Bravais Lattices
&
Crystal Structures

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What we'd (ultimately) like to know:

- What are the allowed energies and wavefunctions of electrons in (periodic) solids?

- *Why consider only periodic structures?*

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- What are the allowed energies and wavefunctions of electrons in (periodic) solids?

- Why consider only periodic structures?

  - They are easier to study, because of some special properties of electrons in periodic potentials.

  - Some of the methods we use are applicable only to periodic systems.

  - Very many systems of interest really are crystalline, i.e., they have a periodic structure.

  (Will see later what to do for non-periodic cases!)

Periodic Crystal Structures

(In Real Space)

Crystal Structures

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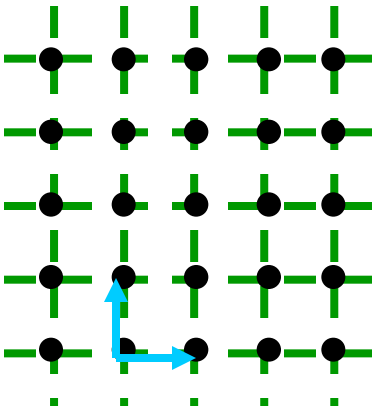
- Every crystal structure consists of:

  (i) a Bravais Lattice (shape of unit cell & how it repeats).

  Specified by primitive lattice vectors $\boldsymbol{a, b, c}$.



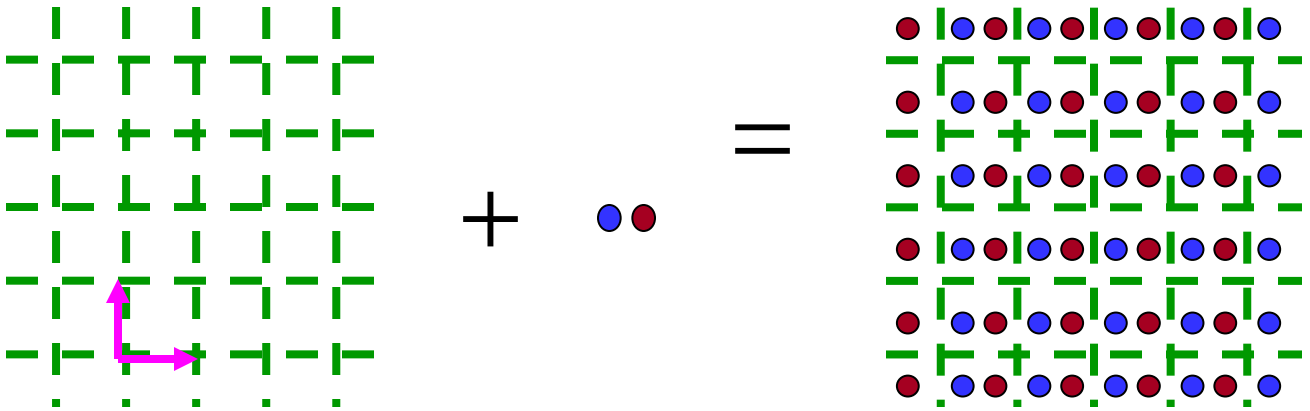
Crystal Structures

- Crystals possess a structure that is built up out of translationally repeating units (unit cells).
- Every crystal structure consists of:

  (i) a Bravais Lattice (shape of unit cell & how it repeats).

  Specified by primitive lattice vectors a, b, c.

  (ii) an Atomic Basis (how many atoms are in the unit cell, and how they are arranged).



a. The Bravais Lattice

Input parameters in pwscf

`ibrav`

`celldm`

OR

`A, B, C, cosAB, cosBC, cosAC`

Bravais Lattices

- Enumerated by *Auguste Bravais* (~1850).

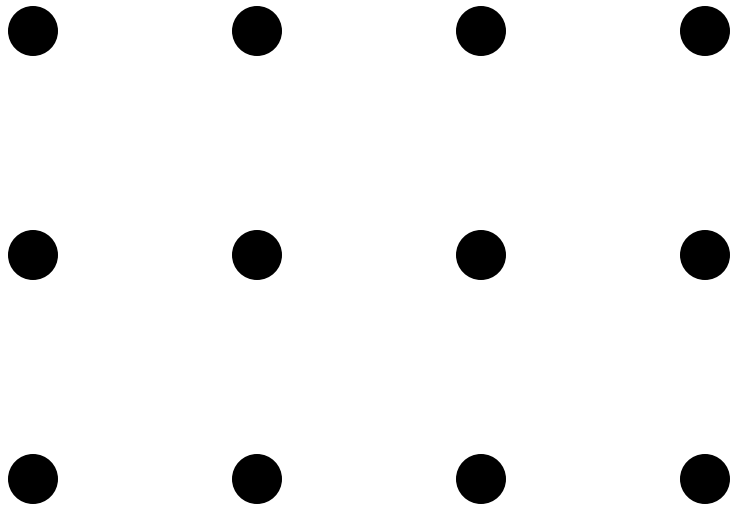
- Infinite lattice of discrete points.
- Arrangement AND Orientation IDENTICAL from all points.
- All points can be specified by:

  $\boldsymbol{R} = n_1\boldsymbol{a} + n_2\boldsymbol{b} + n_3\boldsymbol{c}$, where n_1, n_2, n_3 are integers.

- $\{\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}\}$ = PRIMITIVE LATTICE VECTORS (PLVs)
- In 2-D: $\boldsymbol{a}$ & $\boldsymbol{b}$ should not be parallel (or anti-parallel).
- In 3-D: $\boldsymbol{a}$, $\boldsymbol{b}$ & $\boldsymbol{c}$ should not <u>all</u> be in the same plane.

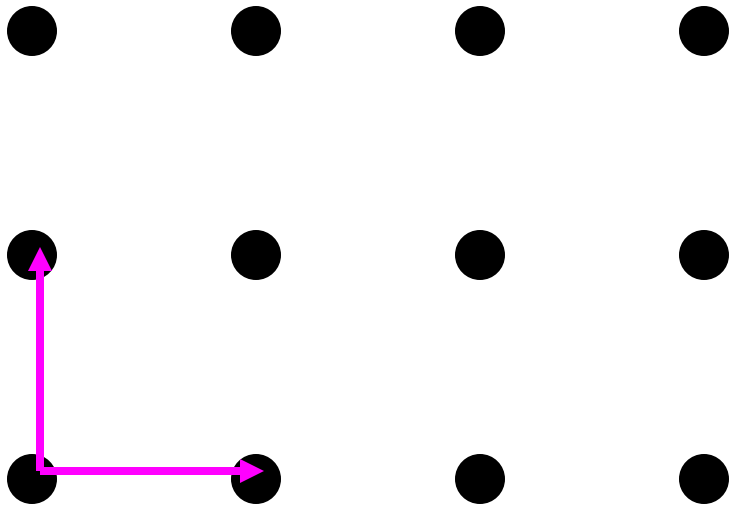
Bravais Lattices (2-D)

- *Is this a Bravais Lattice?*



Bravais Lattices (2-D)

- Yes, 2-D Square Lattice



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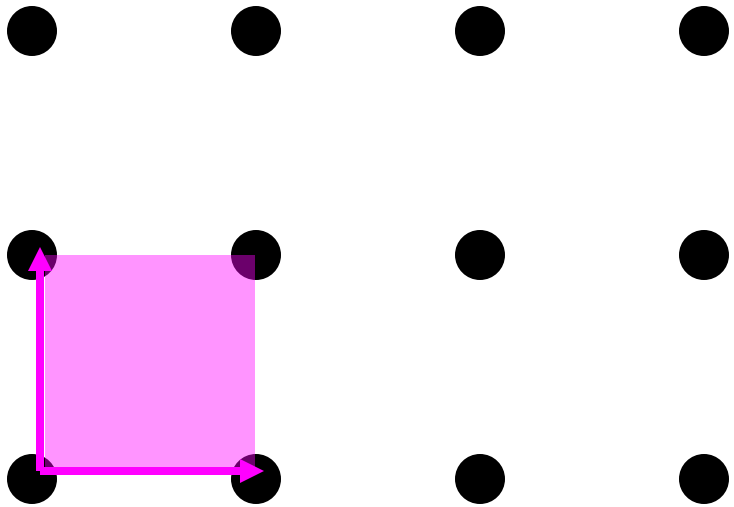

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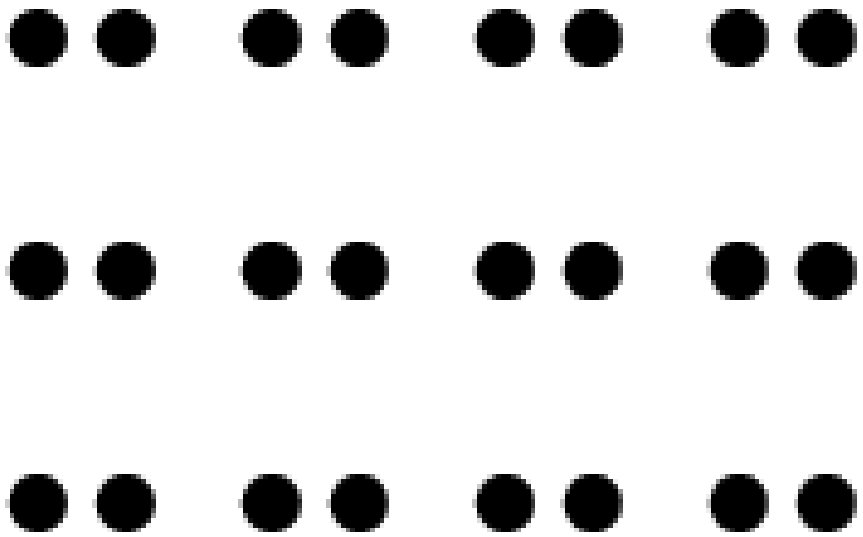
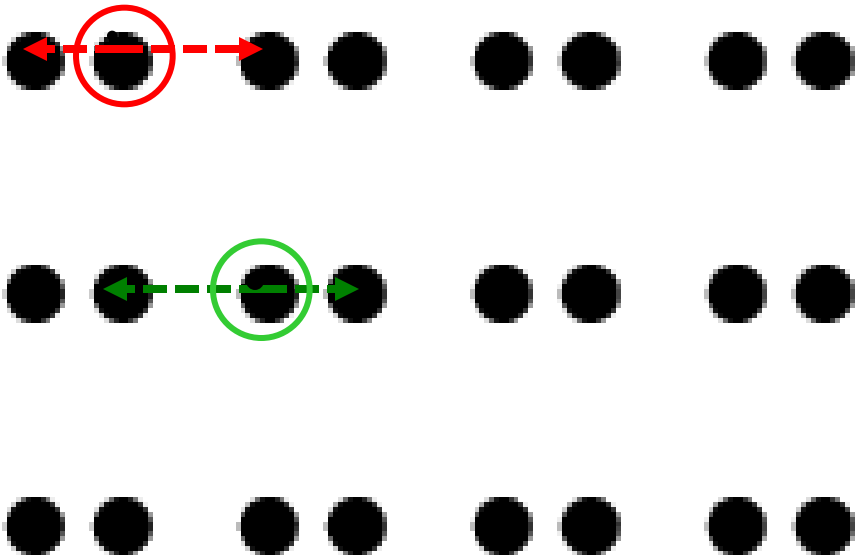


Bravais Lattices (2-D)

- No.



