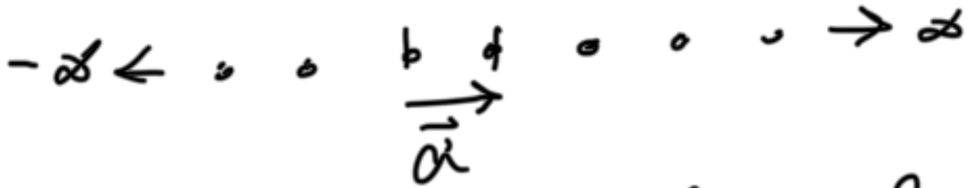
Periodic arrangement of atoms in crystalline solids.

Bravais Lattice: Arrangement of infinite number of points where any point chosen randomly can be translated by a linear combination of "n" linearly independent set of vectors of finite length in "n" dimensional space to completely cover all the points.

1 D: 

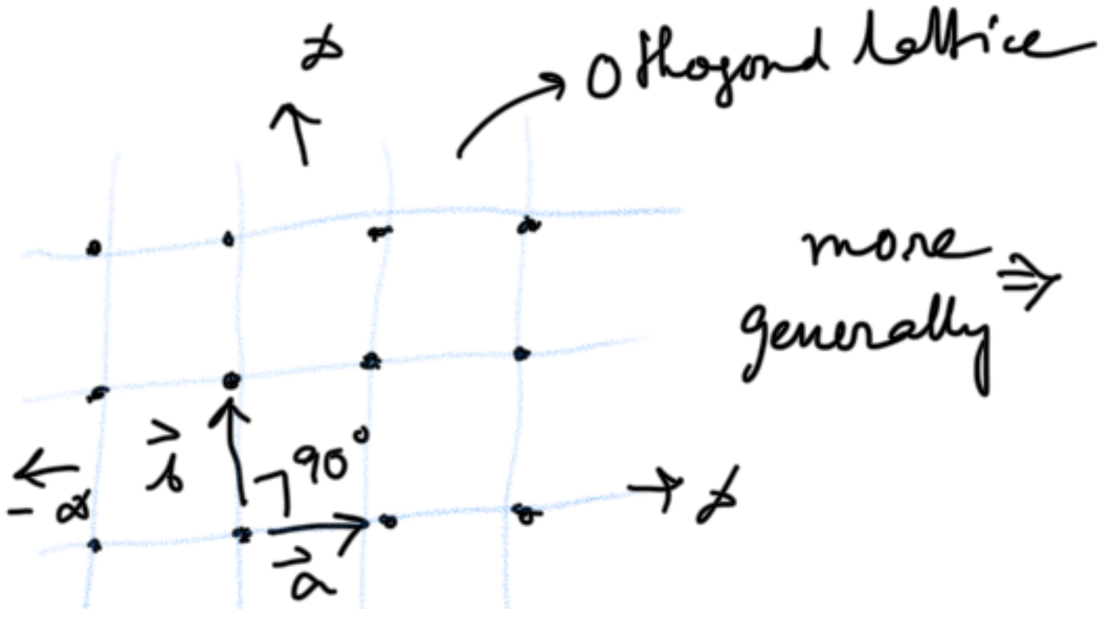
All points can be covered by $n\vec{a}$, $n = 0, \pm 1, \pm 2 \ldots \pm\infty$ after starting from any point.

Corrolary: All points of a Bravais lattice must have exactly same neighbourhood.

