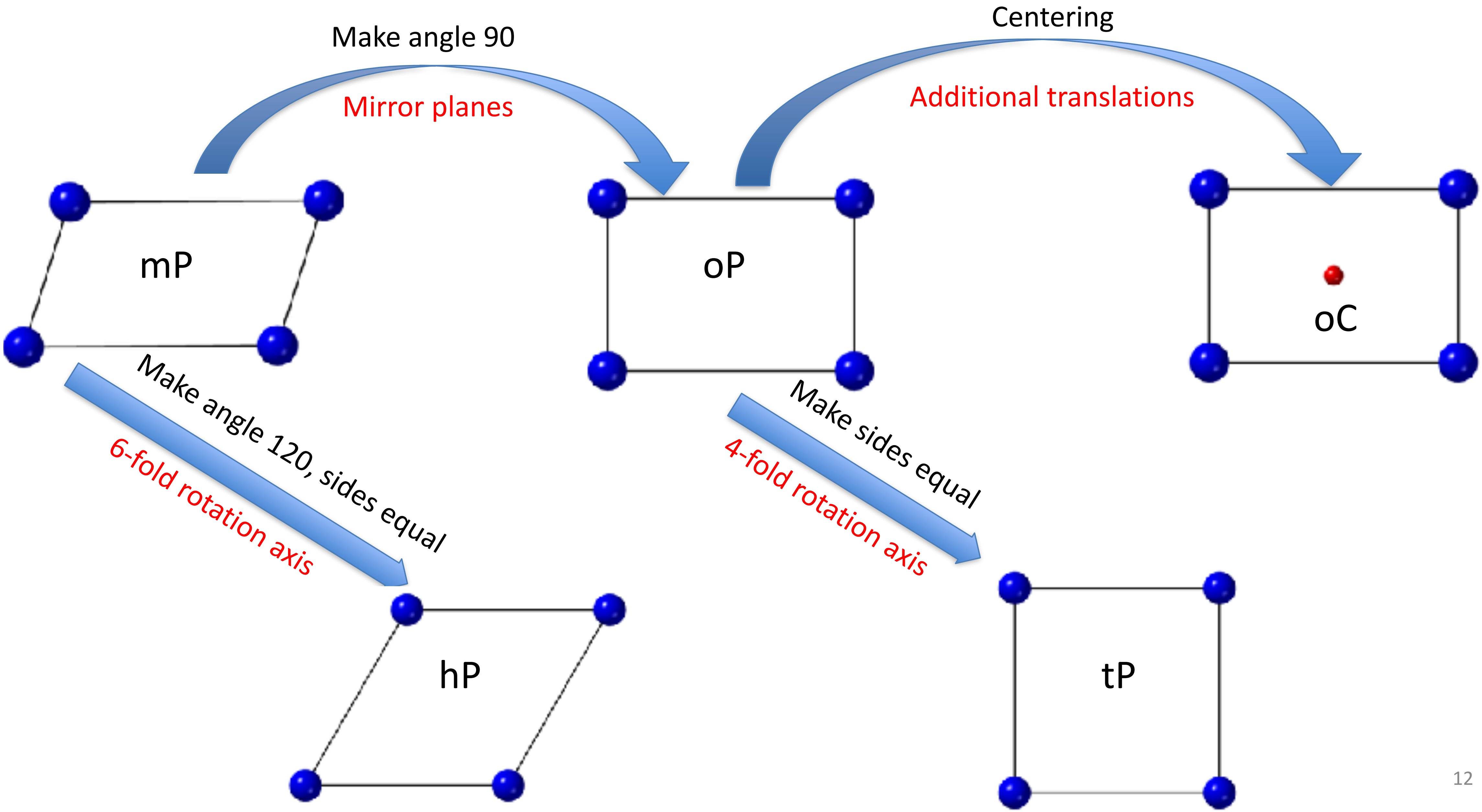




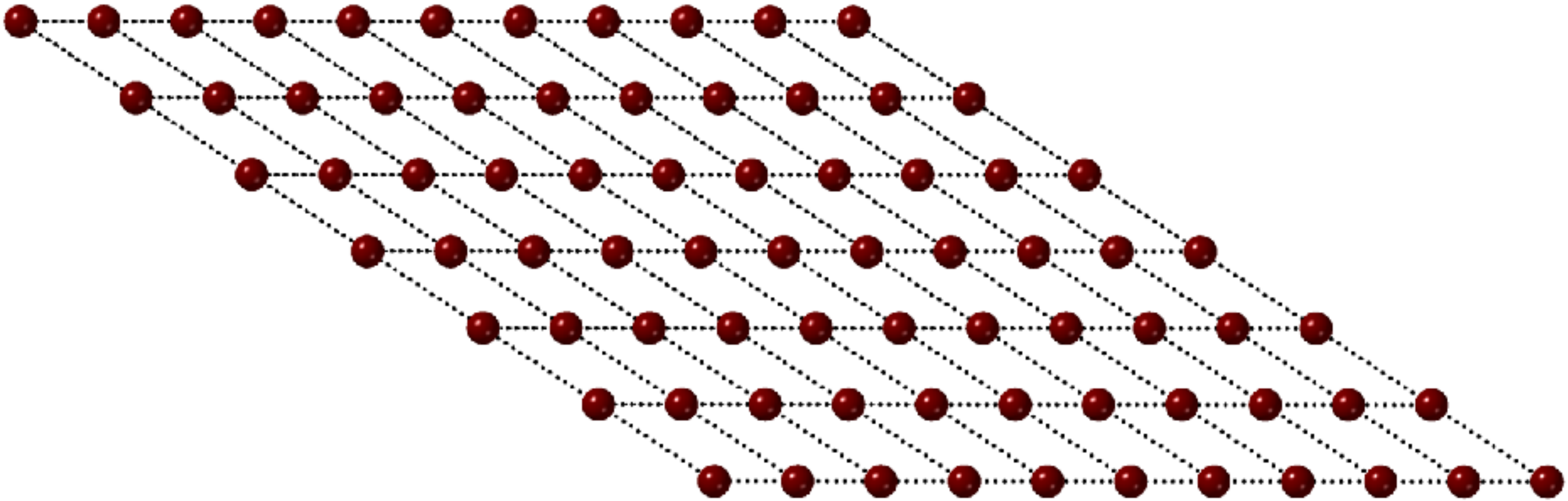
The 2D Bravais nets



The 2D Bravais nets



Which net to choose?



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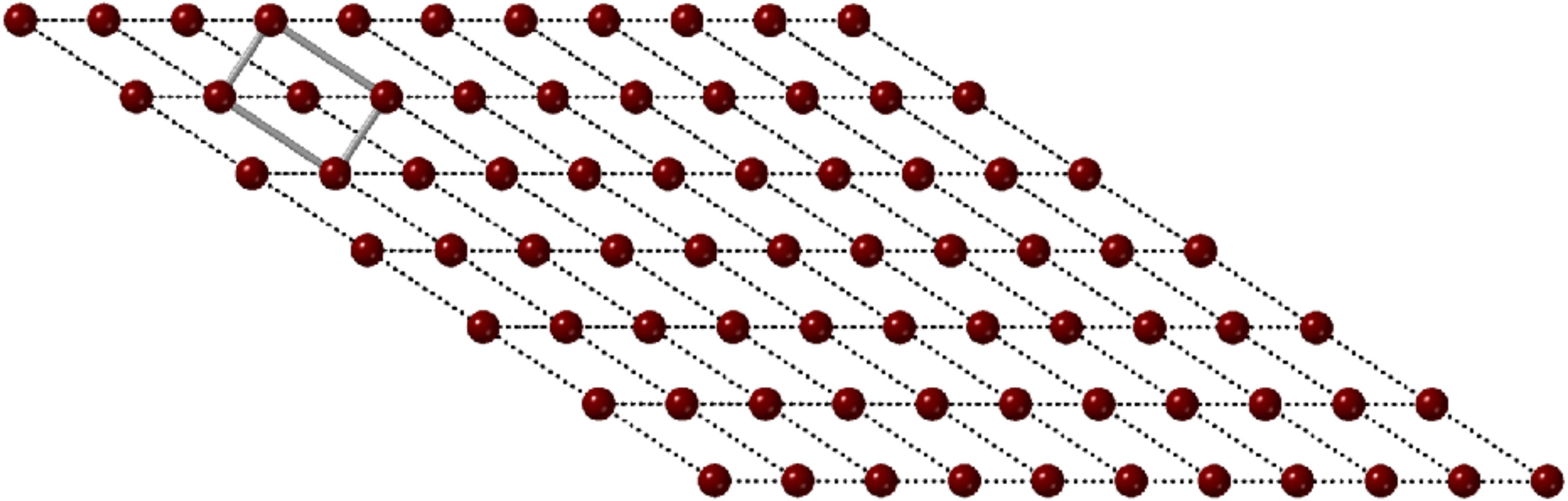

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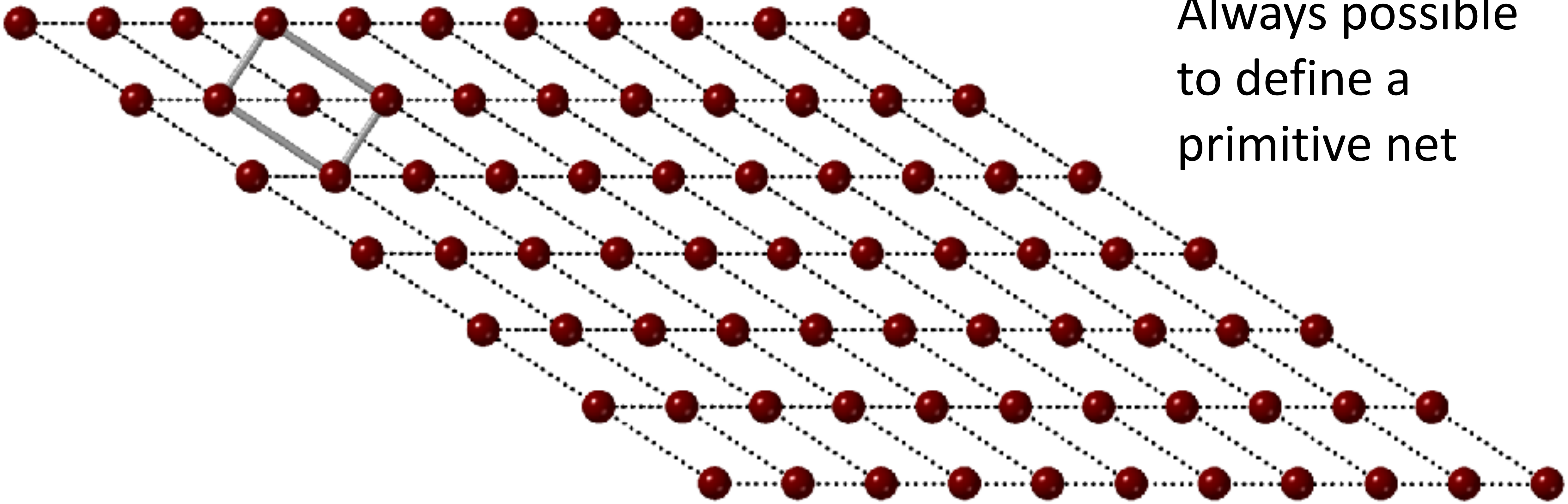
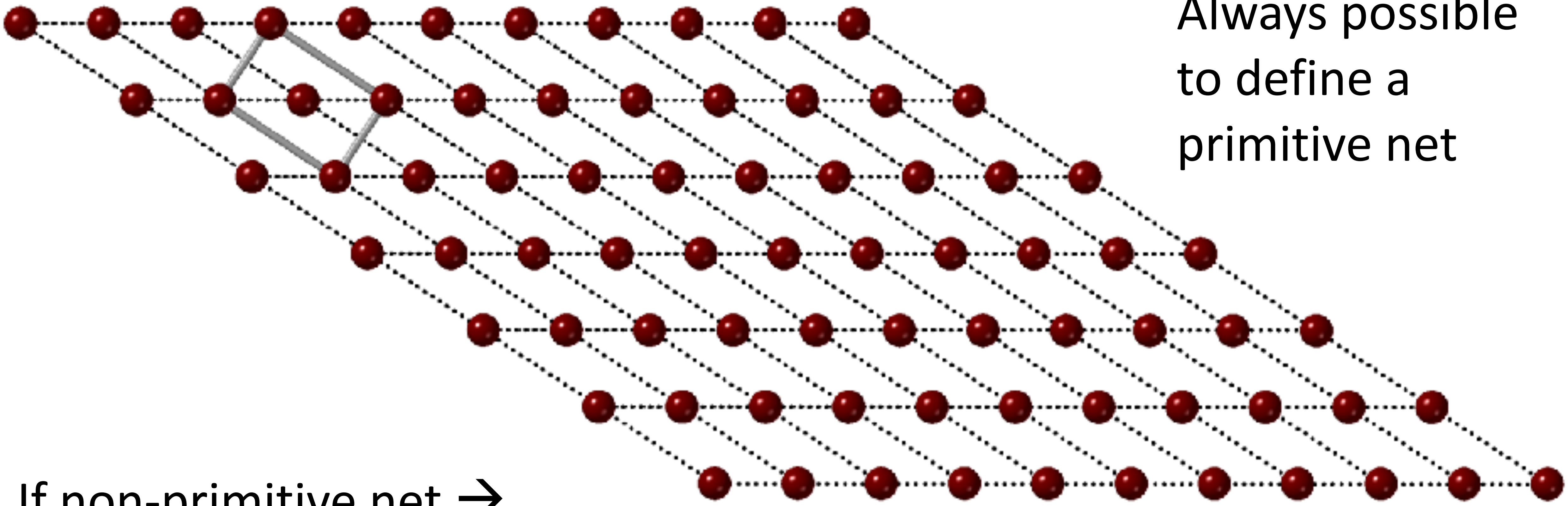


Always possible to define a primitive net

Which net to choose?