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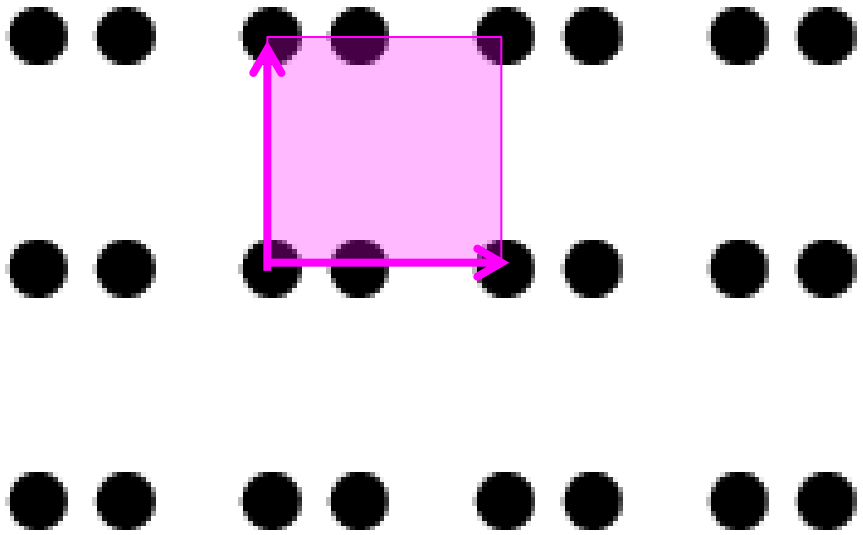
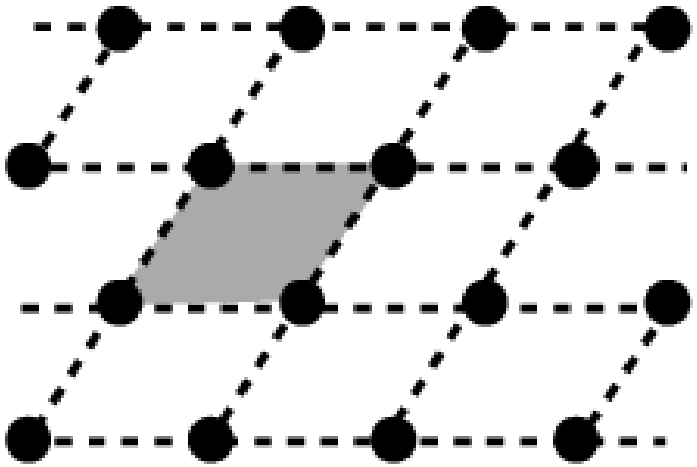


Note that lattice vectors start and end at identical points.

Unit Cells for Bravais Lattices

Primitive (non-primitive) unit cells contain 1 (>1) lattice pt. and generate the whole lattice by translation, without overlapping and without space missing.

e.g., consider the 2-D Hexagonal Lattice:



Unit cell?
Primitive?

Unit Cells for Bravais Lattices

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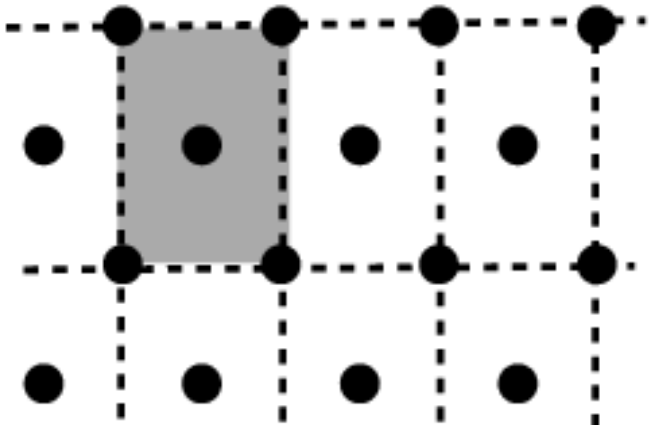
e.g., consider the 2-D Triangular Lattice:



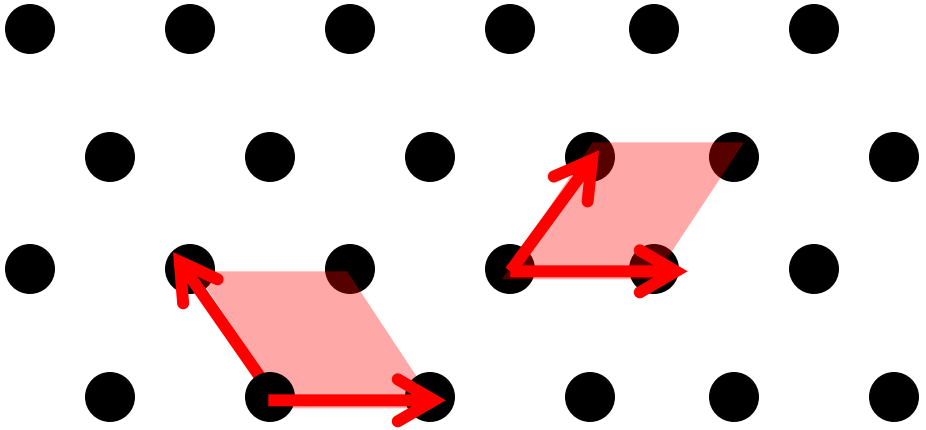
Unit cell?
Primitive?

Here we will do “worksheet 1”
on 2D Bravais Lattices

WORKSHEET 1

Bravais Lattices (2-D)

- Is this a Bravais Lattice? (assume pattern extends to infinity)
- Draw 2 primitive lattice vectors $\underline{a}$ and $\underline{b}$.
- Note: Lattice vectors always start and end at identical points!
- Shade a primitive unit cell.



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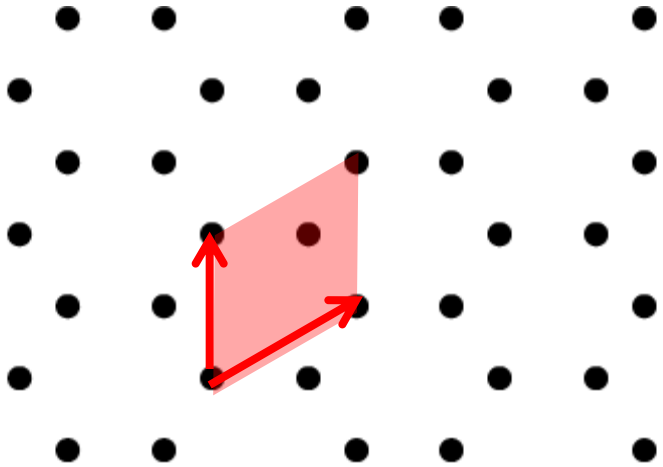