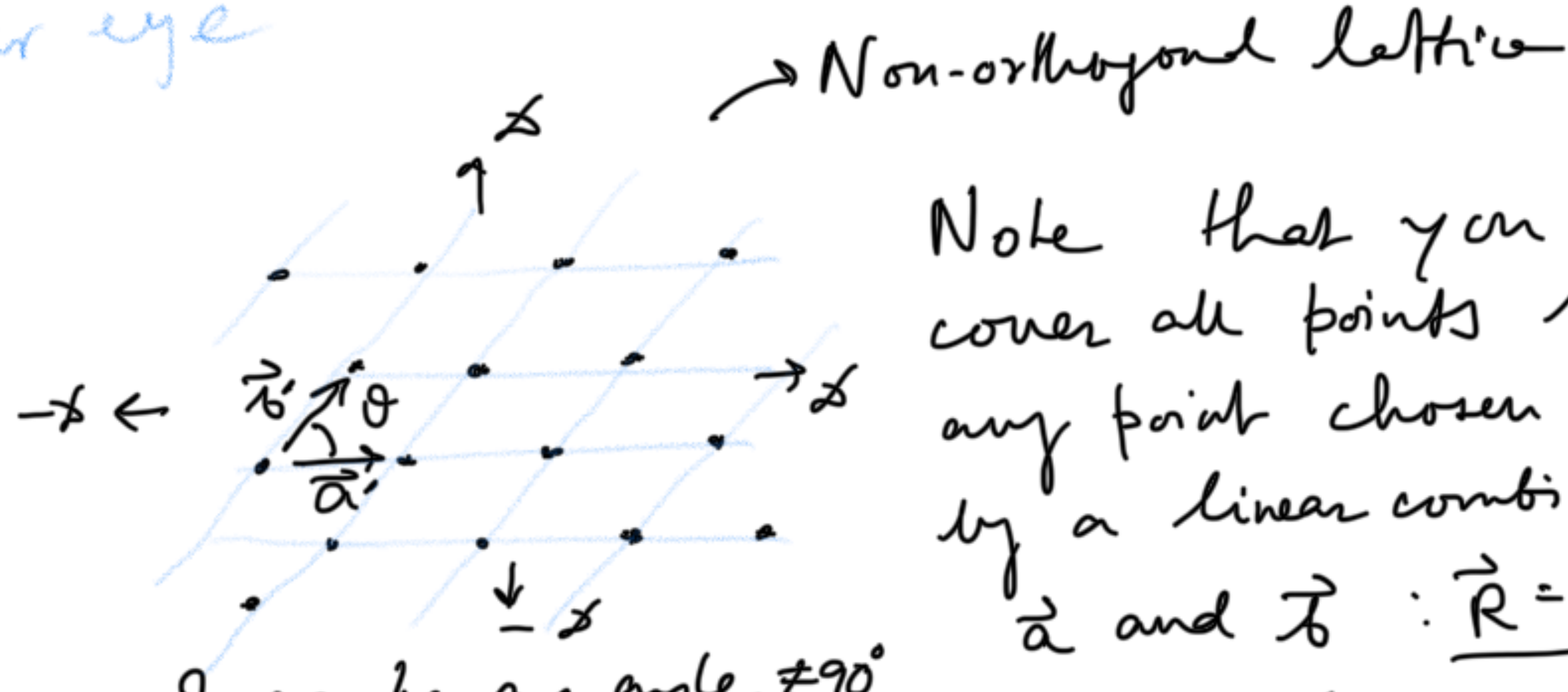
Lattice vector: $\vec{R} = n\vec{a}$.

— guide for eye

2D:



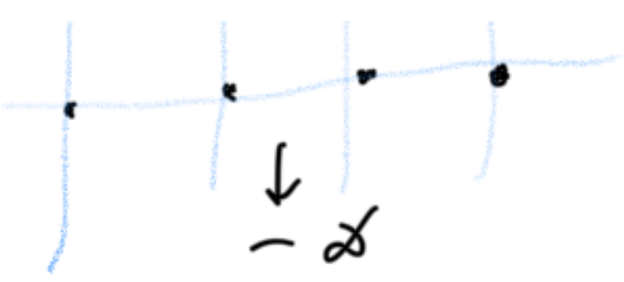
more generally ⇒



θ can be any angle ≠ 90°

Note that you can cover all points by translating any point chosen randomly by a linear combination of $\vec{a}$ and $\vec{b}$: $\vec{R} = l\vec{a} + m\vec{b}$