Always possible to define a primitive net

If non-primitive net → higher symmetry of lattice, choose it.

Problem

Show that an arrangement of points in 2-D, which on a cursory glance, you identify as *tC*, is not a new lattice.

The space lattice

01

Move on to 3 dimensions

02

Introduce new rotational symmetry elements

- Relationships between lattice parameters
- Special values of angles

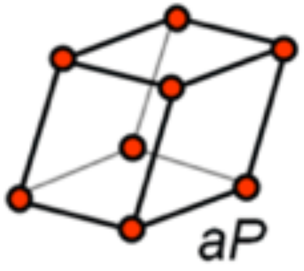
03

Introduce new translational symmetry

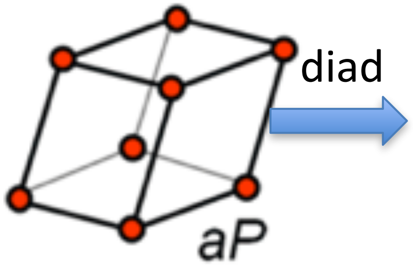
- Additional lattice points in the unit cell

The primitive space lattices

The primitive space lattices



The primitive space lattices



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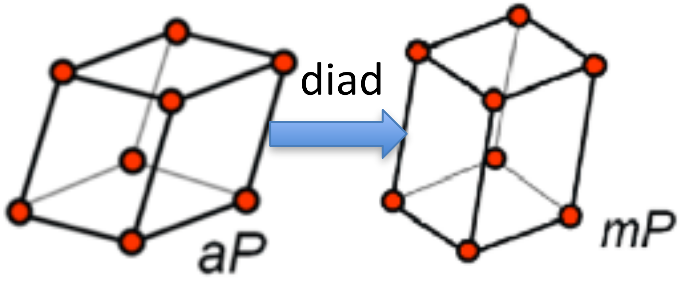

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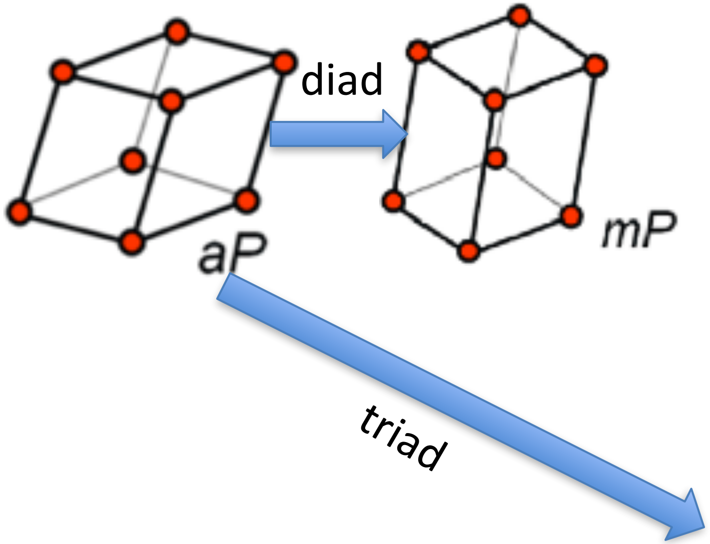

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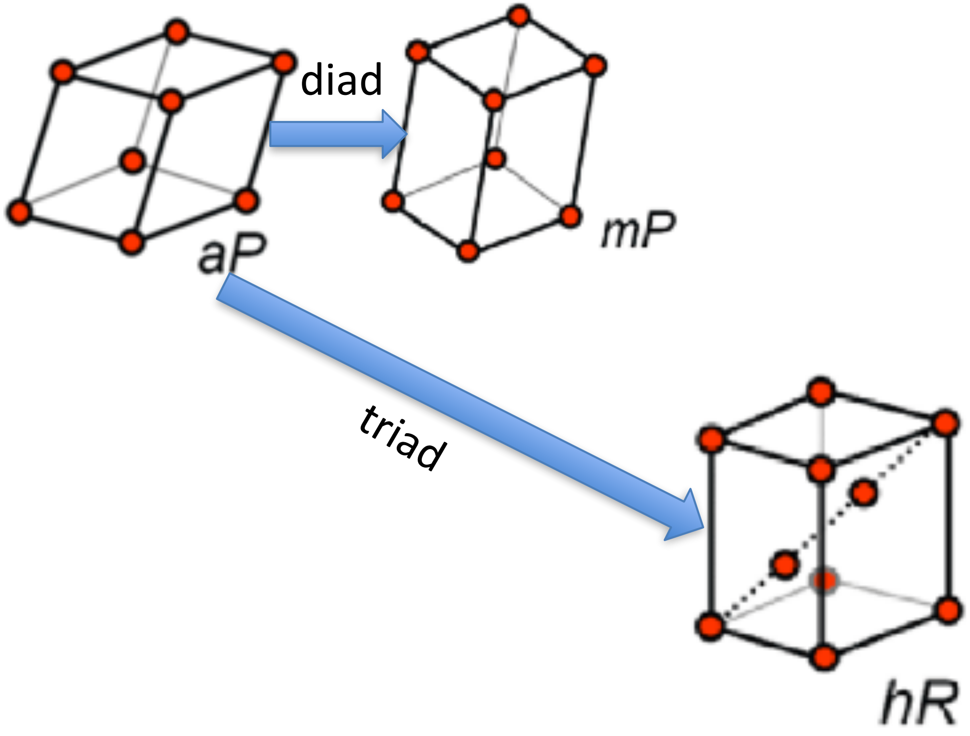

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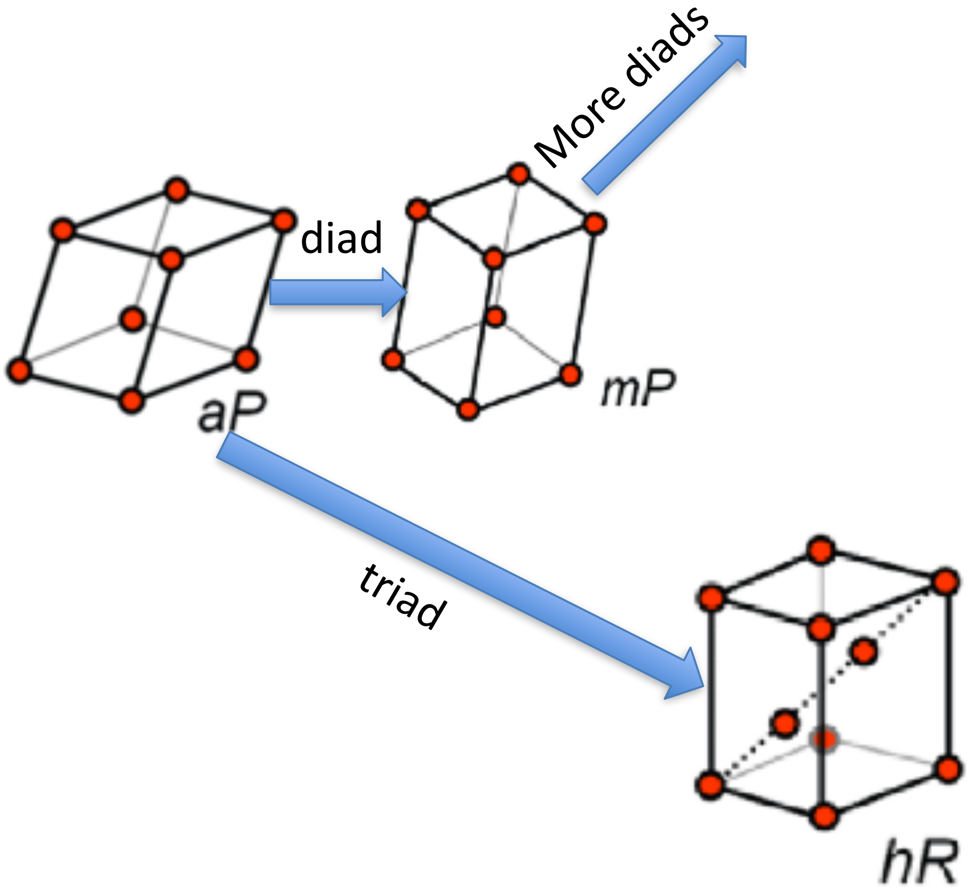

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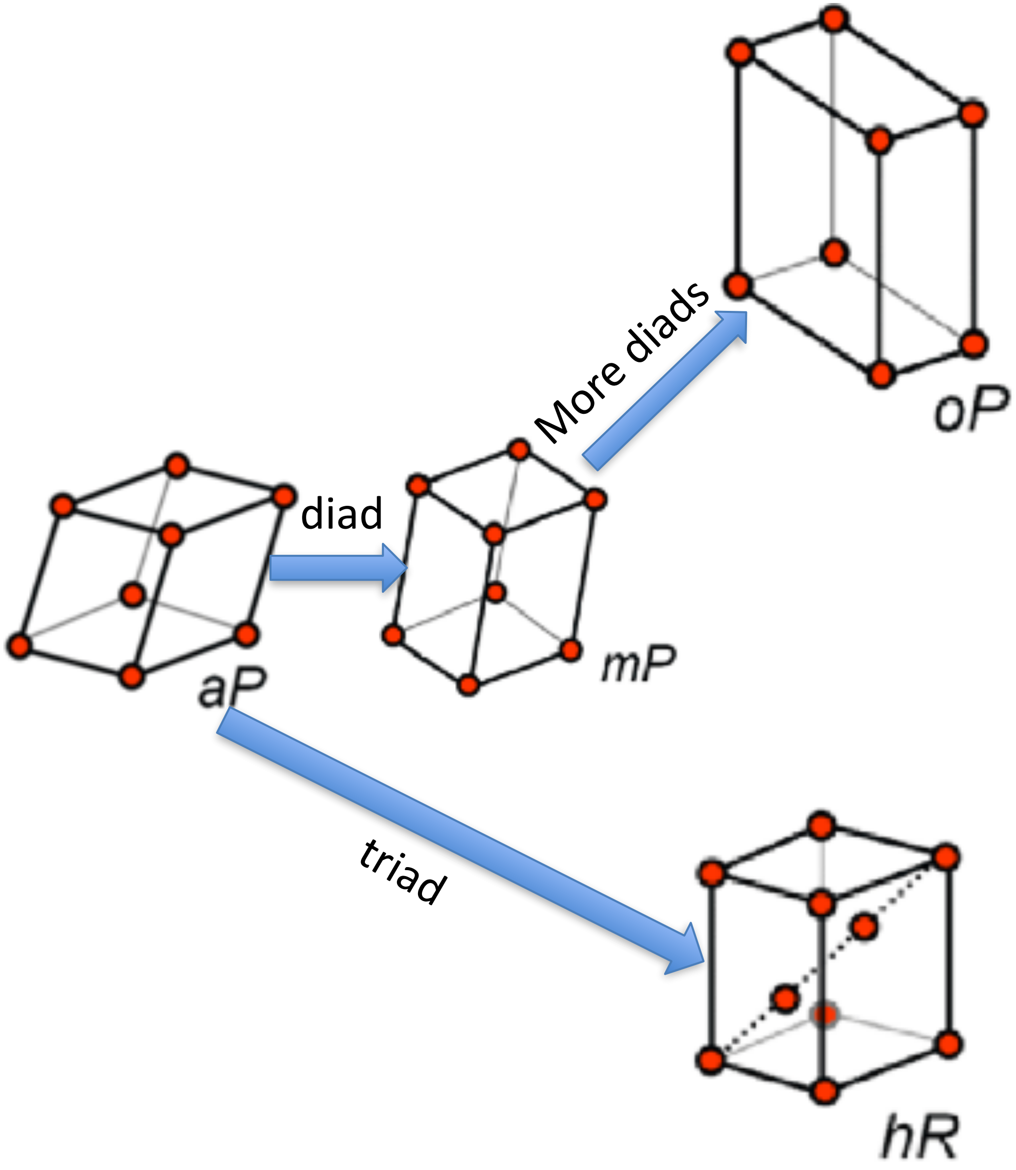