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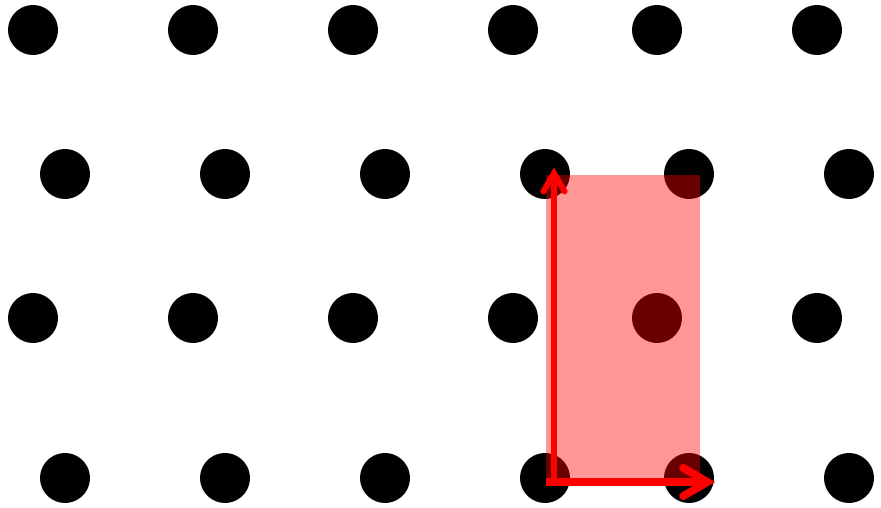
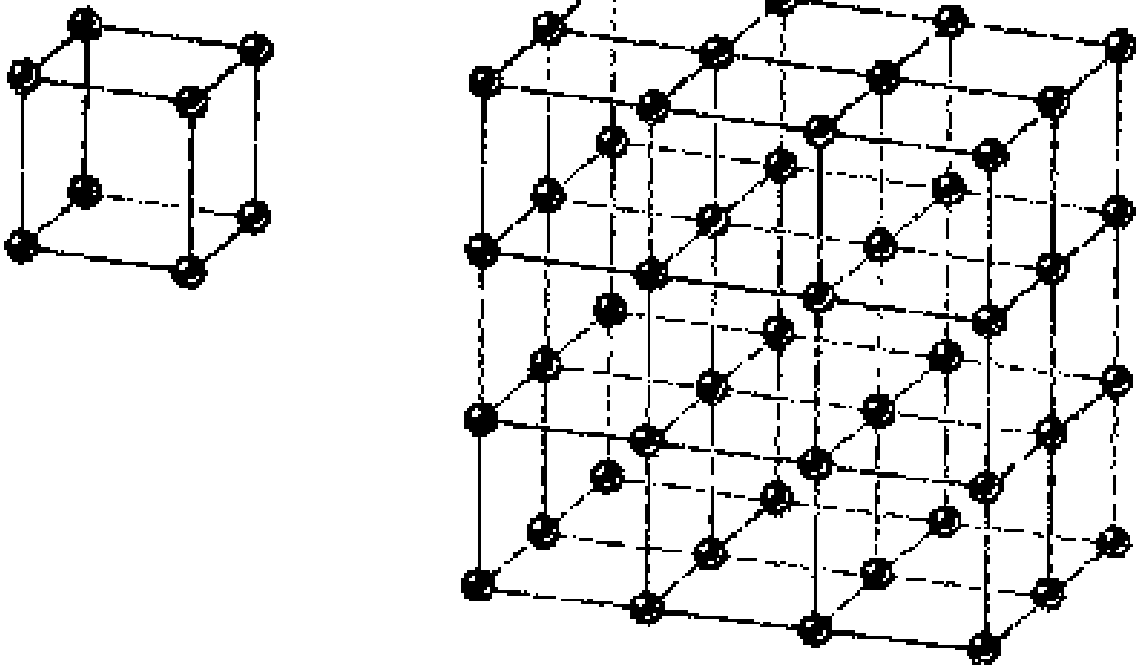


The Simple Cubic Lattice



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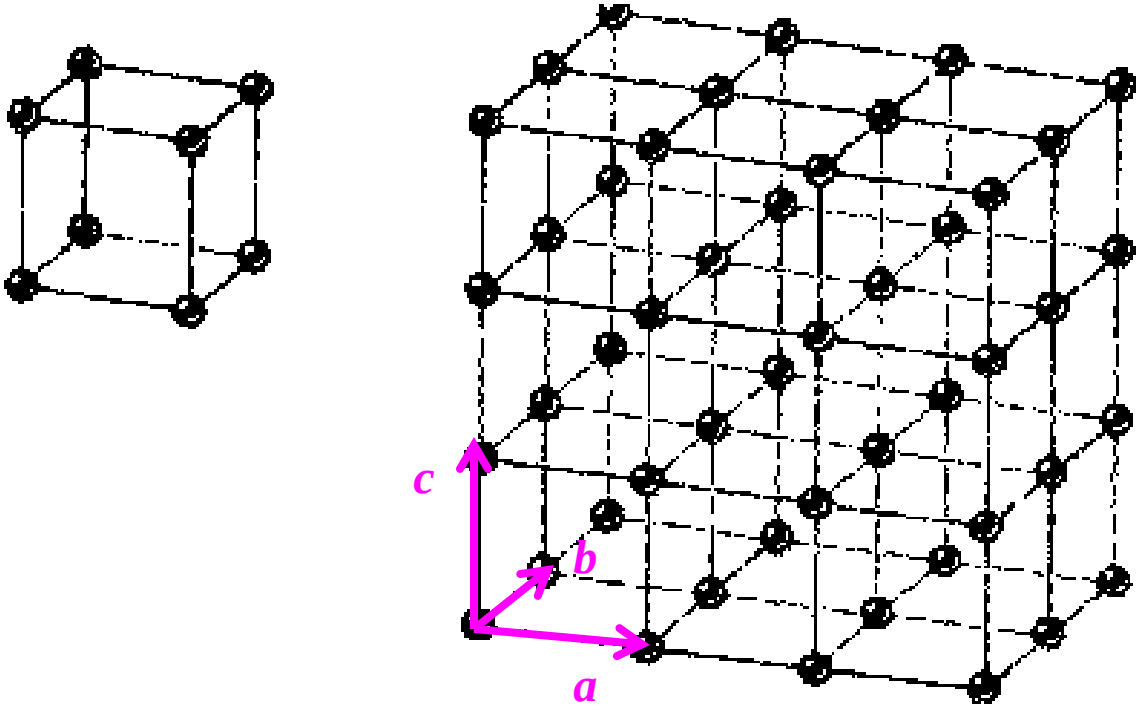
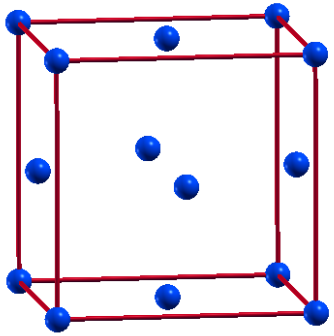
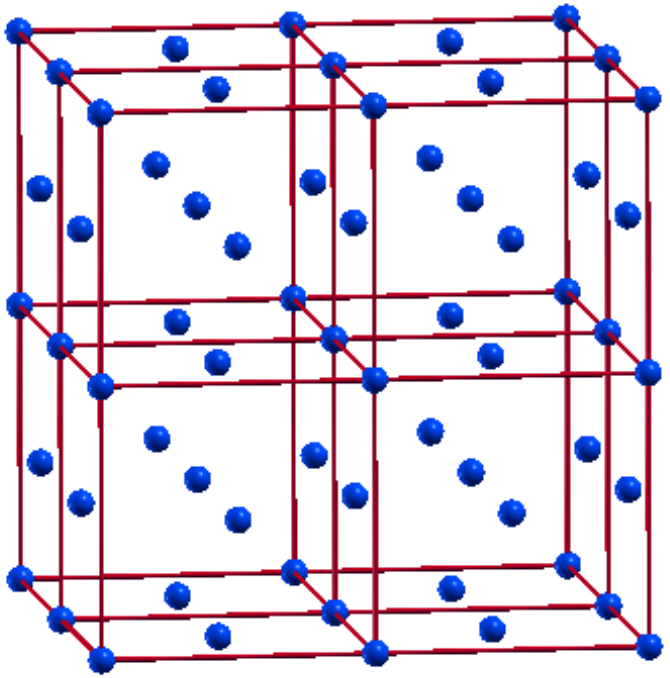
The Simple Cubic Lattice



- Yes, it is a Bravais Lattice.
- ***a, b, c*** are on possible set of primitive lattice vectors.

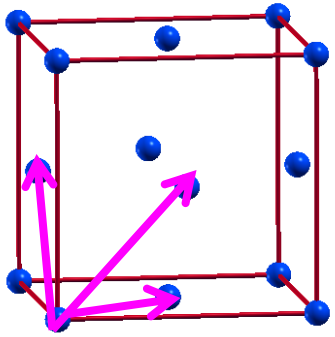
The Face Centered Cubic Lattice

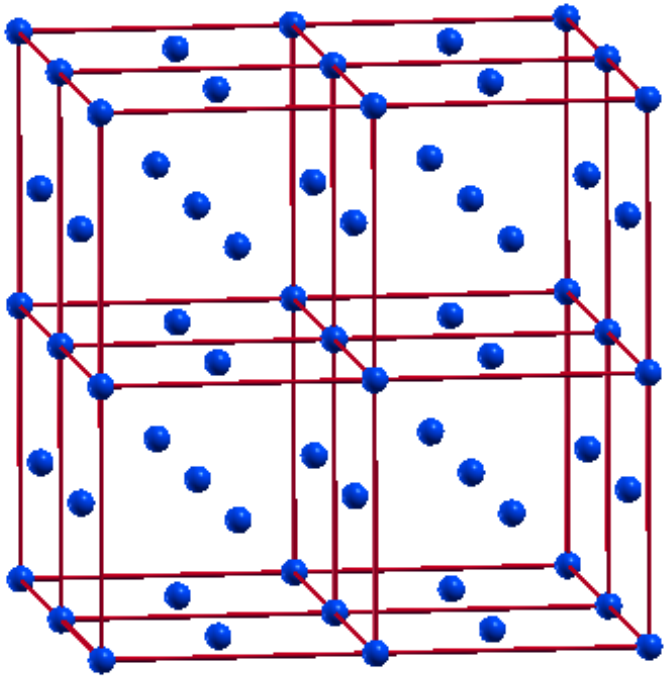




- Is this a Bravais Lattice?

The Face Centered Cubic Lattice





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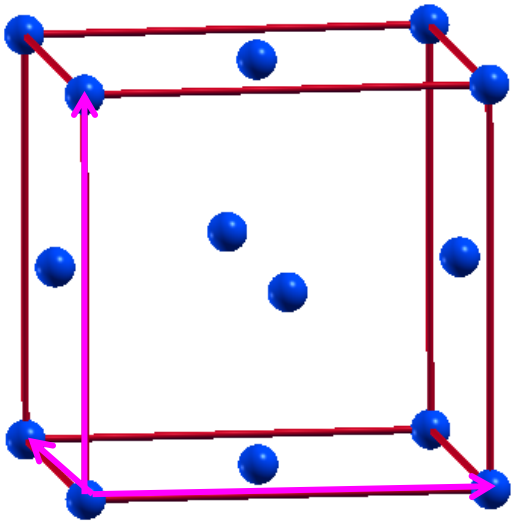
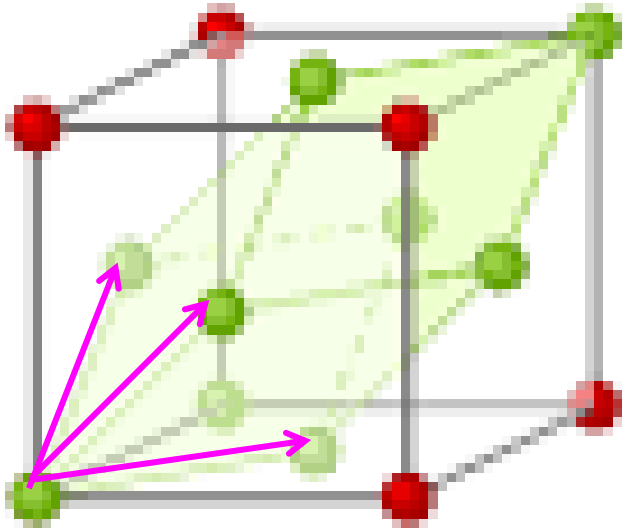
The Face Centered Cubic Lattice



Conventional Cubic Unit Cell



Primitive Unit Cell

How to Specify the Bravais Lattice

In the most general case:

Have to specify the 3 vectors a, b, c

To do this, we need to specify SIX numbers.