$\{l, m\} = \{0, \pm 1, \pm 2 \ldots \pm \infty\}$



In 3D Bravais lattice lattice vector $\vec{R} = l\vec{a} + m\vec{b} + n\vec{c}$

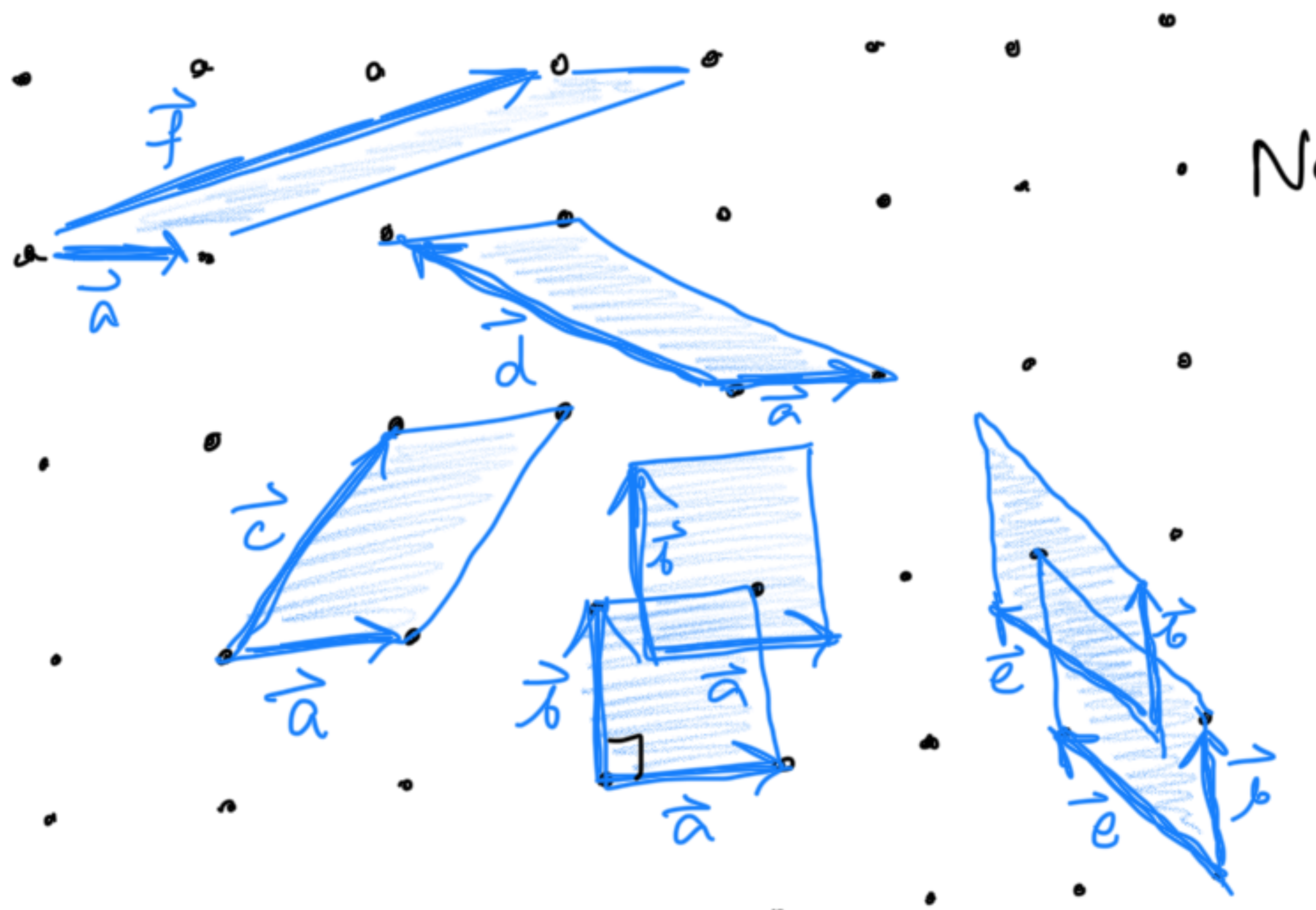
PUC : Primitive unit cell : smallest periodic unit.