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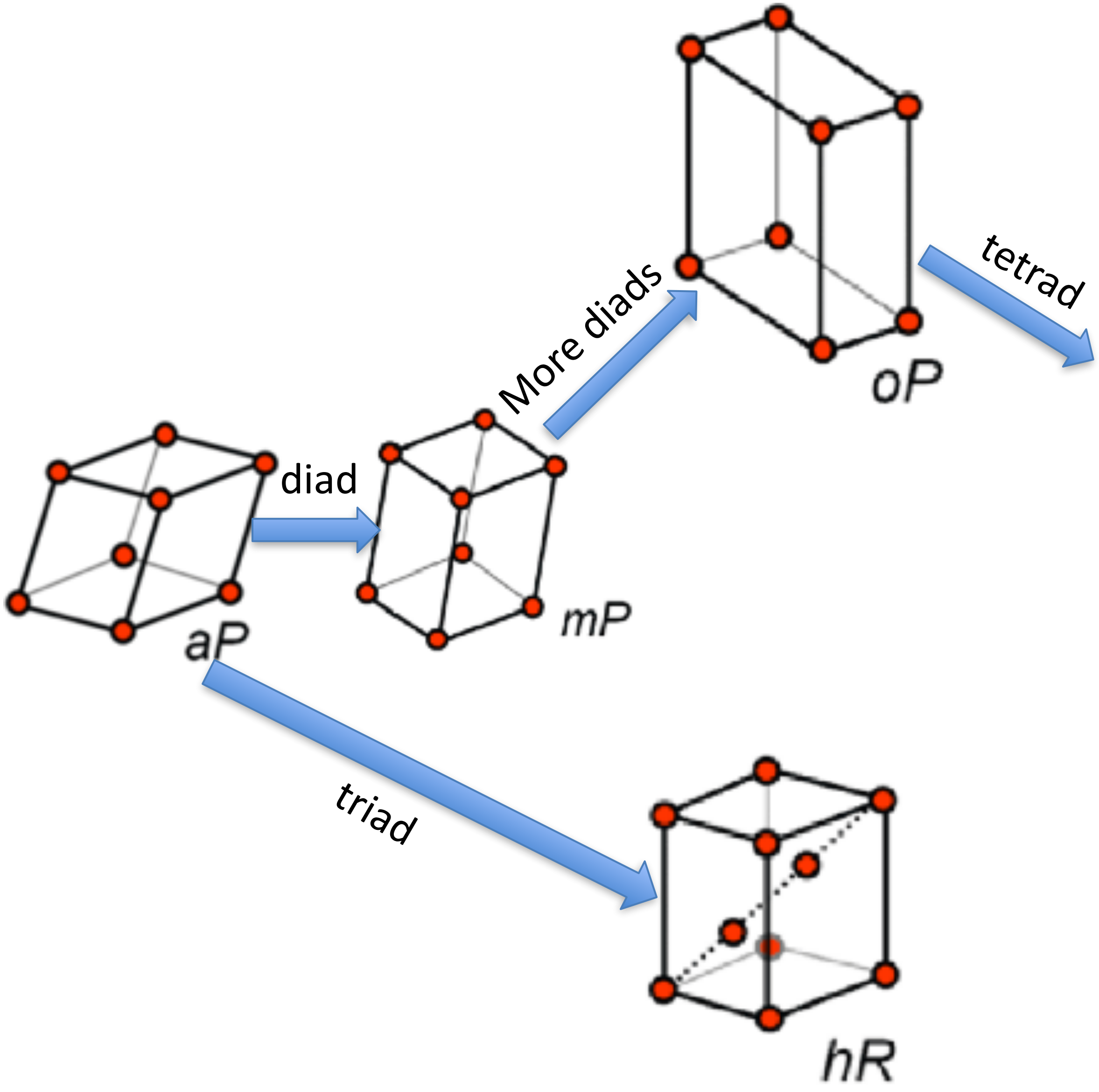

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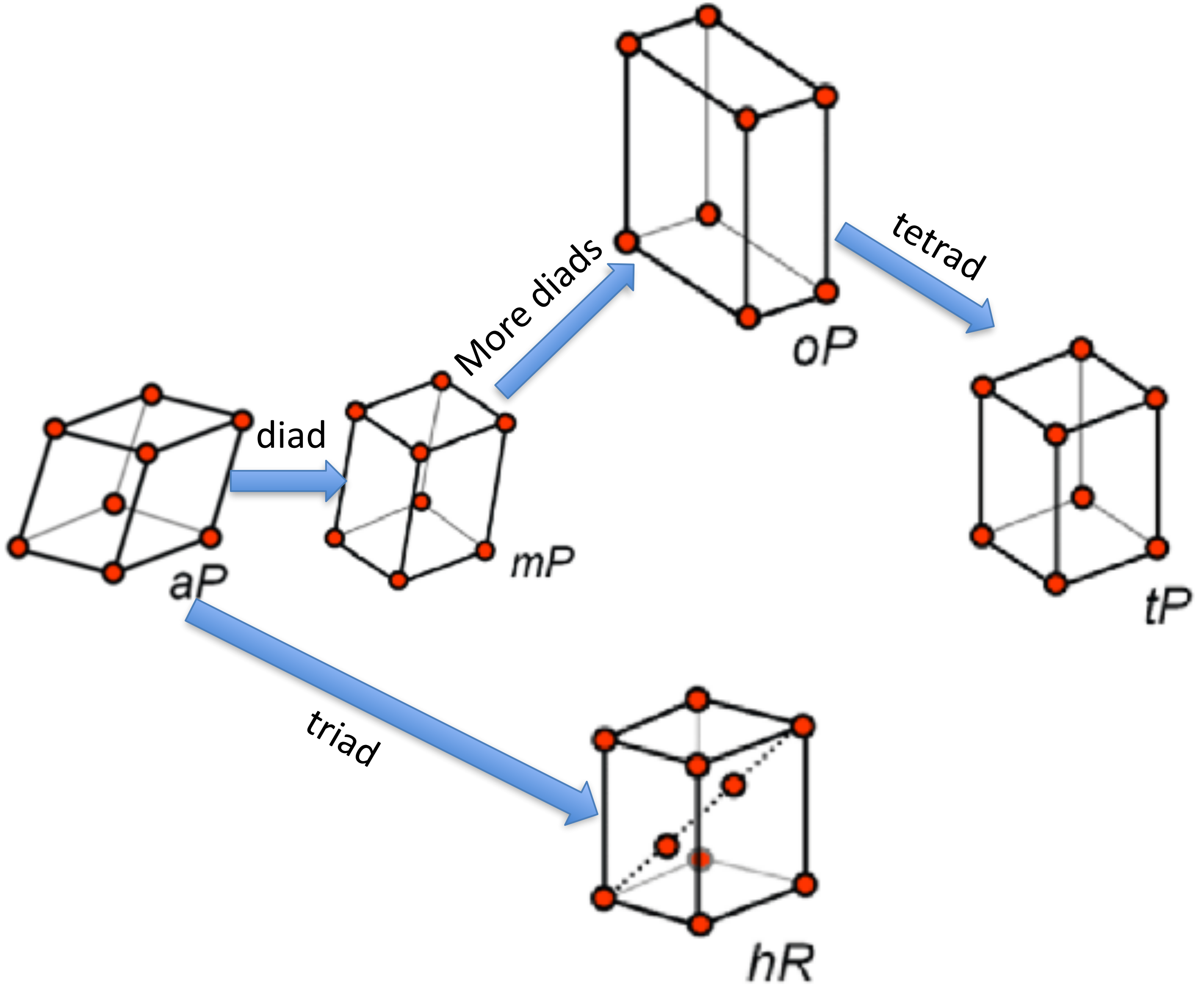

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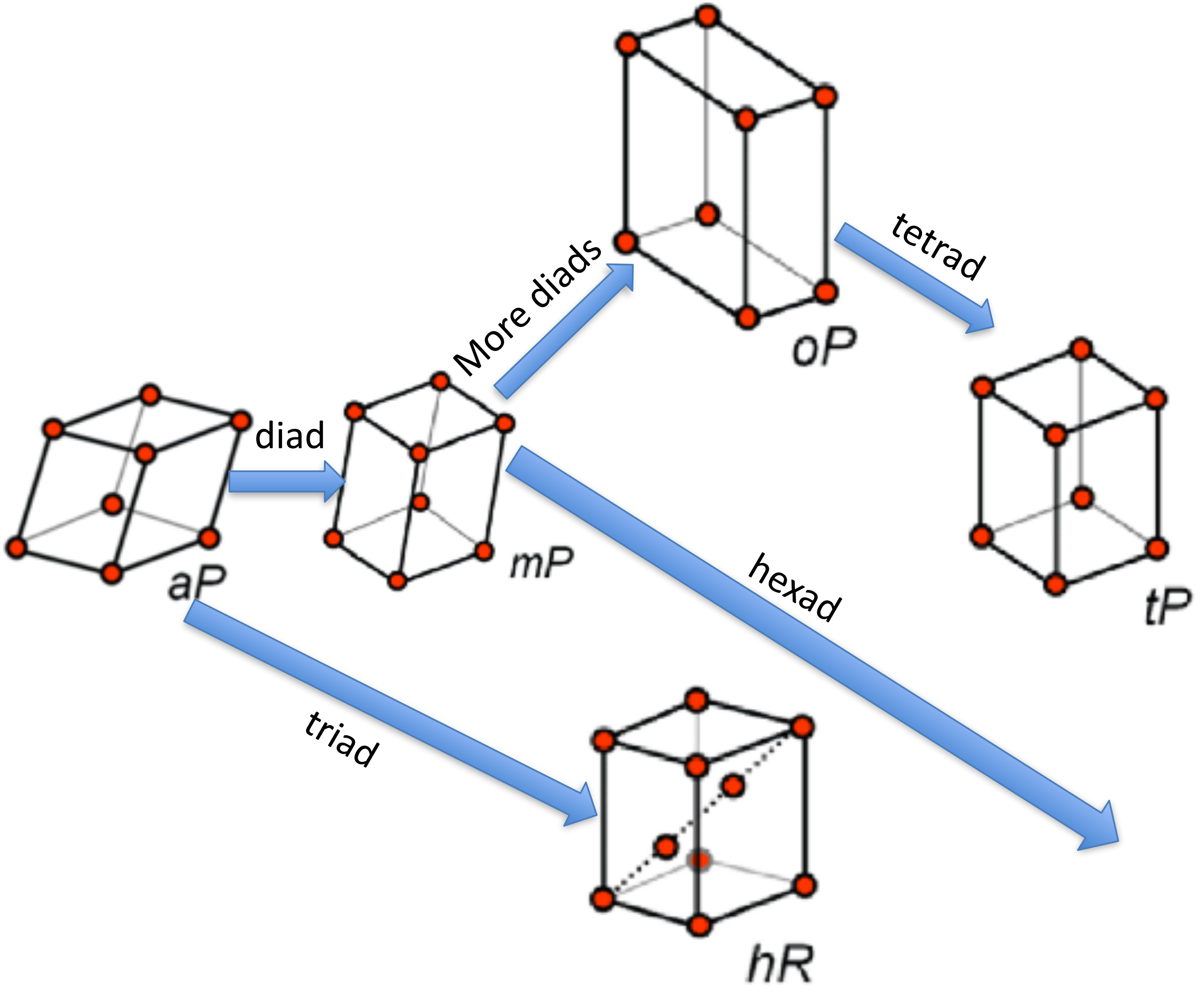