- a = Length of a --- **A** or **celldm(1)**
- b = Length of b or b/a --- **B** or **celldm(2)**
- c = Length of c or c/a --- **C** or **celldm(3)**
- Angle between b & c --- **cosBC** or **celldm(4)**
- Angle between a & c --- **cosAC** or **celldm(5)**
- Angle between a & b --- **cosAB** or **celldm(6)**

For Quantum ESPRESSO (pwscf)

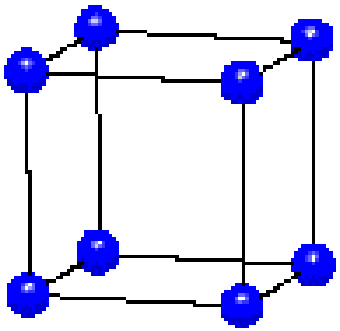
Specify the 6 numbers in green or brown if you put **ibrav = 0**

How to Specify the Bravais Lattice

3-D Bravais lattices are classified into 14 types

- Cubic
- $a = b = c$, $\alpha=\beta=\gamma = 90$

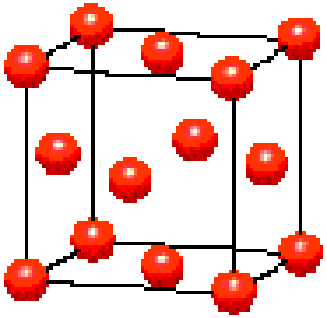
(1)



SC

`ibrav=1`

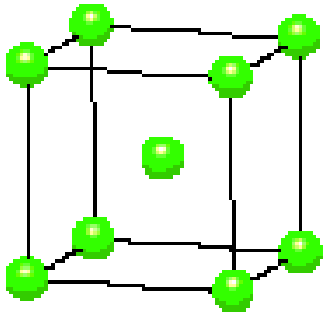
(2)



FCC

`ibrav=2`

(3)



BCC

`ibrav=3`

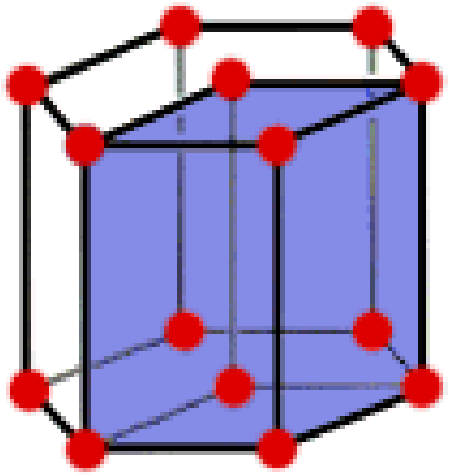
Need to specify only a = length of a = **`celldm(1)`**

How to Specify the Bravais Lattice

3-D Bravais lattices are classified into 14 types

- Hexagonal
- $a = b \neq c$, $\alpha=\beta=90$ $\gamma = 120$

(4)



ibrav=4

Need to specify

a = **celldm(1)**

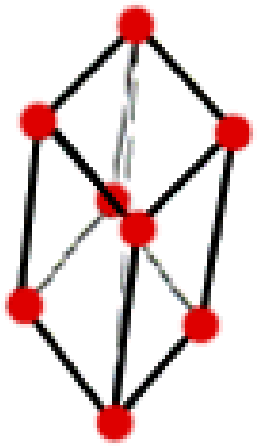
c/a = **celldm(3)**

How to Specify the Bravais Lattice

3-D Bravais lattices are classified into 14 types

- Trigonal (Rhombohedral)
- $a = b = c$, $\alpha = \beta = \gamma \neq 90$

(5)



ibrav=5

Need to specify

a = **celldm(1)**

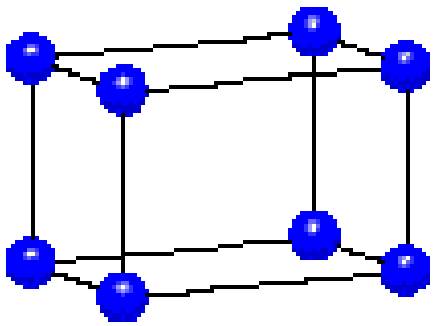
cos(γ) = **celldm(4)**

How to Specify the Bravais Lattice

3-D Bravais lattices are classified into 14 types

- Tetragonal
- $a = b \neq c$, $\alpha=\beta=\gamma = 90$

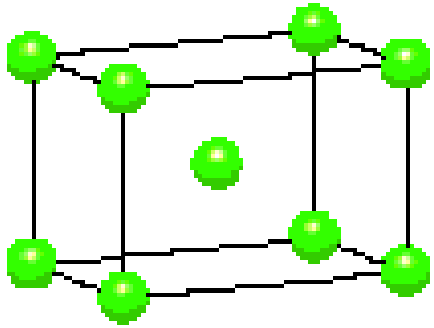
(6)



ST

ibrav=6

(7)



BCT

ibrav=7

Need to specify

a = **celldm(1)**

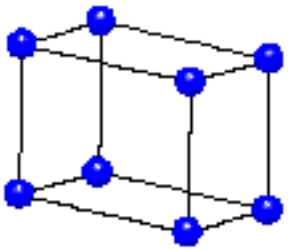
c/a = **celldm(3)**

How to Specify the Bravais Lattice

3-D Bravais lattices are classified into 14 types

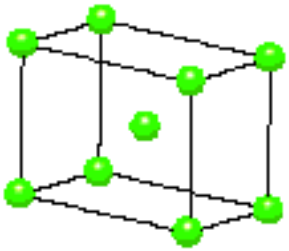
- Orthorhombic
- $a \neq b \neq c$, $\alpha=\beta=\gamma = 90$

(8)



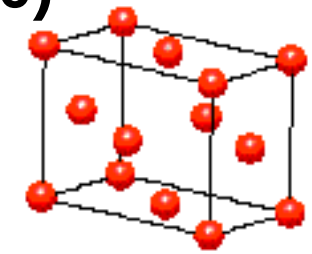
SO
ibrav=8

(9)



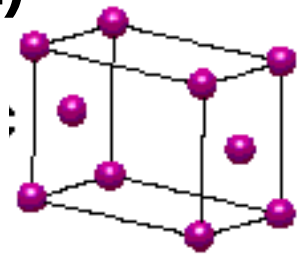
BCO
ibrav=9

(10)



FCO
ibrav=10

(11)



1-FCO
ibrav=11

Need to specify

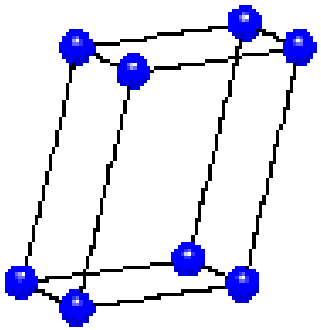
a = **celldm(1)**; b/a = **celldm(2)**; c/a = **celldm(3)**

How to Specify the Bravais Lattice

3-D Bravais lattices are classified into 14 types

- Monoclinic
- $a \neq b \neq c$, $\alpha=\beta=90 \neq \gamma$

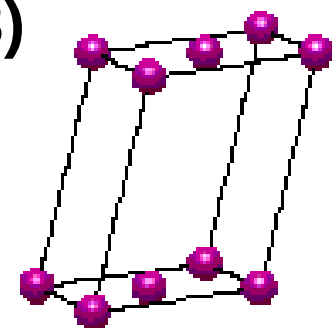
(12)



Monoclinic P

ibrav=12

(13)



Base-centered monoclinic

ibrav=13

Need to specify a = **celldm(1);** b/a = **celldm(2);**

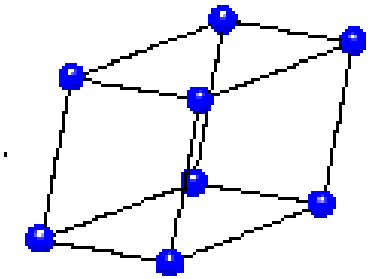
c/a = **celldm(3);** cos(γ) = **celldm(4)**

How to Specify the Bravais Lattice

3-D Bravais lattices are classified into 14 types

- Triclinic
- $a \neq b \neq c$, $\alpha \neq \beta \neq \gamma \neq 90$

(14)