PUC can be translated by lattice vector $\vec{R}$

To completely cover all the infinite number of points

PUC is spanned by primitive lattice vectors (PLV)

Infinitely many choices of PUCs and PLVs



$\vec{c} = \vec{a} + \vec{b}$

$\vec{d} = -2\vec{a} + \vec{b}$

$\vec{e} = -\vec{a} + \vec{b}$

$\vec{f} = 3\vec{a} + \vec{b}$

Note: All PUCs have same area $= (|\vec{a}||\vec{b}|)$

PUCs spanned by $\vec{a}$ and $\vec{b}$ are orthogonal choices of PUC (all angles 90°)

Other choices of PUCs shown here are non-orthogonal PUCs

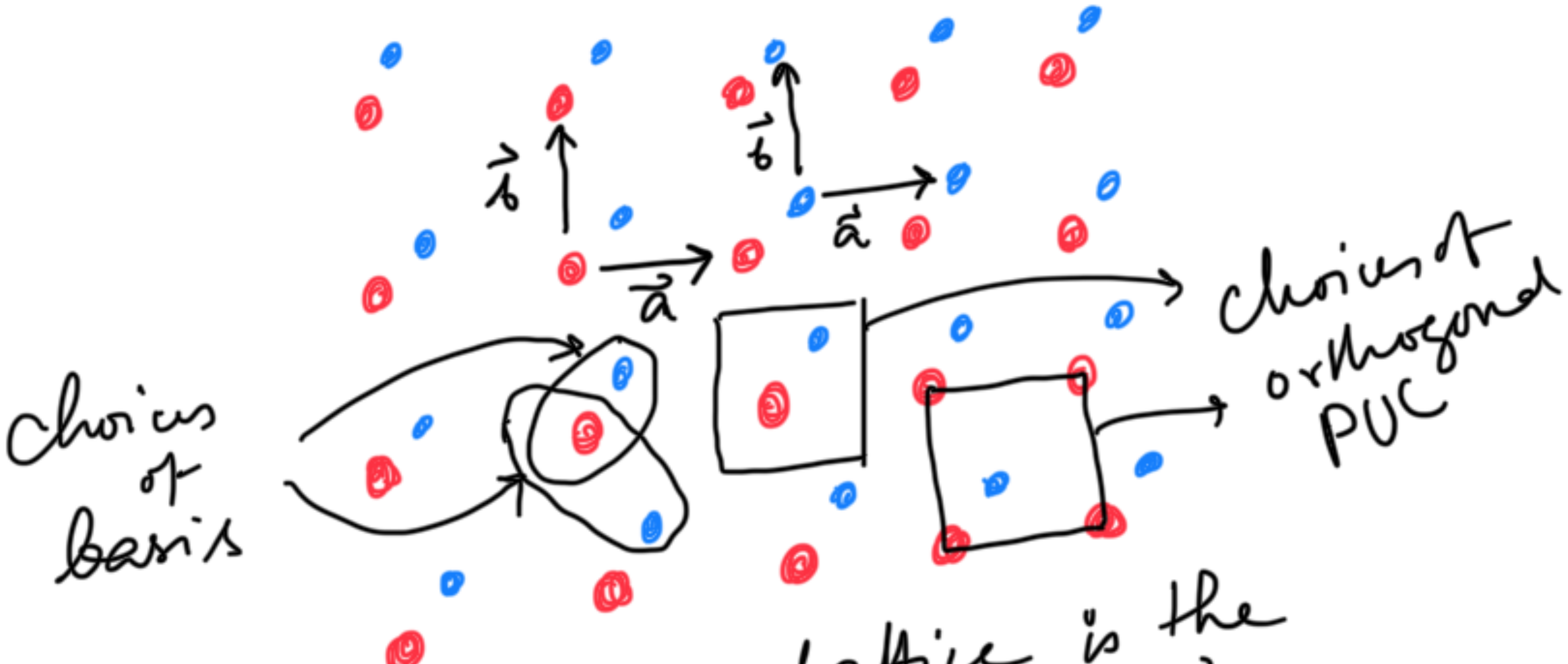
* All choices of PUCs must have same area (2D) / vol (3D).

Unit cell (UC): Any multiple of PUC.