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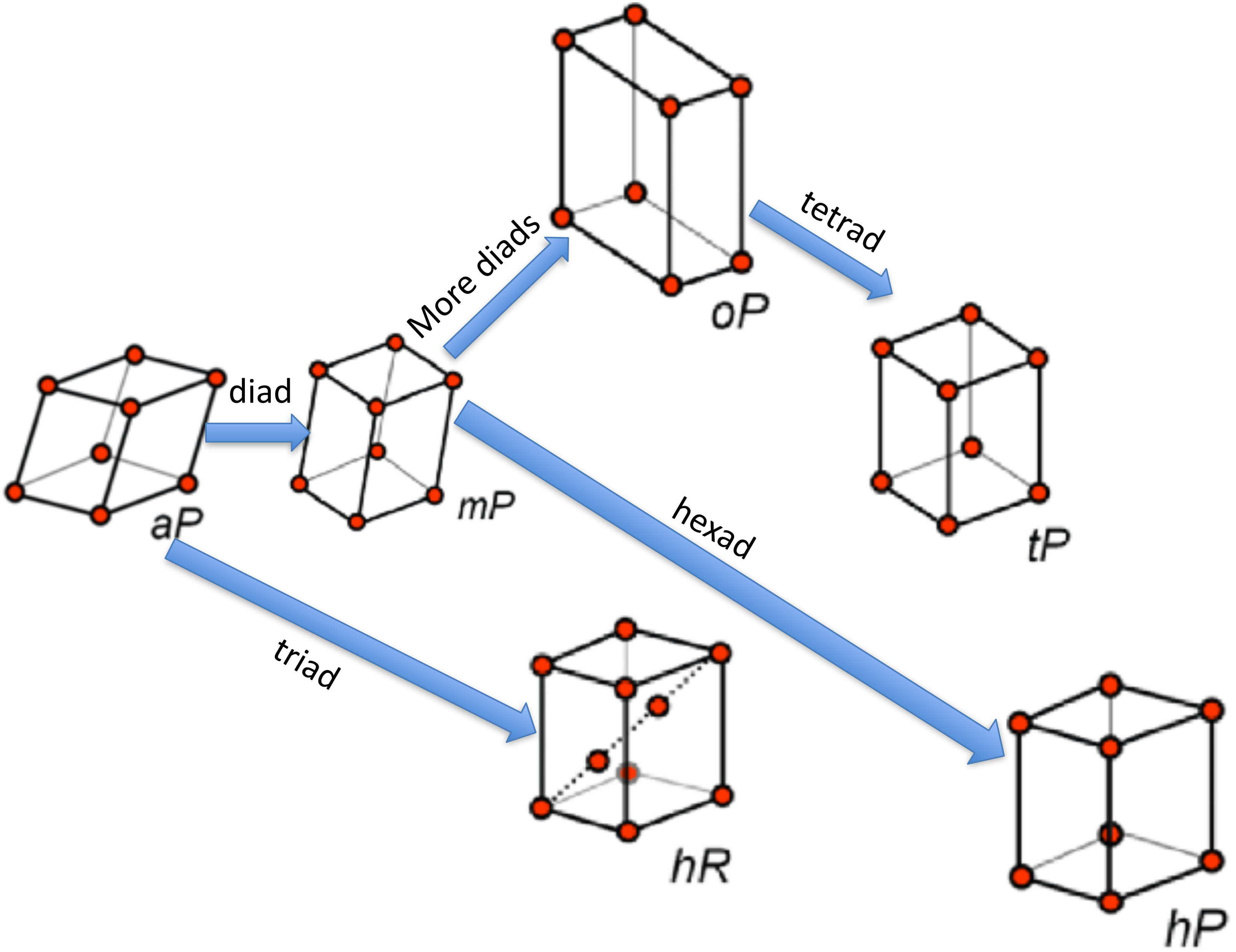

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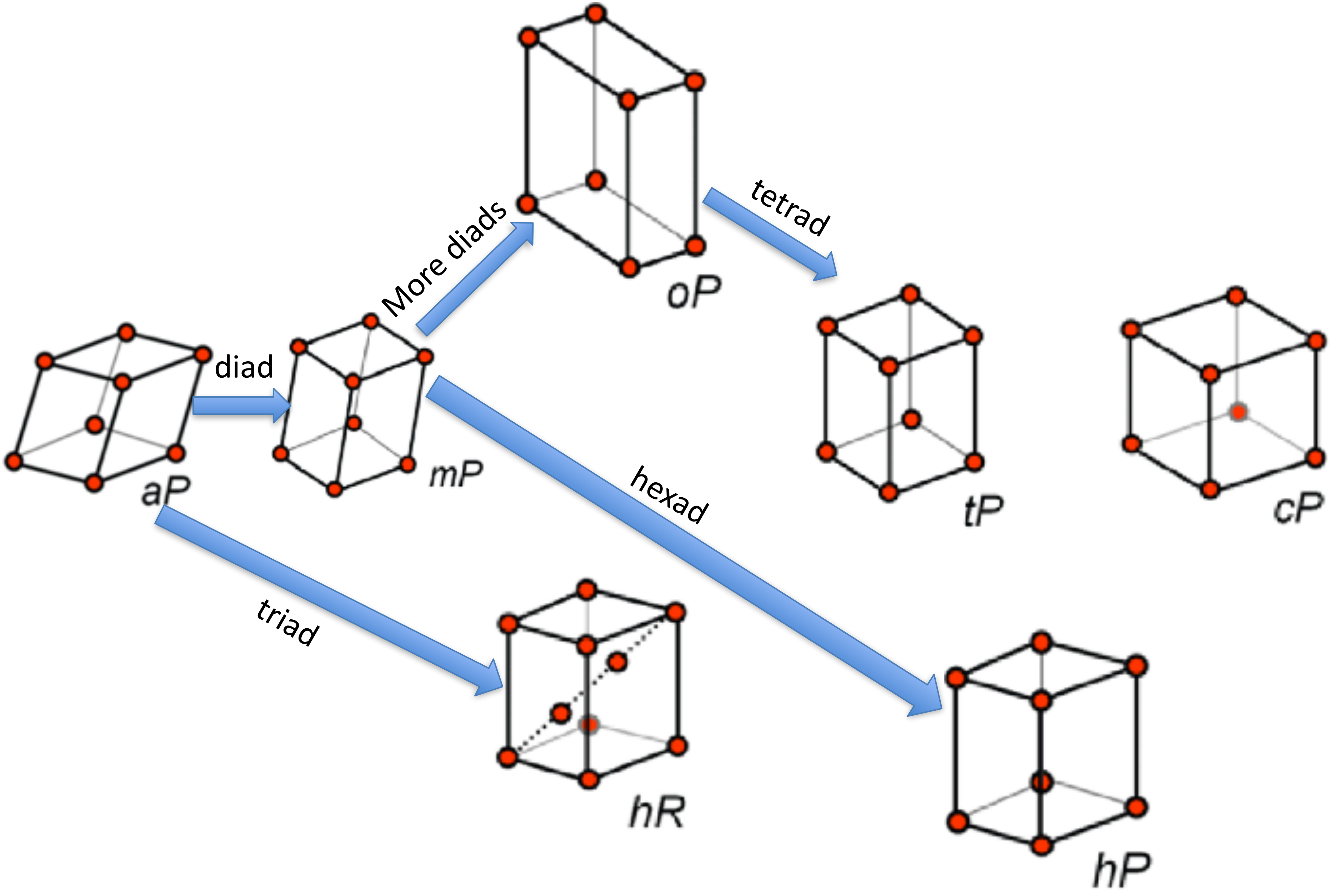

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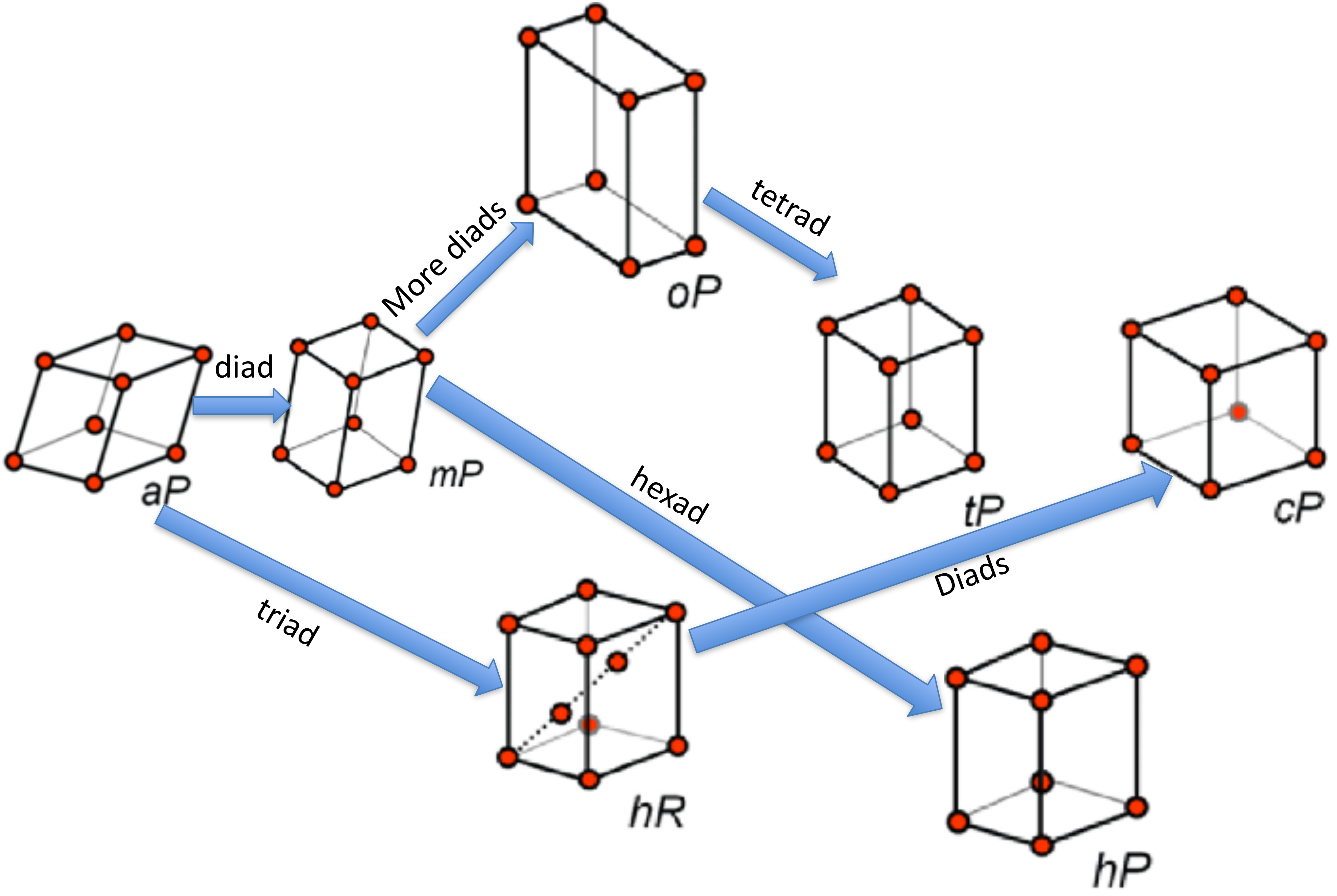