Triclinic

ibrav=14

Need to specify

a = **celldm(1);** b/a = **celldm(2);** c/a = **celldm(3);**

cos**(γ)=celldm(4);** cos**(β)=celldm(5);** cos**(α)= celldm(6)**

b. The Crystal Structure

Input parameters in pwscf

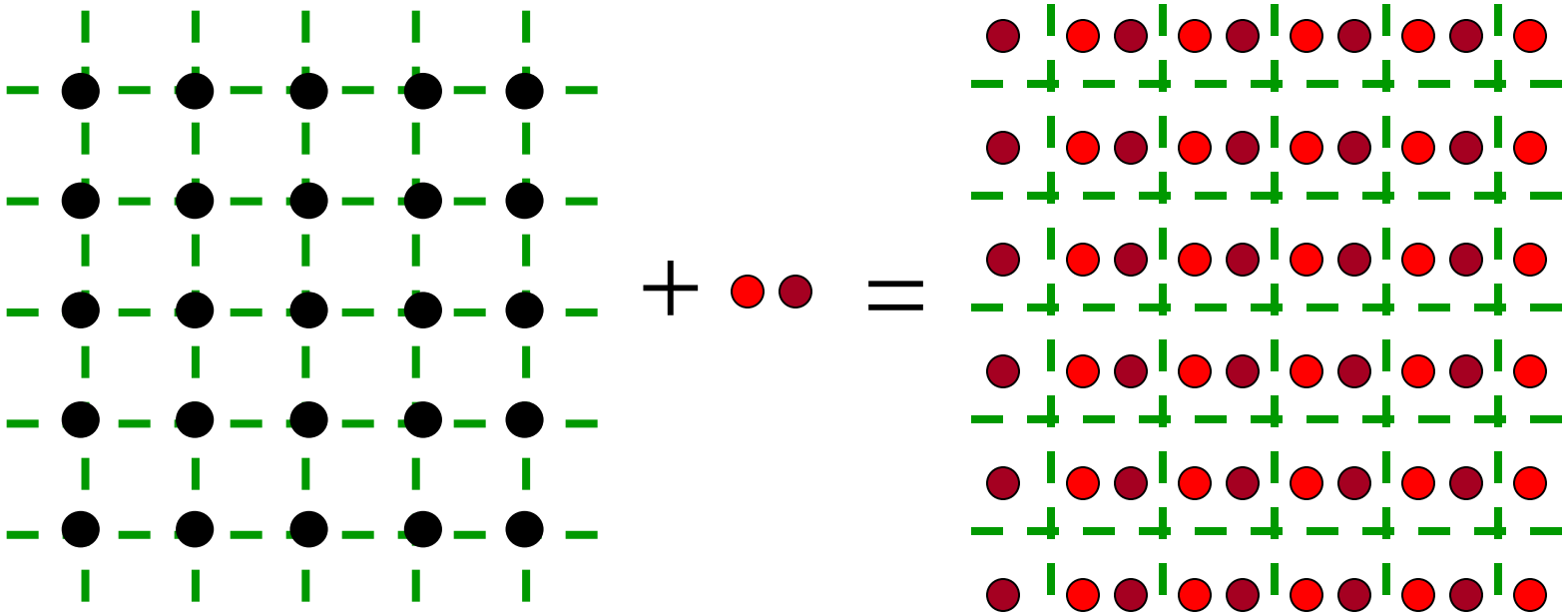
`nat`

`ntyp`

`ATOMIC_POSITIONS`

Crystal Structures

- To get the crystal structure, one attaches an atomic basis every point in the Bravais Lattice.



Primitive Unit Cell

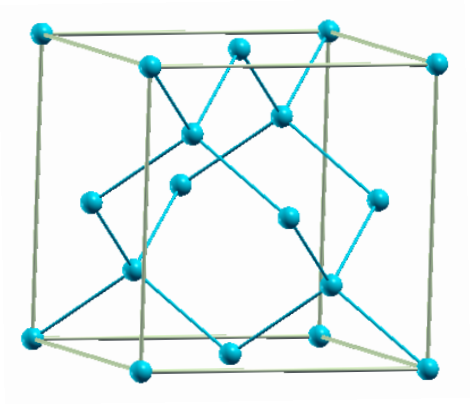
- Smallest possible unit cell for a given crystal structure.
- Depending on the crystal structure, it may contain only one atom, or it may contain more than one atom.

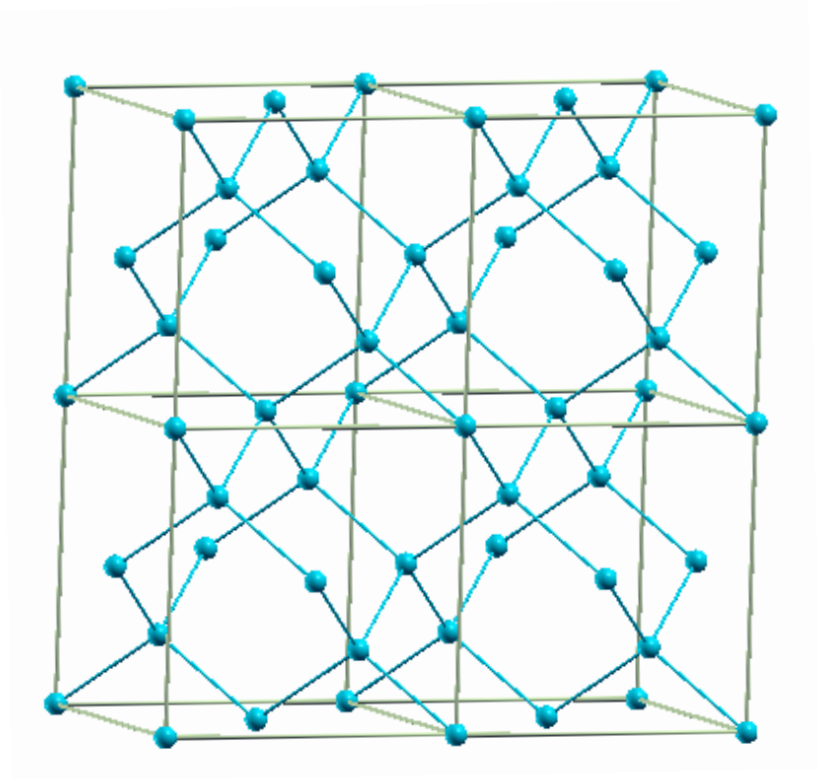
- One can always choose to work with a larger (non-primitive) unit cell. Such a cell is called a supercell.

Crystal Structures that are also Bravais lattice types

- In many cases, the crystal structure itself is a Bravais lattice type (e.g., BCC or FCC)
- Then (and ONLY THEN) there is only one atom in the primitive unit cell.
- THEN (in input for pwscf):
- `nat = 1`
- `ntyp = 1`
- `ATOMIC_POSITIONS`: put one atom anywhere you want (usually at `0.0 0.0 0.0`)

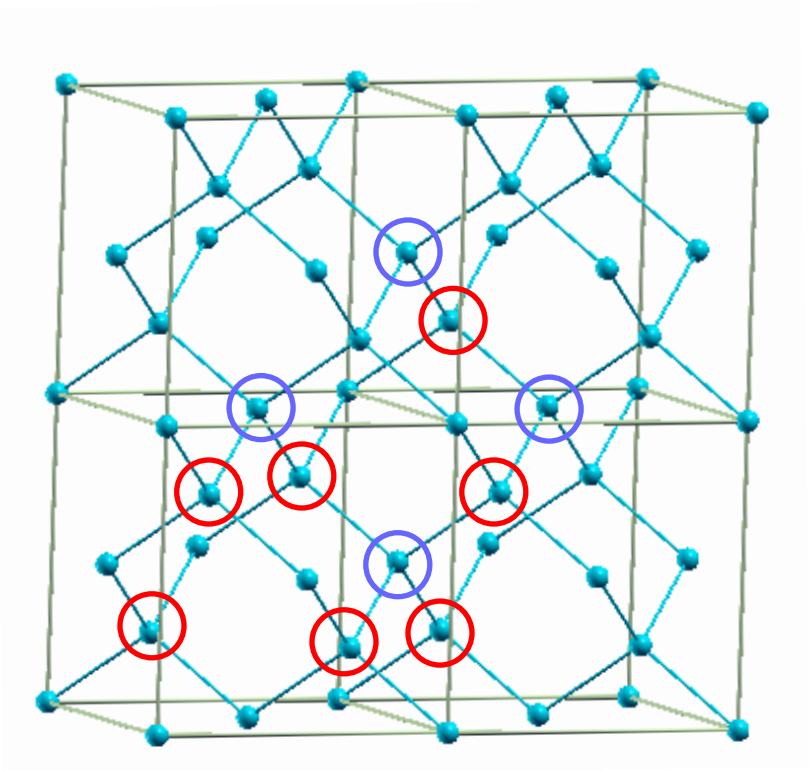
The Diamond Structure





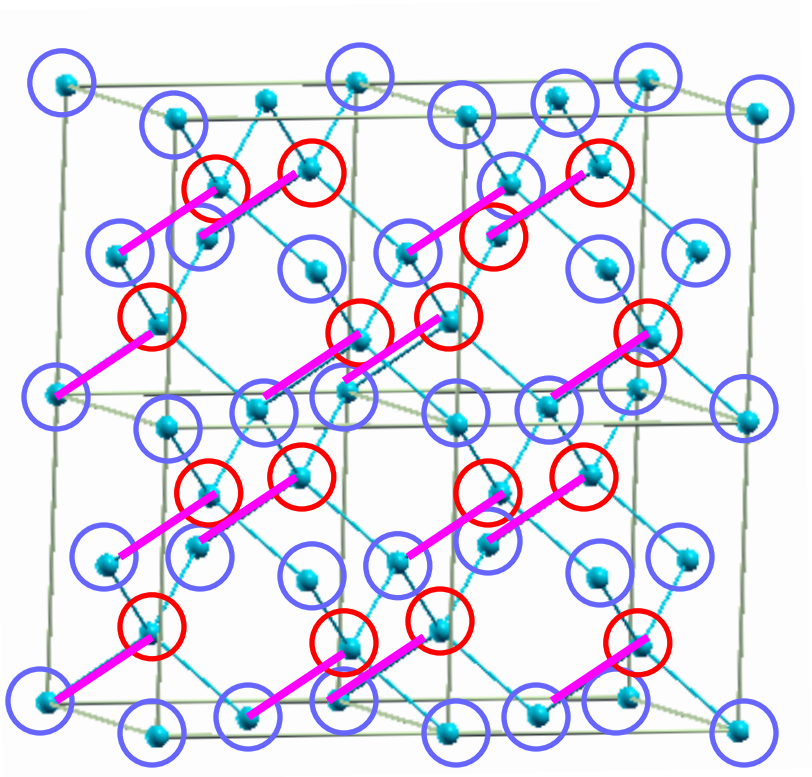
- Is this a Bravais Lattice?
- If yes, find a set of primitive lattice vectors.
- If no, find the Bravais lattice and basis.