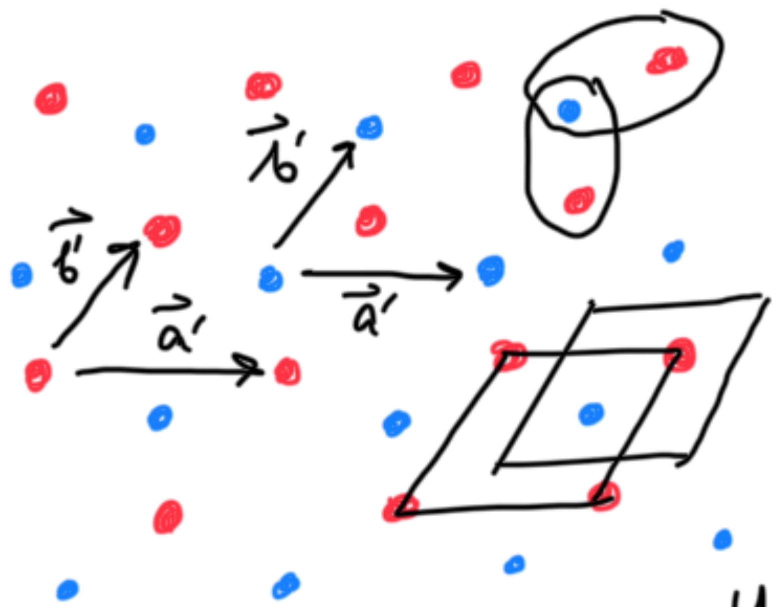
We choose PUC and UC for a given lattice as per the convenience of our understanding.

Real crystal: lattice + basis.

Each lattice point is "decorated" by a basis which can be a single atom or a group of similar or different atoms.



The associated lattice is the same lattice spanned by $\{\vec{a}, \vec{b}\}$ shown above

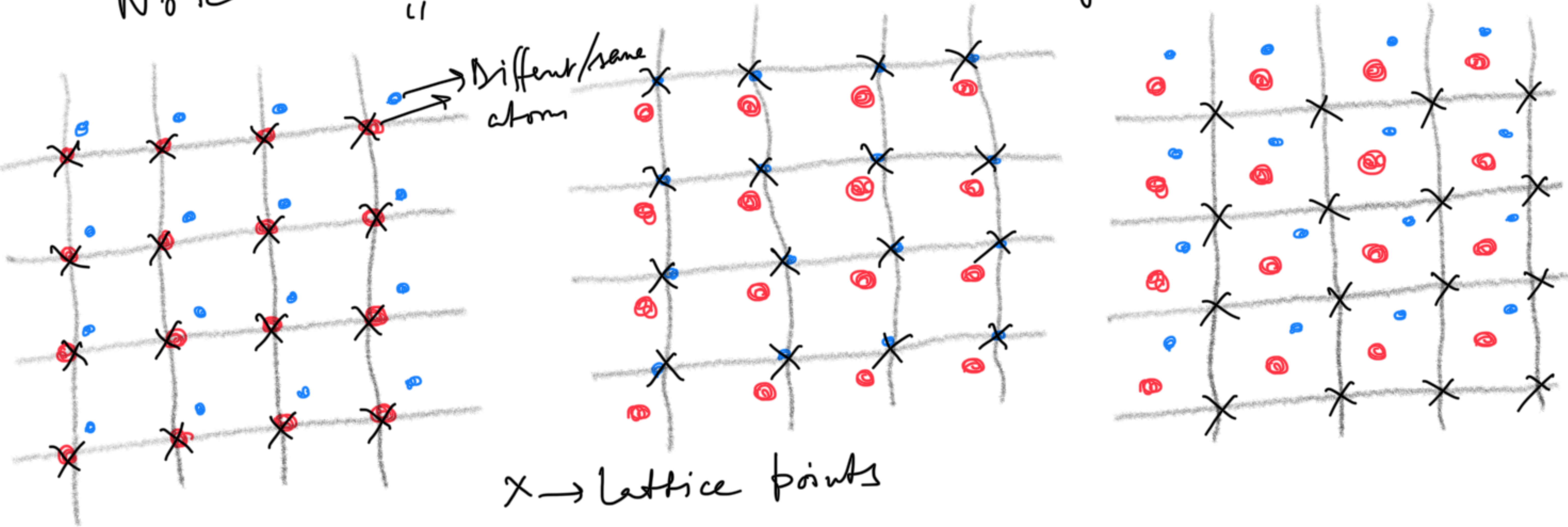


The lattice is the same one spanned by $\vec{a'}$ and $\vec{b'}$ shown above.

known

Note: Lattice points are abstract but basis are real.