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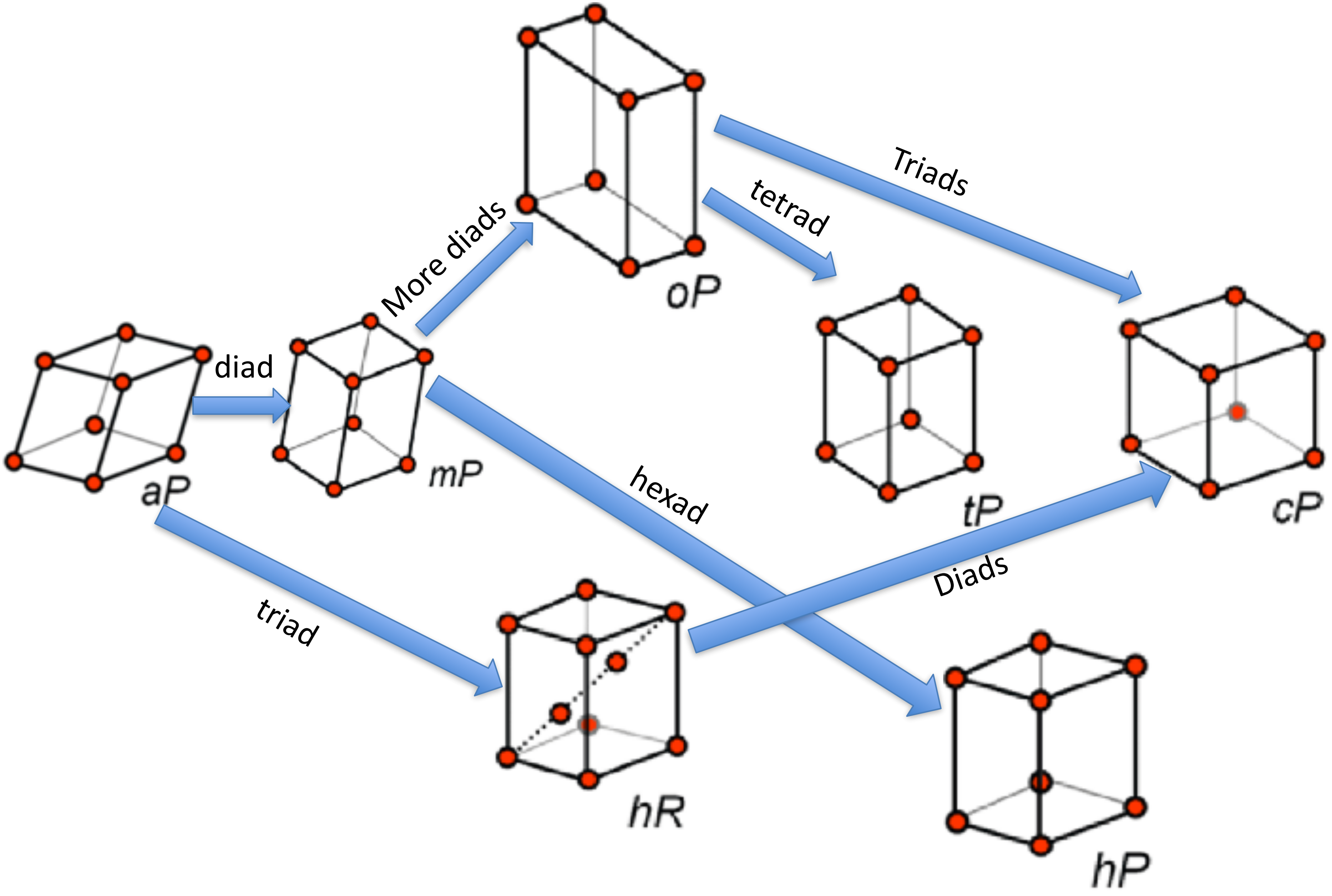

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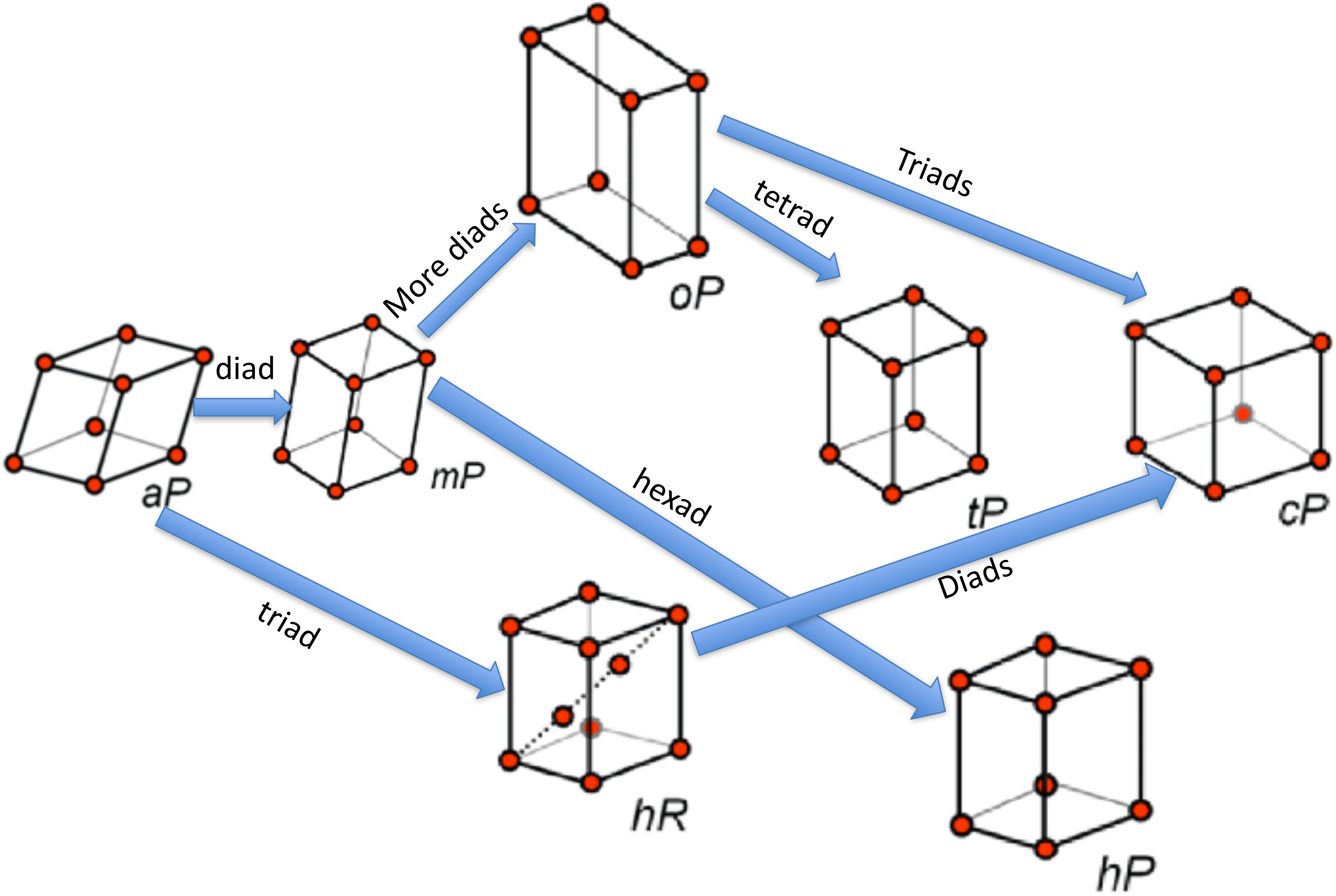
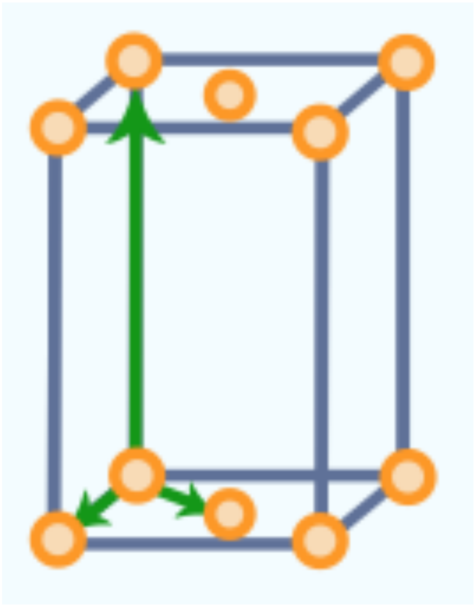


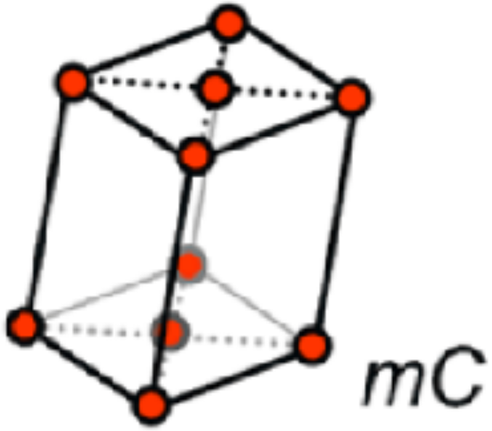
What Next?

Additional Lattice points in 3-D

Base-centering:

(A, B, or C -centered)





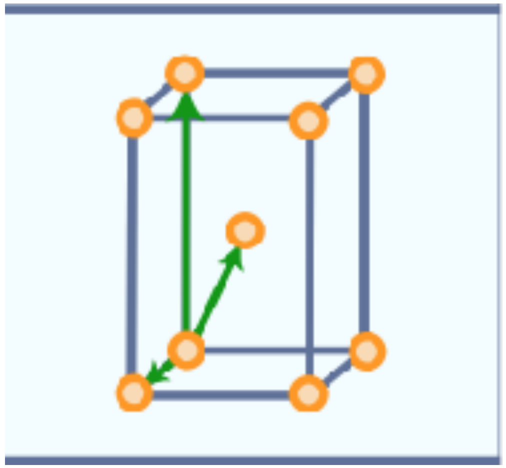
$$\vec{t} \Rightarrow \vec{t} + \frac{(\vec{a_2} + \vec{a_3})}{2}$$ or

$$\vec{t} \Rightarrow \vec{t} + \frac{(\vec{a_1} + \vec{a_3})}{2}$$ or

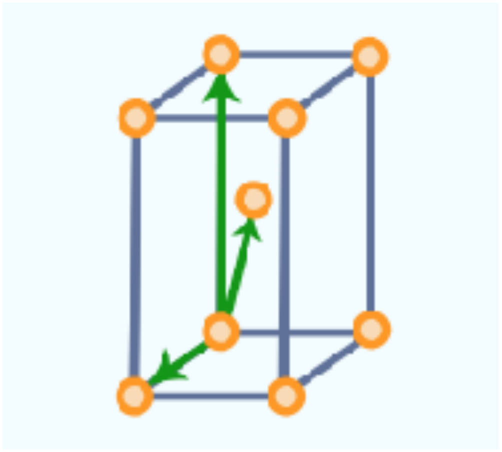
$$\vec{t} \Rightarrow \vec{t} + \frac{(\vec{a_1} + \vec{a_2})}{2}$$

Additional Lattice points in 3-D

Body-centering
(Innenzentriert)



tl



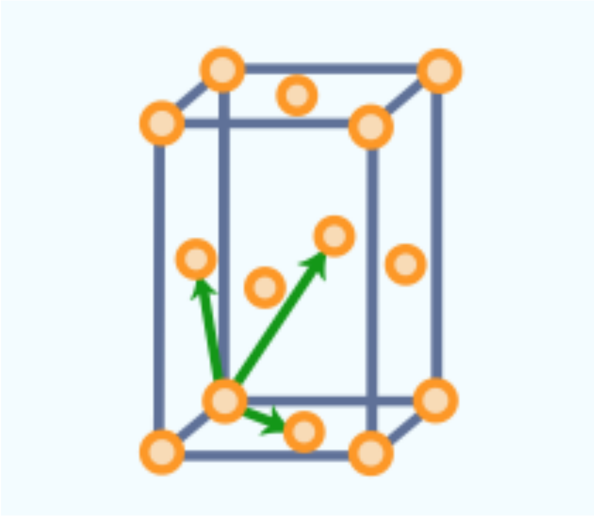
oI

$$\vec{t} \Rightarrow \vec{t} + \frac{(\vec{a_1} + \vec{a_2} + \vec{a_3})}{2}$$

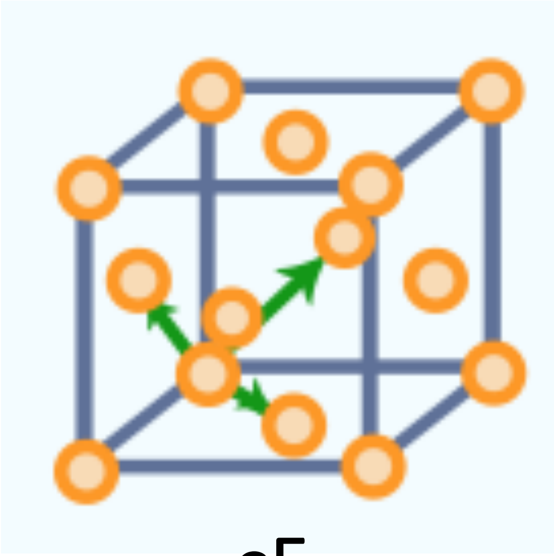
Additional Lattice points in 3-D

Face-centering:

3 additional sites (Face)



oF



cF

$$\vec{t} \Rightarrow \vec{t} + \frac{(\vec{a_2} + \vec{a_3})}{2}$$ and

$$\vec{t} \Rightarrow \vec{t} + \frac{(\vec{a_1} + \vec{a_3})}{2}$$ and

$$\vec{t} \Rightarrow \vec{t} + \frac{(\vec{a_1} + \vec{a_2})}{2}$$

The Bravais space lattices

A, B, C, I, F centering applied to the 7 crystal systems yields 35 additional lattices

The Bravais space lattices

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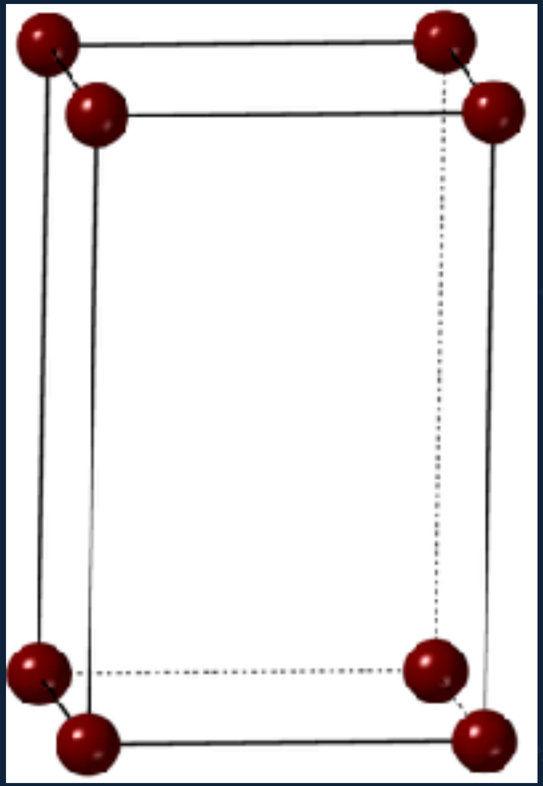

The Bravais space lattices

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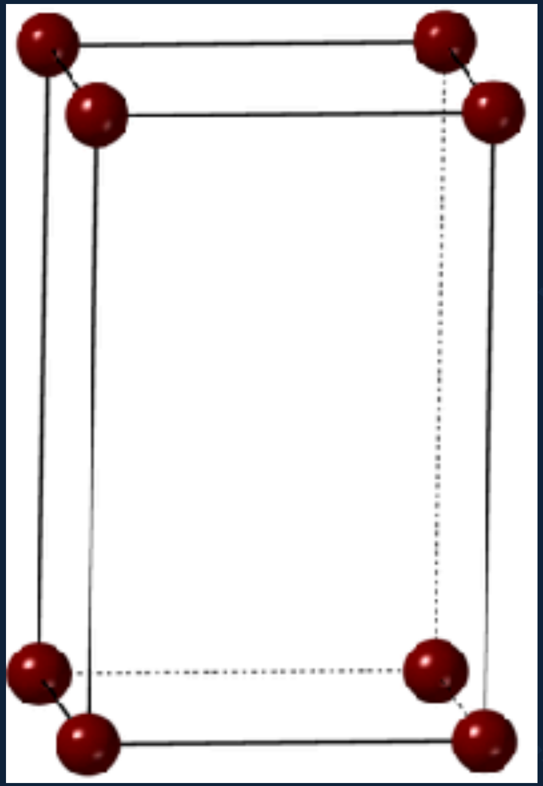

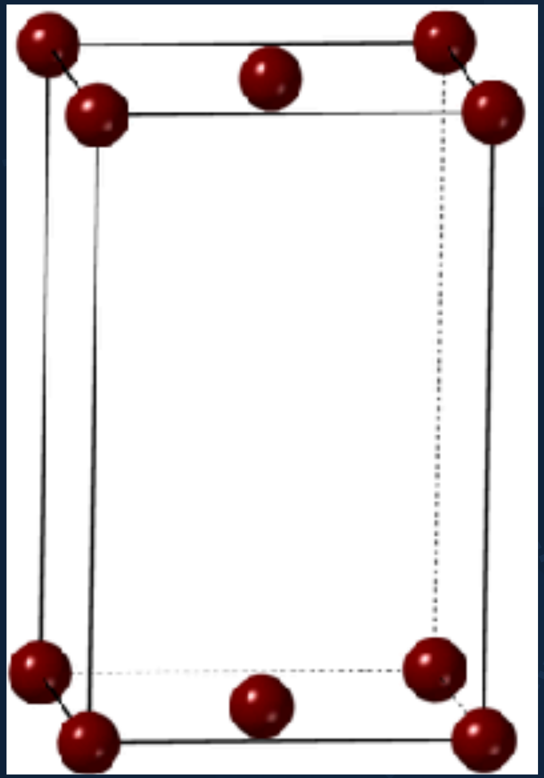

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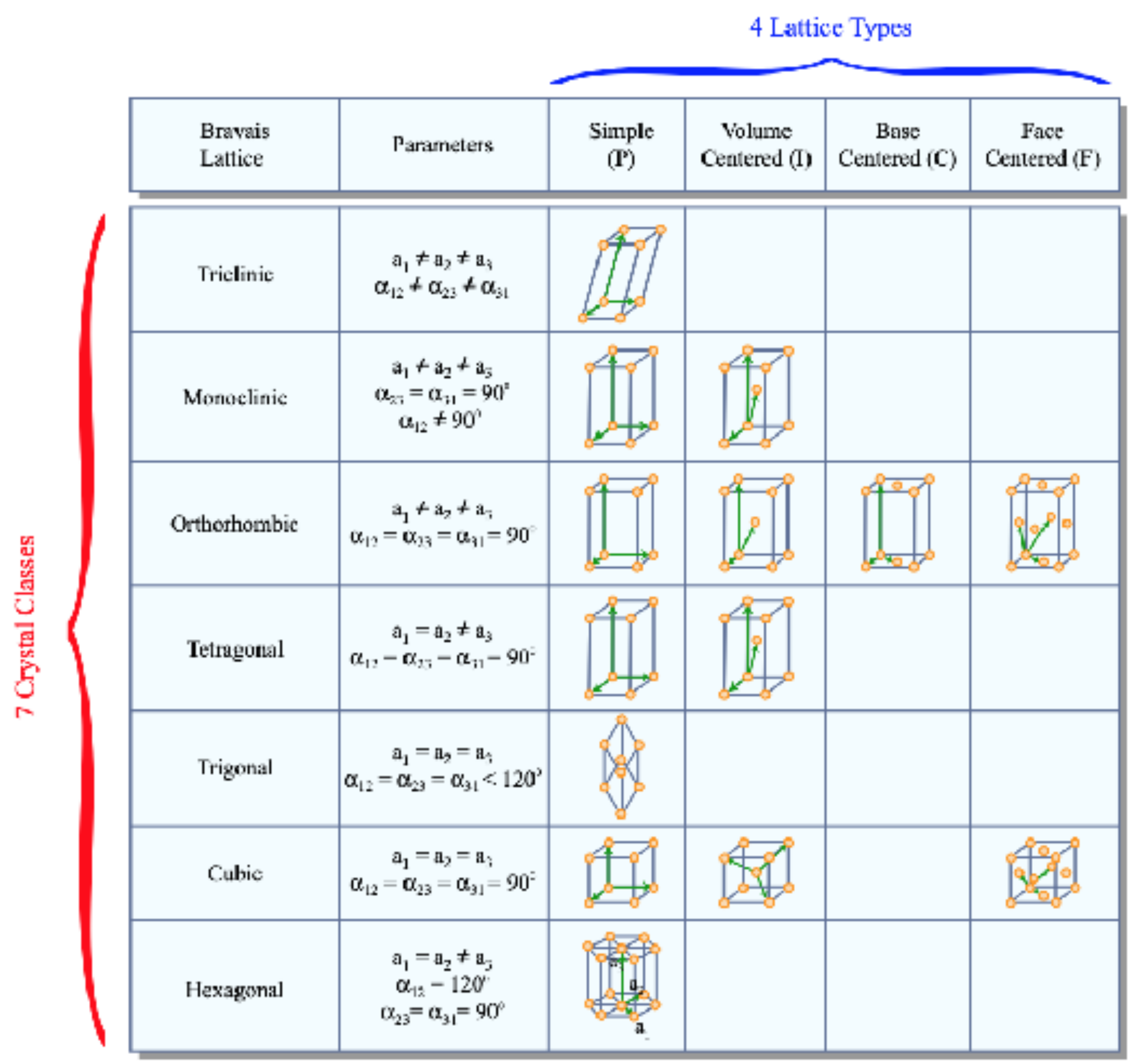
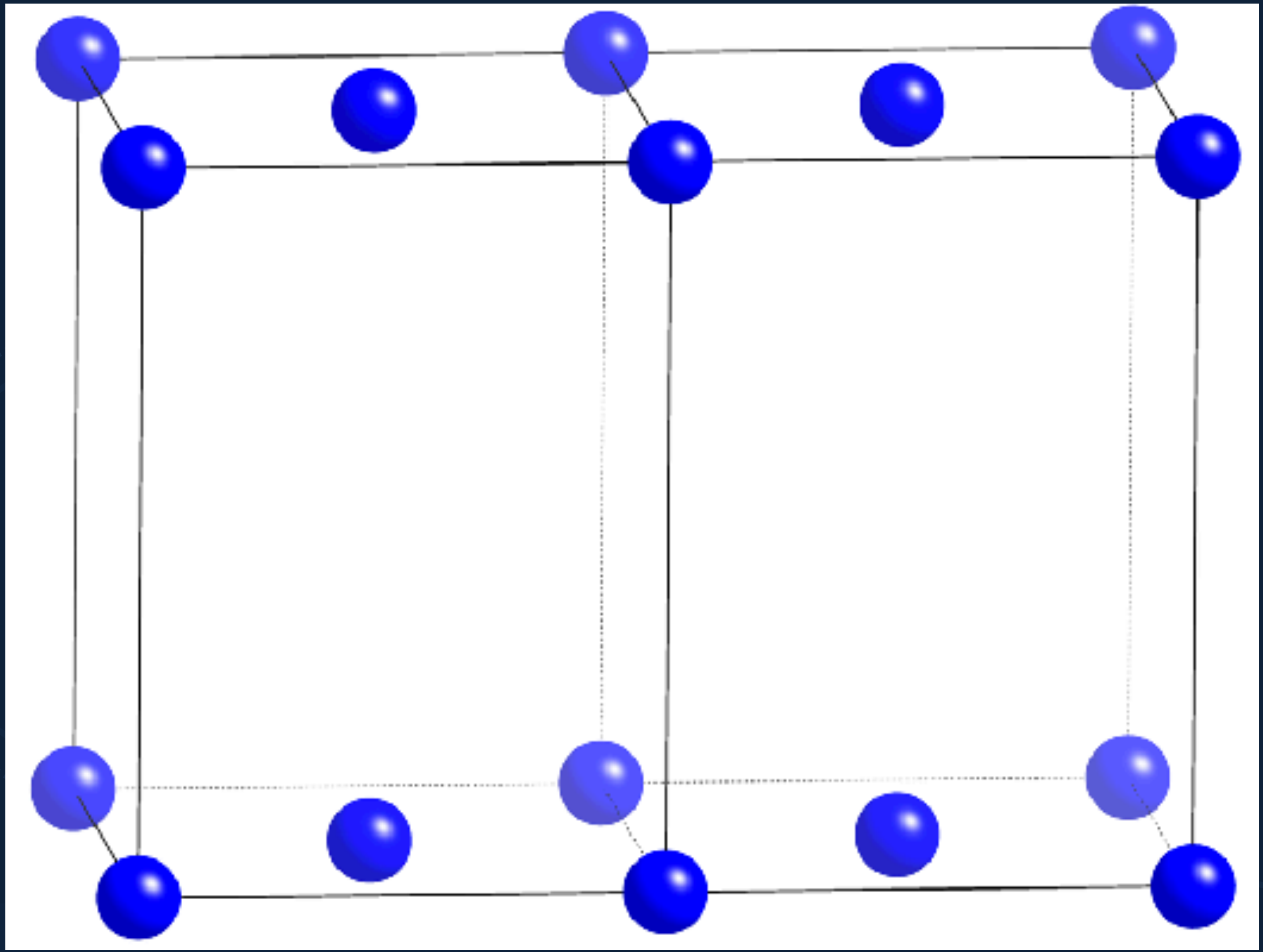


Can we always use the primitive unit cell?