The Diamond Structure



No, it is not a Bravais lattice.
View from red and blue points is different!

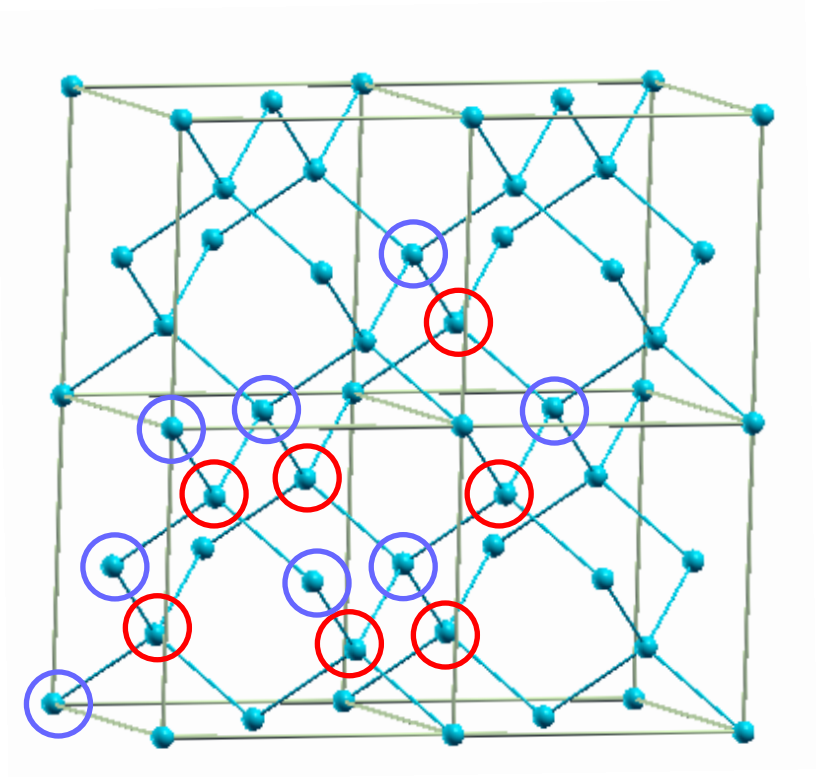
The Diamond Structure



To generate whole structure:

FCC Bravais lattice + 2-atom basis: (0,0,0) + (¼, ¼, ¼)

The Diamond Structure



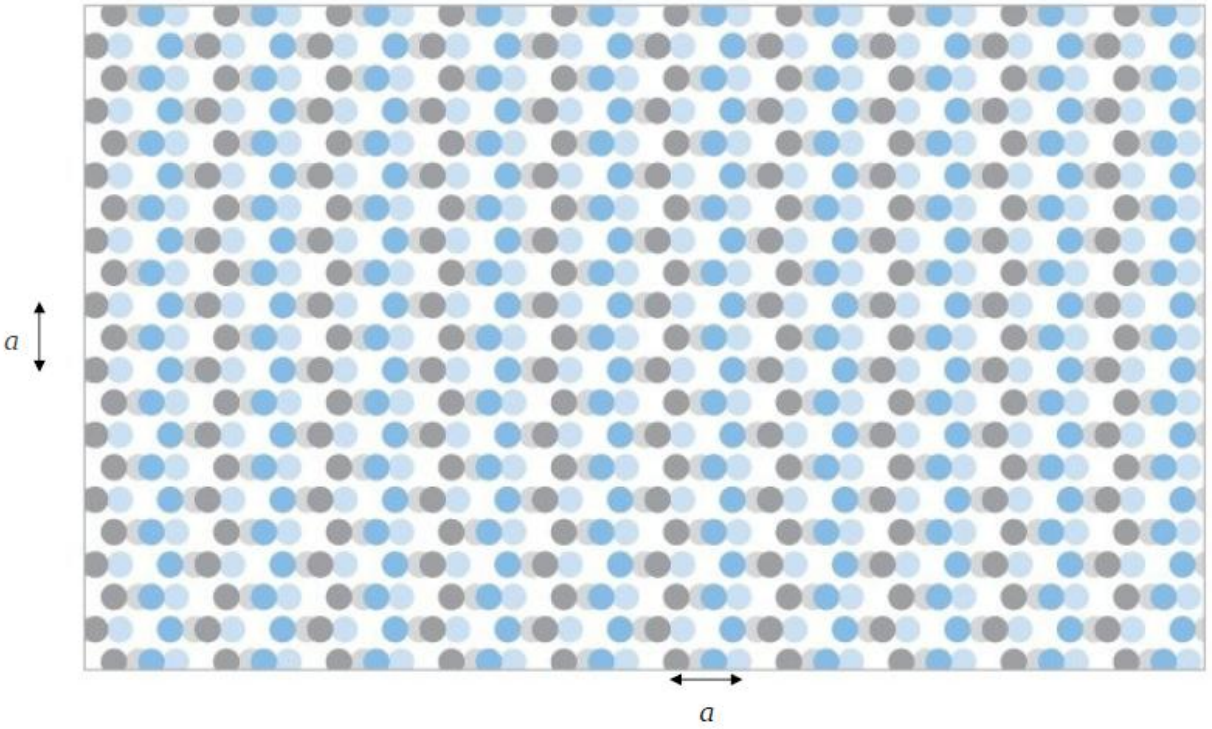
FCC

```
ibrav = 2
nat = 2
ntyp = 1
ATOMIC_POSITIONS
... 0.0 0.0 0.0
... 0.25 0.25 0.25
```

Here we will do “worksheet 2”
on crystal structures

WORKSHEET 2

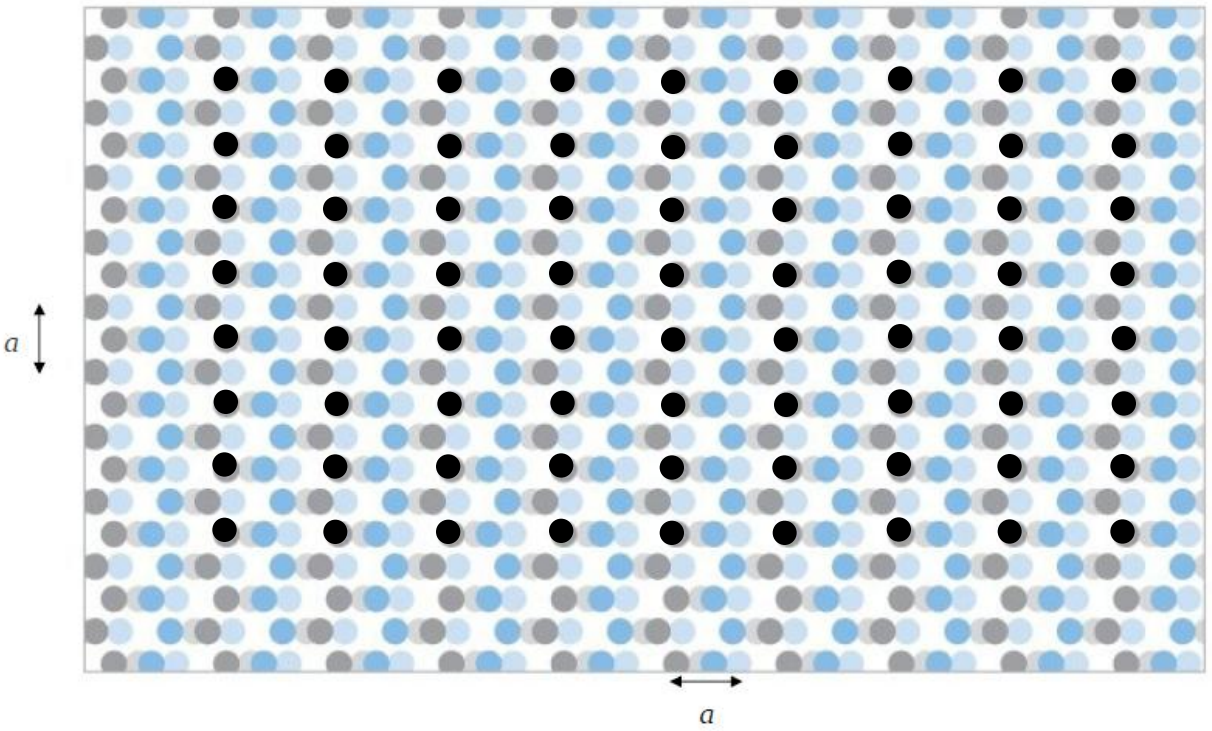
2D Crystals



- Find the 2D Bravais lattice and basis for this (infinite) pattern.
- Draw two (primitive) lattice vectors.
- Find the primitive unit cell. How many atoms (dots) does it contain?

WORKSHEET 2

2D Crystals

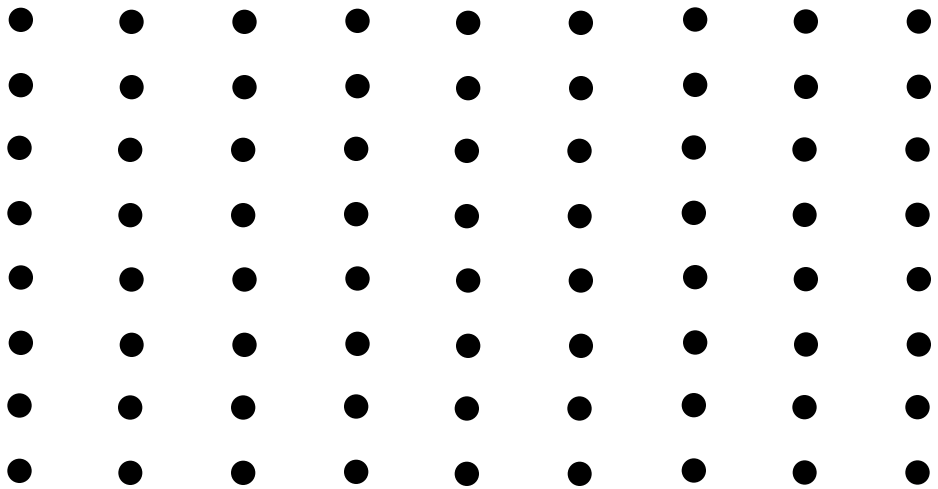


- Find the 2D Bravais lattice and basis for this (infinite) pattern.
- Draw two (primitive) lattice vectors.
- Find the primitive unit cell. How many atoms (dots) does it contain?