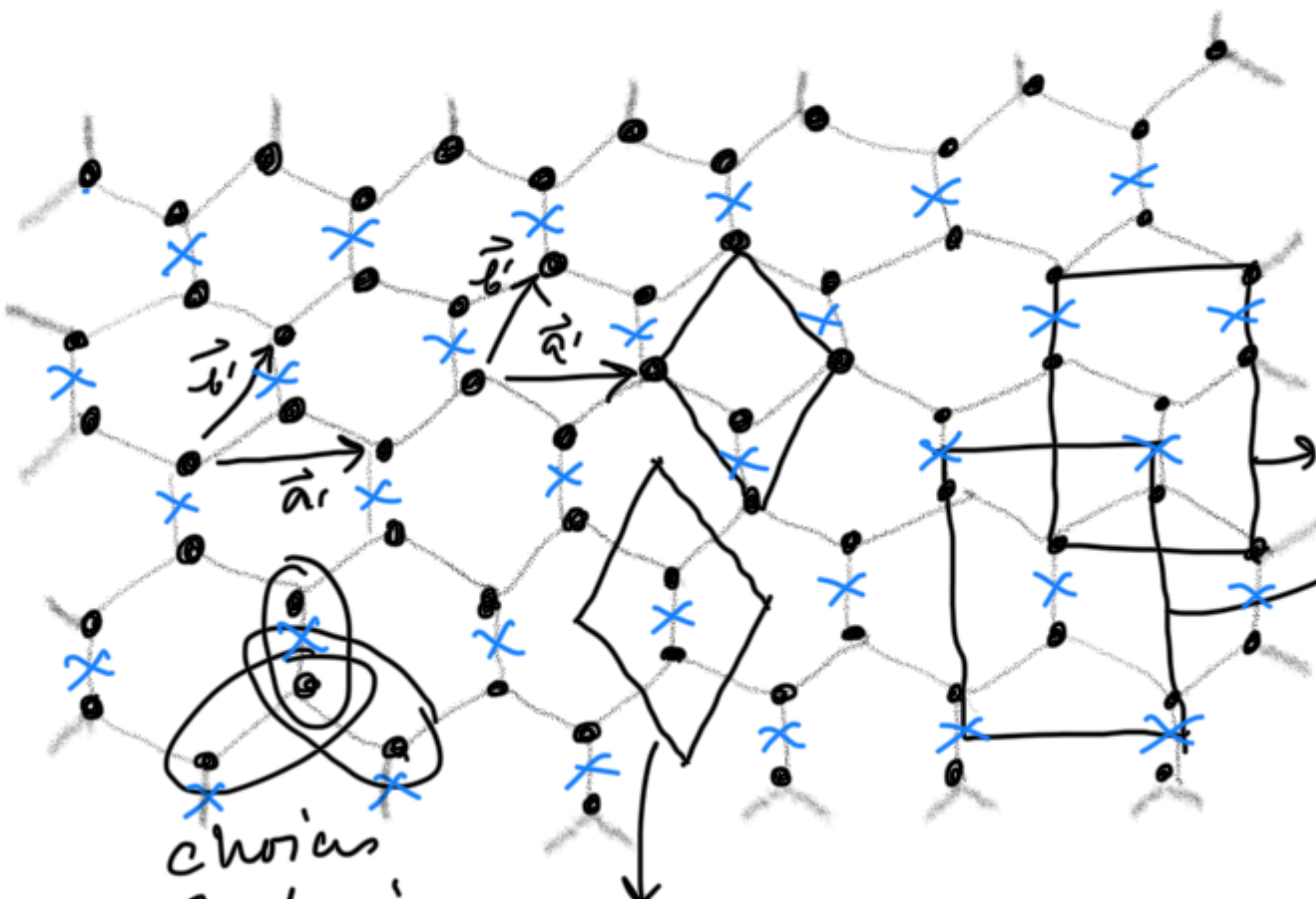
" " can be chosen anywhere in space



x → lattice points

Graphene:

Each lattice point (x) is decorated by a basis of two carbon atoms.