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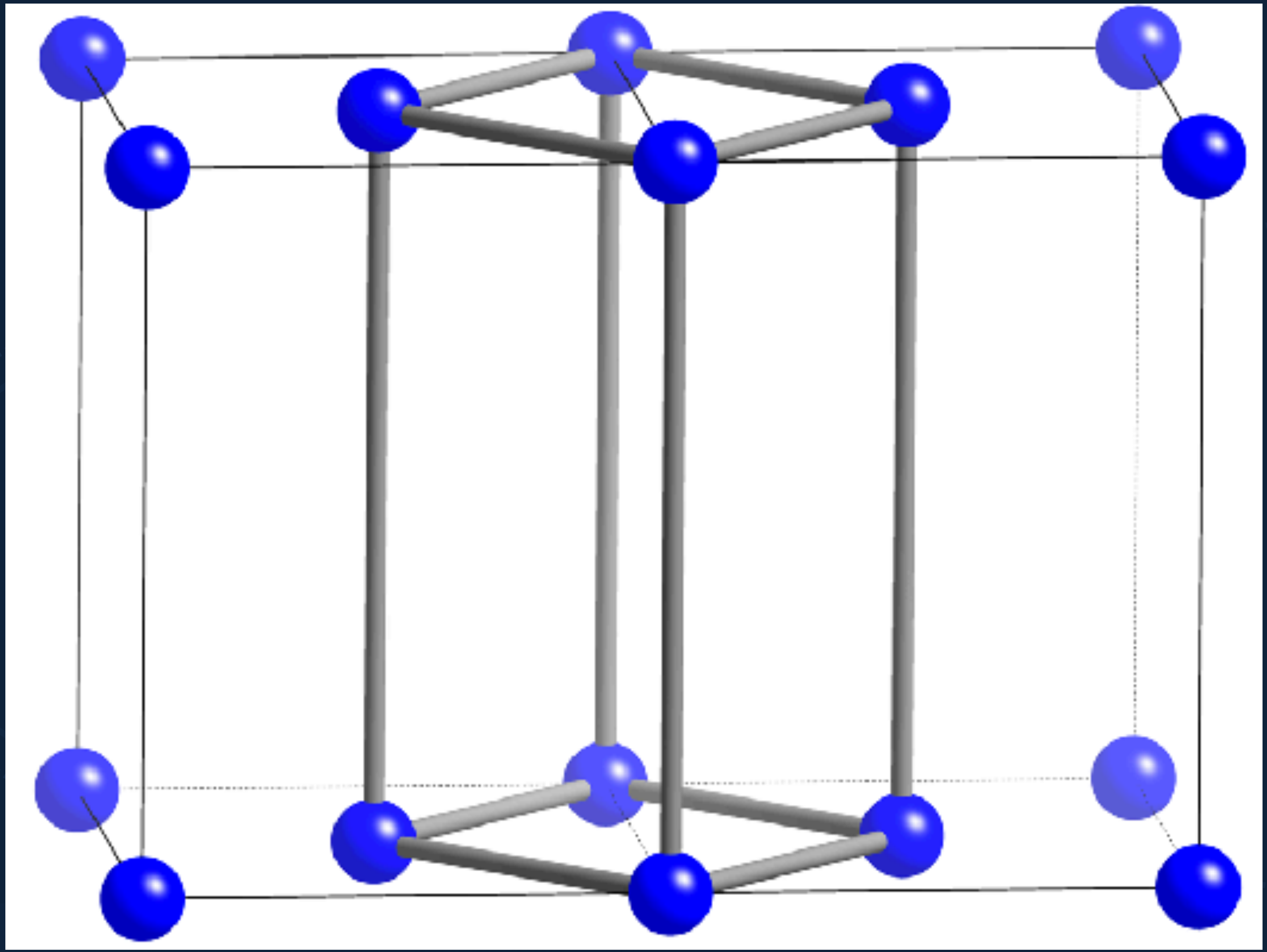
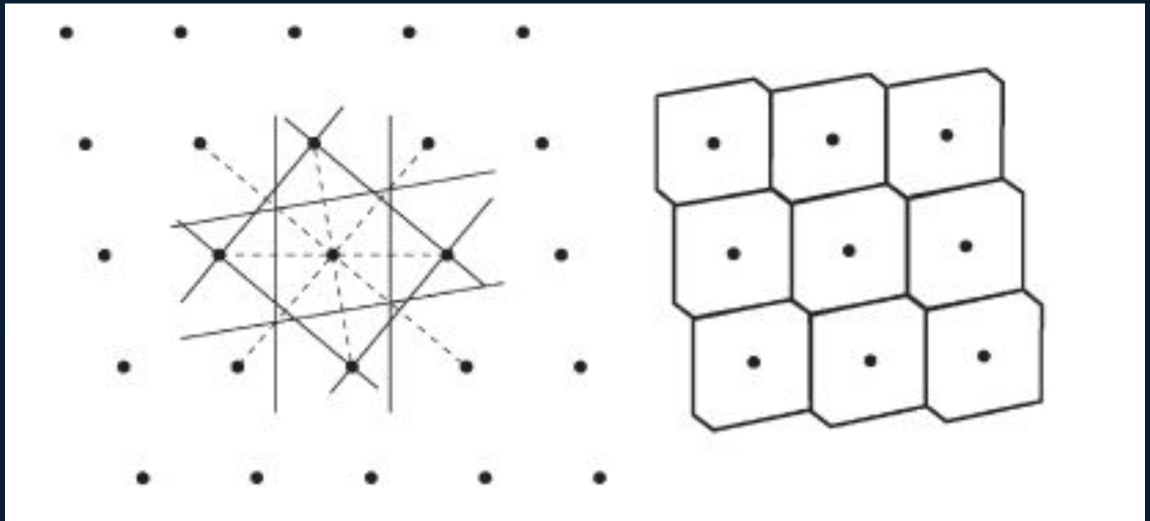


Iso-symmteric Primitive Unit Cell

Wigner-Seitz cell

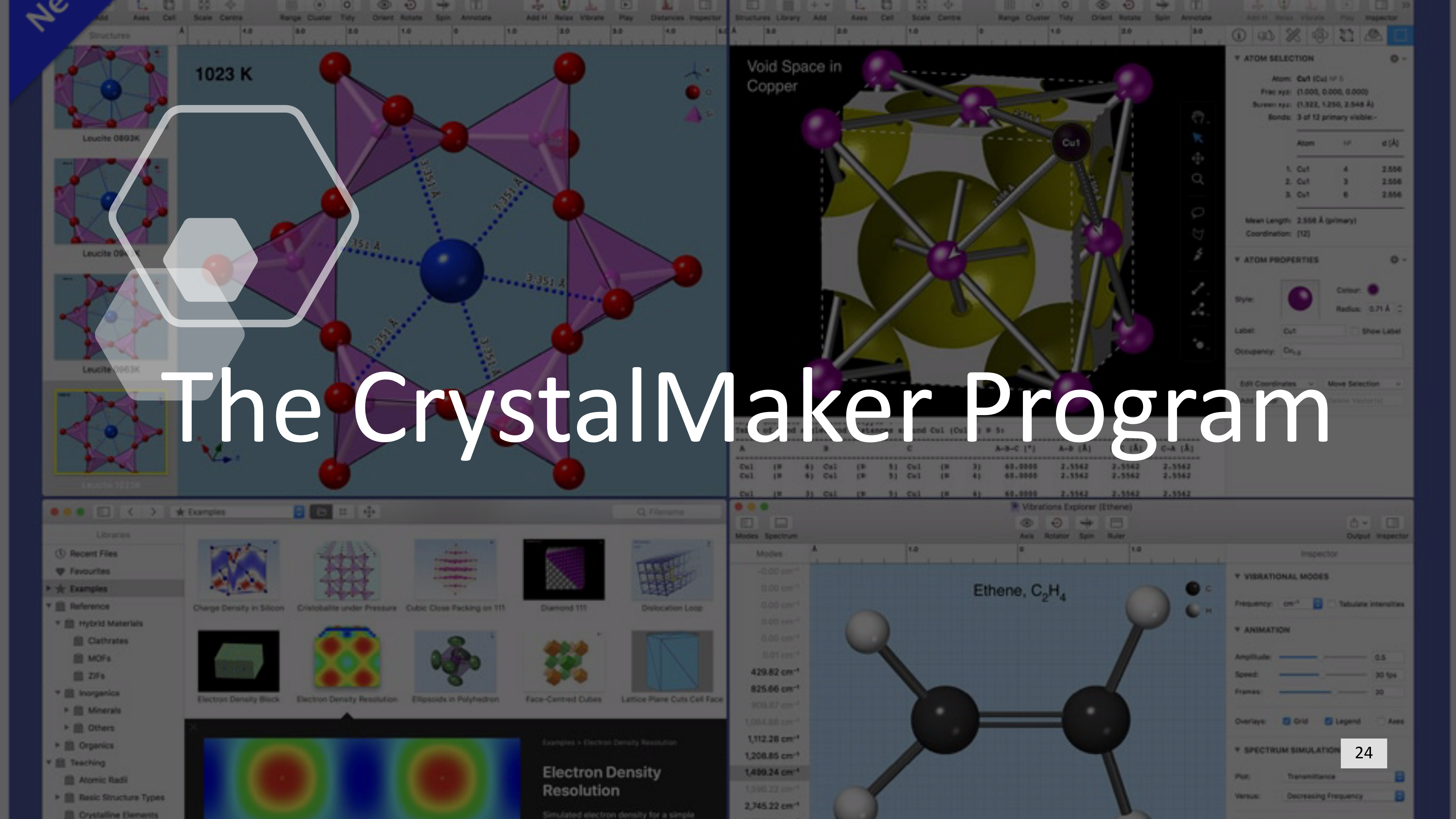


Region of space closer to a lattice point than to any other lattice point

Reproduced from “Structure of Materials”, Marc DeGraef and Michael McHenry

Crystalline Materials

- Standardized way to describe lattices
- Symmetry to create classifications
- Mathematical techniques
  - Unambiguous and clear description
  - Rules and tools to perform crystallographic computations