WORKSHEET 2

2D Crystals

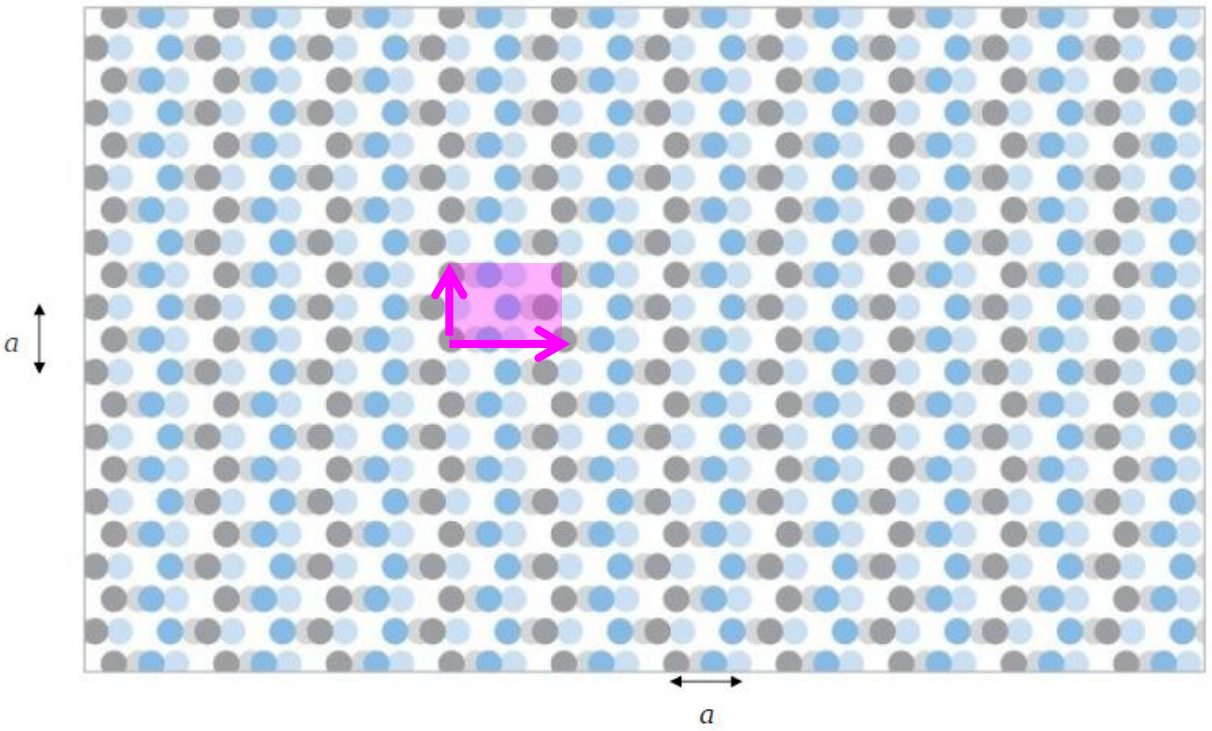
2D Bravais lattice:



- 8-atom basis:

WORKSHEET 2

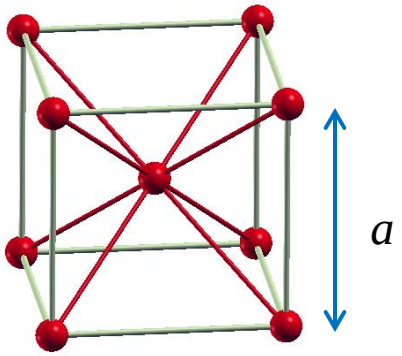
2D Crystals

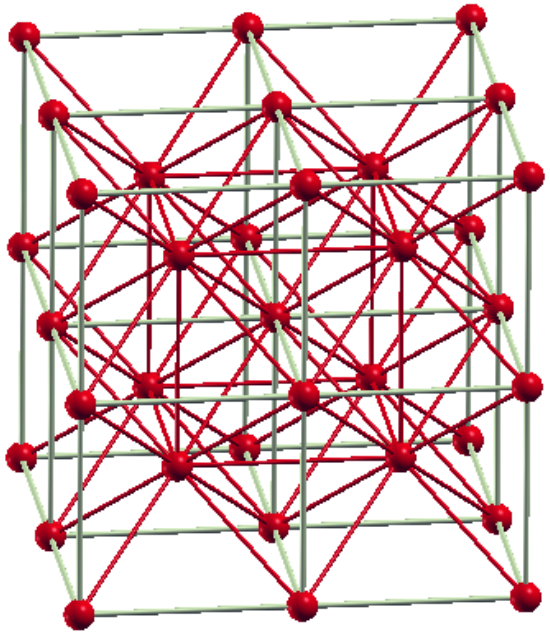


- Find the 2D Bravais lattice and basis for this (infinite) pattern.
- Draw two (primitive) lattice vectors.
- Find the primitive unit cell. How many atoms (dots) does it contain?

WORKSHEET 2

The Body Centered Cubic Structure



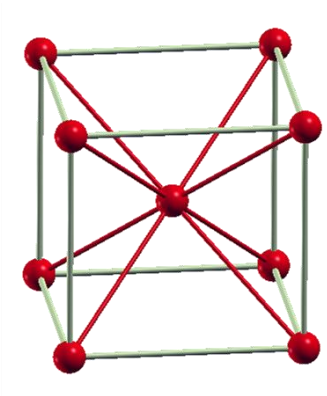


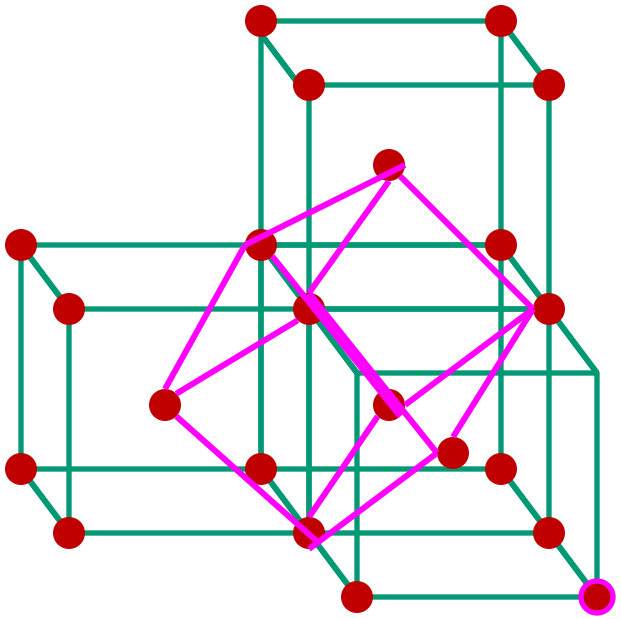
This is a Bravais lattice.
You can do a pwscf calculation with
`ibrav=3`, `nat=1`,`nytp=1`, one atom placed at `0.0 0.0 0.0`

If you instead choose to work with a supercell and `ibrav=1`, give
`nat, ntyp` and `ATOMIC_POSITIONS`

WORKSHEET 2

The Body Centered Cubic Structure



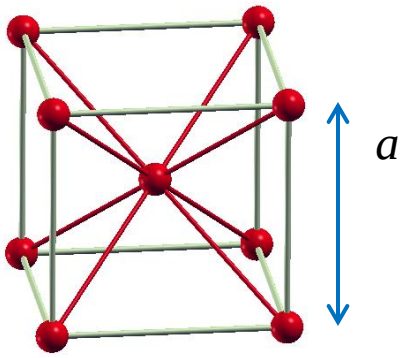


Conventional Cubic Unit Cell

Primitive Unit Cell

WORKSHEET 2

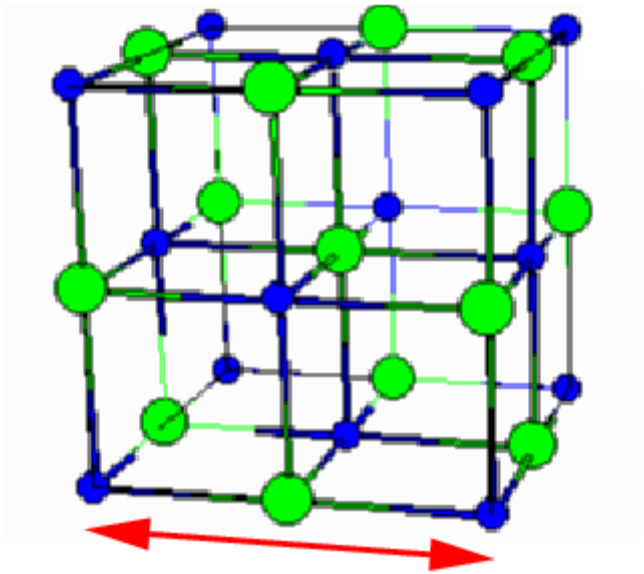
The Body Centered Cubic Structure




```
ibrav = 1
nat = 2
ntyp = 1
ATOMIC_POSITIONS
... 0.0 0.0 0.0
... 0.5 0.5 0.5
```