→ Orthogonal UC (Not PUC)

We can not have any ortho PUC in this case.

Here we chose to

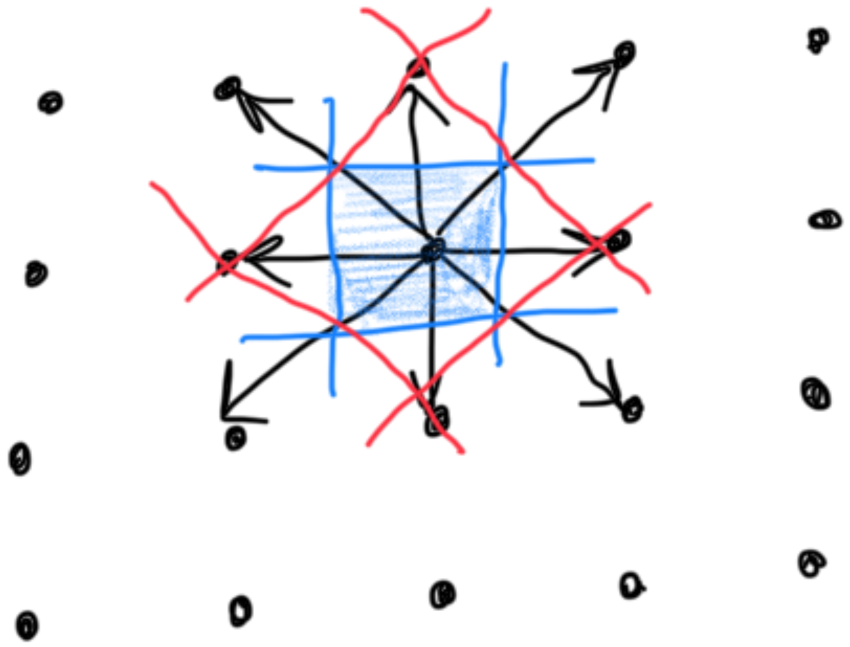
there are
place the lattice points
between two C atoms.

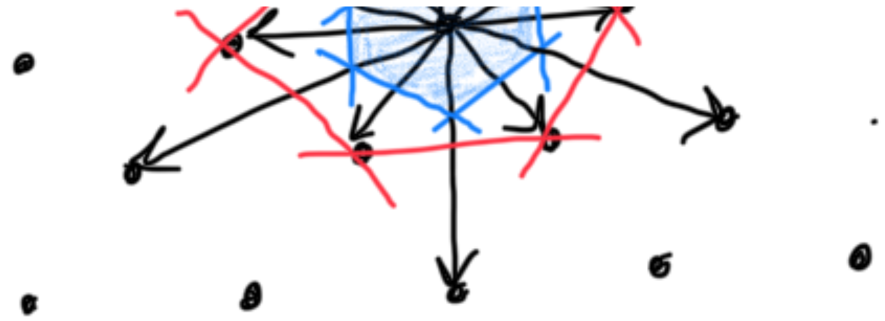
of basis
PUC

Note that the environment of the two atoms in the PUC are not same.
You can not translate the environment of one to the other.
∴ Both the atoms in the basis can not simultaneously be Bravais lattice points.
We can choose one of them and then the other one will be part of a two atom basis.
∴ Two atom basis for graphene is unavoidable for PUC.

Wigner Seitz (WS) cells : A method to determine PUC.

In 2D/3D draw perpendicular bisecting line/planes for all lattice vectors around a randomly chosen lattice point (which can be any basis atom) and find the area/volume enclosed by the lines/planes containing the chosen lattice point.





Note that in case of WS cells the PLVs do not explicitly span the WS cell. They need to be determined.