The CrystalMaker Program

$$u \equiv u_1$$

$$v \equiv u_2$$

$$w \equiv u_3$$

$$\tau = \{\vec{t} \mid \vec{t} = u\vec{a} + v\vec{b} + w\vec{c}\}$$

$$u, v, w \in \mathbb{Z}$$

$$\vec{t} = u_i \mathbf{a_i}$$

$$\vec{a} \equiv a_1$$

$$\vec{b} \equiv a_2$$

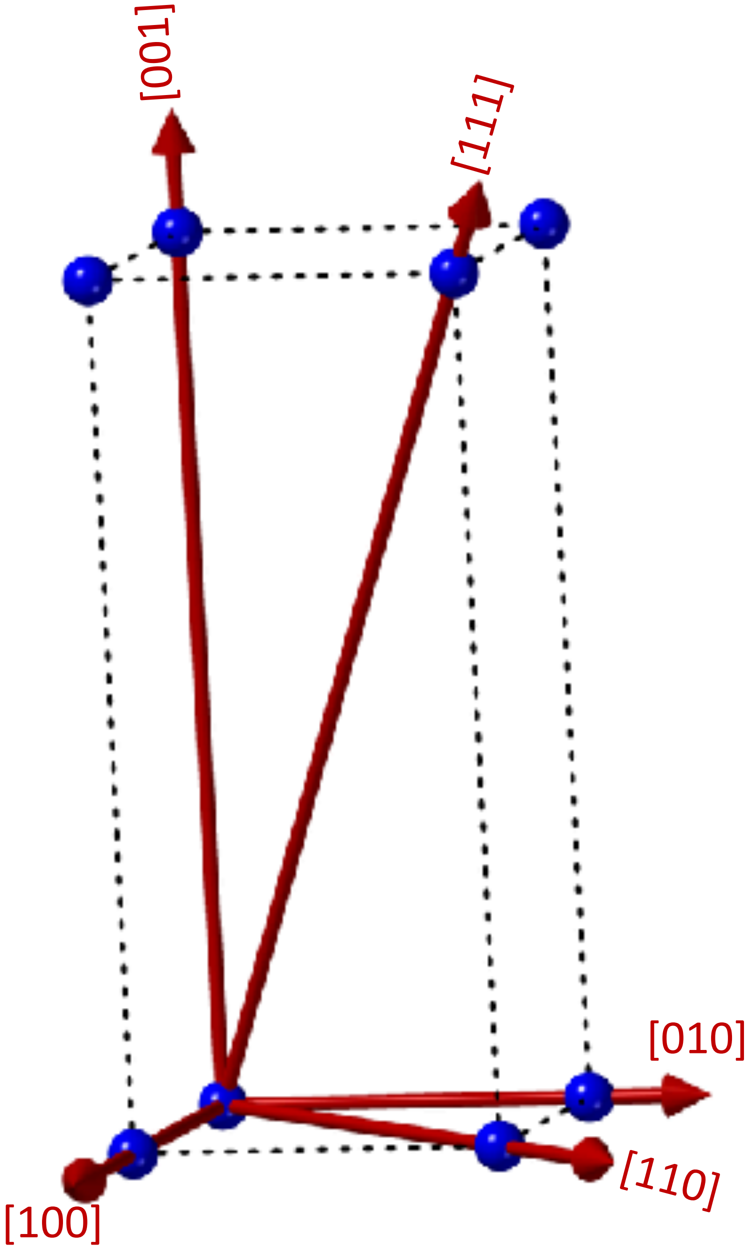
$$\vec{c} \equiv a_3$$

Notation for lattice vectors

Working in real space

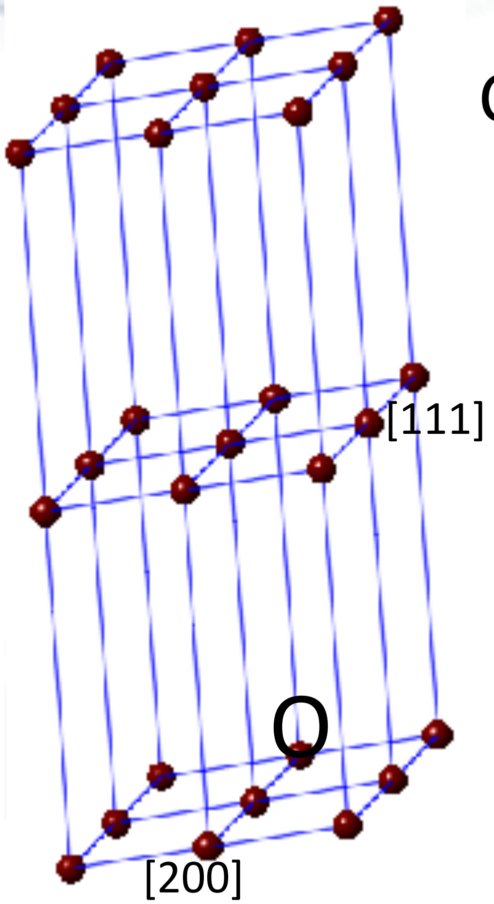
Special symbol for directions: $[u_1u_2u_3]$ Also, [uvw] can be used

u_1, u_2, u_3 are smallest integers proportional to components of the translation vector



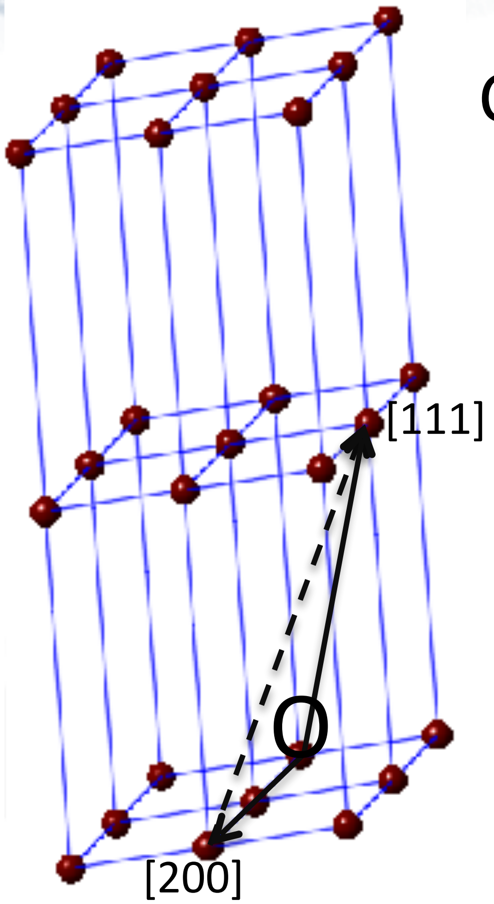
Directions always defined w.r.t. crystallographic basis

The need to work with a non-orthonormal basis



Compute distance between lattice points (2,0,0) and (1,1,1)

The need to work with a non-orthonormal basis



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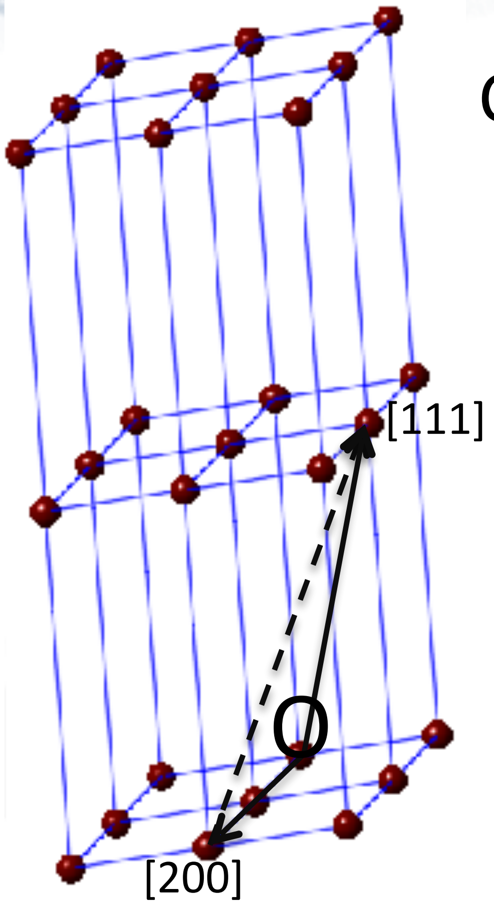
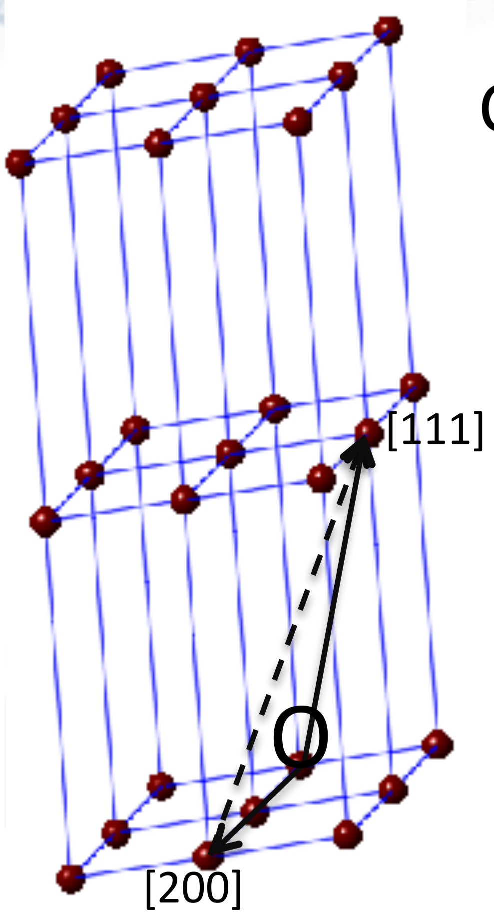


Compute distance between lattice points (2,0,0) and (1,1,1)

$$\vec{d} = [111] - [200]$$

The need to work with a non-orthonormal basis



Compute distance between lattice points (2,0,0) and (1,1,1)

$$\vec{d} = [111] - [200]$$

$$|\vec{d}| = \sqrt{d \cdot d}$$

$$= \sqrt{([111] - [200]) \cdot ([111] - [200])}$$

Distance between two lattice points

$$\mathbf{q} = q_1\mathbf{a_1} + q_2\mathbf{a_2} + q_3\mathbf{a_3}$$

$$\mathbf{p} = p_1\mathbf{a_1} + p_2\mathbf{a_2} + p_3\mathbf{a_3}$$

$$d^2 = (\mathbf{q} - \mathbf{p}) \cdot (\mathbf{q} - \mathbf{p})$$

The real space "metric tensor"

$$(\mathbf{q} - \mathbf{p}) \cdot (\mathbf{q} - \mathbf{p})$$

The real space "metric tensor"

$$(\mathbf{q}-\mathbf{p})\cdot(\mathbf{q}-\mathbf{p}) = \begin{pmatrix} q_1-p_1 & q_2-p_2 & q_3-p_3 \end{pmatrix} \begin{pmatrix} \mathbf{a_1}\cdot\mathbf{a_1} & \mathbf{a_1}\cdot\mathbf{a_2} & \mathbf{a_1}\cdot\mathbf{a_3} \\ \mathbf{a_2}\cdot\mathbf{a_1} & \mathbf{a_2}\cdot\mathbf{a_2} & \mathbf{a_2}\cdot\mathbf{a_3} \\ \mathbf{a_3}\cdot\mathbf{a_1} & \mathbf{a_3}\cdot\mathbf{a_2} & \mathbf{a_3}\cdot\mathbf{a_3} \end{pmatrix} \begin{pmatrix} q_1-p_1 \\ q_2-p_2 \\ q_3-p_3 \end{pmatrix}$$

The real space "metric tensor"

$$(\mathbf{q}-\mathbf{p})\cdot(\mathbf{q}-\mathbf{p}) = \begin{pmatrix} q_1 - p_1 & q_2 - p_2 & q_3 - p_3 \end{pmatrix} \begin{pmatrix} \mathbf{a_1}\cdot\mathbf{a_1} & \mathbf{a_1}\cdot\mathbf{a_2} & \mathbf{a_1}\cdot\mathbf{a_3} \\ \mathbf{a_2}\cdot\mathbf{a_1} & \mathbf{a_2}\cdot\mathbf{a_2} & \mathbf{a_2}\cdot\mathbf{a_3} \\ \mathbf{a_3}\cdot\mathbf{a_1} & \mathbf{a_3}\cdot\mathbf{a_2} & \mathbf{a_3}\cdot\mathbf{a_3} \end{pmatrix} \begin{pmatrix} q_1 - p_1 \\ q_2 - p_2 \\ q_3 - p_3 \end{pmatrix}$$

$$g_{ij}$$

Real space metric tensor

The real space "metric tensor"

$$(\mathbf{q}-\mathbf{p})\cdot(\mathbf{q}-\mathbf{p}) = \begin{pmatrix} q_1-p_1 & q_2-p_2 & q_3-p_3 \end{pmatrix} \begin{pmatrix} \mathbf{a_1}\cdot\mathbf{a_1} & \mathbf{a_1}\cdot\mathbf{a_2} & \mathbf{a_1}\cdot\mathbf{a_3} \\ \mathbf{a_2}\cdot\mathbf{a_1} & \mathbf{a_2}\cdot\mathbf{a_2} & \mathbf{a_2}\cdot\mathbf{a_3} \\ \mathbf{a_3}\cdot\mathbf{a_1} & \mathbf{a_3}\cdot\mathbf{a_2} & \mathbf{a_3}\cdot\mathbf{a_3} \end{pmatrix} \begin{pmatrix} q_1-p_1 \\ q_2-p_2 \\ q_3-p_3 \end{pmatrix}$$

$$g_{ij}$$

Real space metric tensor

$$d^2 = (q-p)_i \, g_{ij} \, (q-p)_j$$

Uses of real space metric tensor

- Computation of length of a vector
- Computation of angle between lattice directions
- Computation of the distance between atoms
- Computation of the angle between atomic bonds

Problem

- A crystal has lattice parameters: (3,3,3,68°,68°,68°)
  - Atoms are present at (½, 1/3, ¼) and (1/3, ½, ¾). Compute distance between the two atoms.
  - Compute length of the body diagonal.
  - What is the angle between the [101] and [201] directions.