WORKSHEET 2

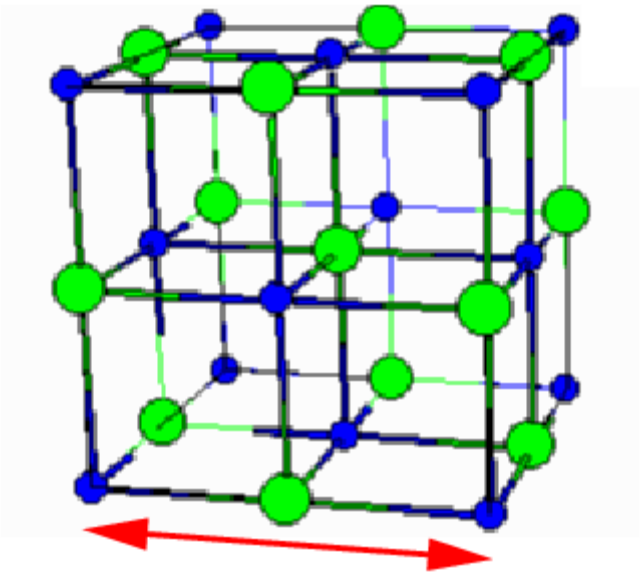
The Rock Salt (NaCl) Structure



- This is obviously not a Bravais lattice! (Why?)
- Find a Bravais lattice and basis.
- Give `nat,ntyp` and `ATOMIC_POSITIONS`

WORKSHEET 2

The Rock Salt (NaCl) Structure




```
ibrav = 2
nat = 2
ntyp = 2
ATOMIC_POSITIONS
... 0.0 0.0 0.0
... 0.5 0.5 0.5
```

OR

```
... 0.0 0.0 0.0
... 0.5 0.0 0.0
```

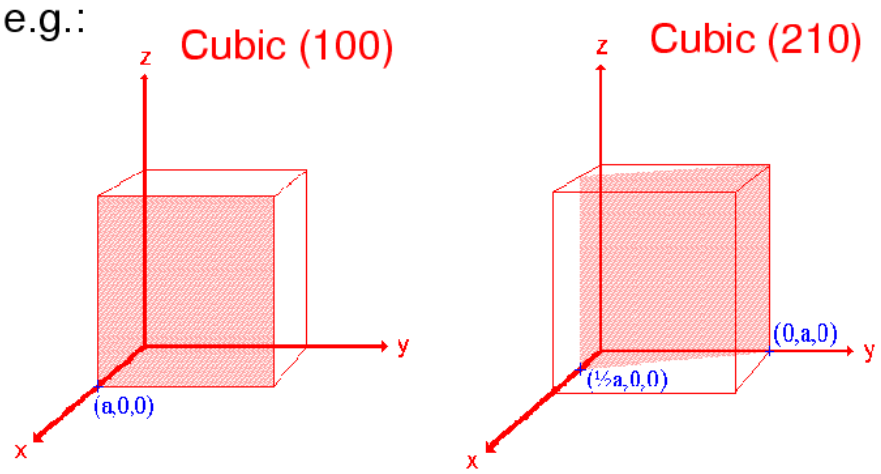
Miller Indices

Way of specifying planes/directions in crystal.

Plane: (hkl)

1) Take intercepts on the LVs *a, b, c* = n_1, n_2, n_3
2) Take reciprocals of intercepts = $1/n_1, 1/n_2, 1/n_3$
3) [Usually] multiply by factor m so that all 3 nos. are now integers: $h = m/n_1, k = m/n_2, l = m/n_3$.

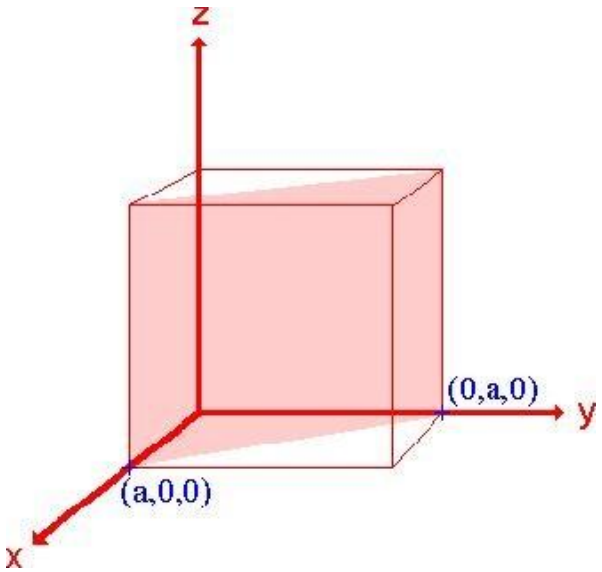
e.g.:

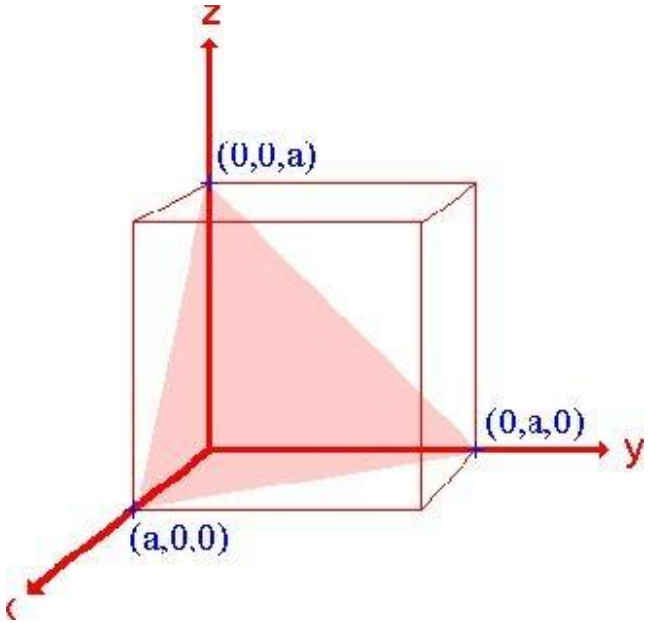


Note: For FCC,BCC, usually use *a, b, c* *for conventional cubic cell (non–primitive).*

Miller Indices

- Consider the following 2 planes in a cubic crystal.
- What are their Miller indices?

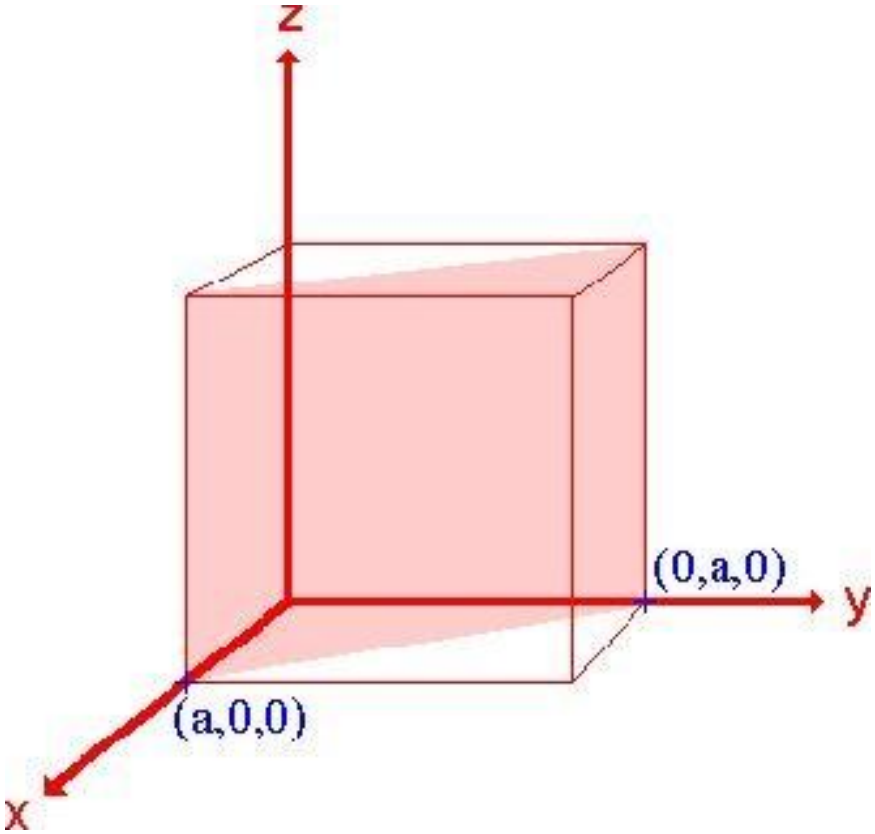




Here we will do “worksheet 3”
on Miller indices

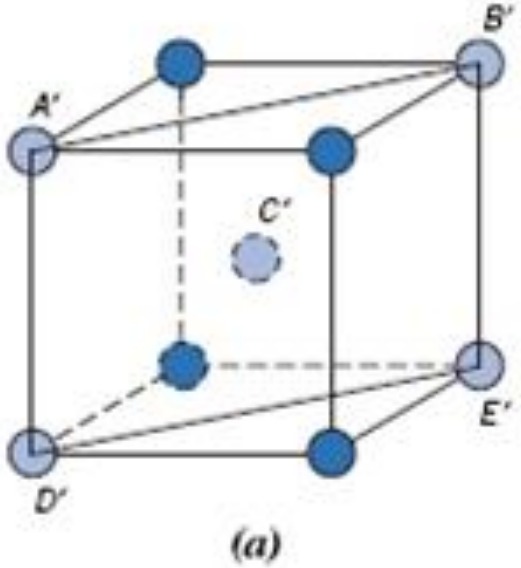
WORKSHEET 3

BCC (110) Surface

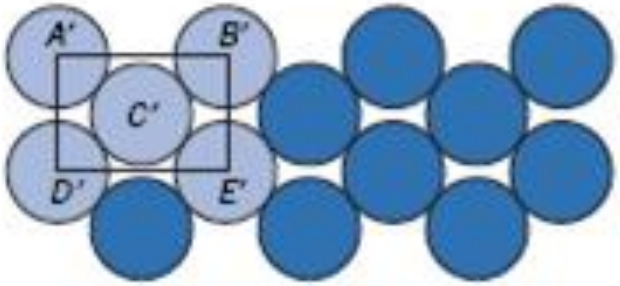


- Draw the 2D arrangement of atoms on a BCC(110) surface.
- Make sure you mark lengths in units of a (side of conventional cubic unit cell of BCC)
- Draw two PLVs.
- Draw the boundaries of a primitive unit cell.
- To do later: get the coordinates of atoms in the top 3 layers.

WORKSHEET 3

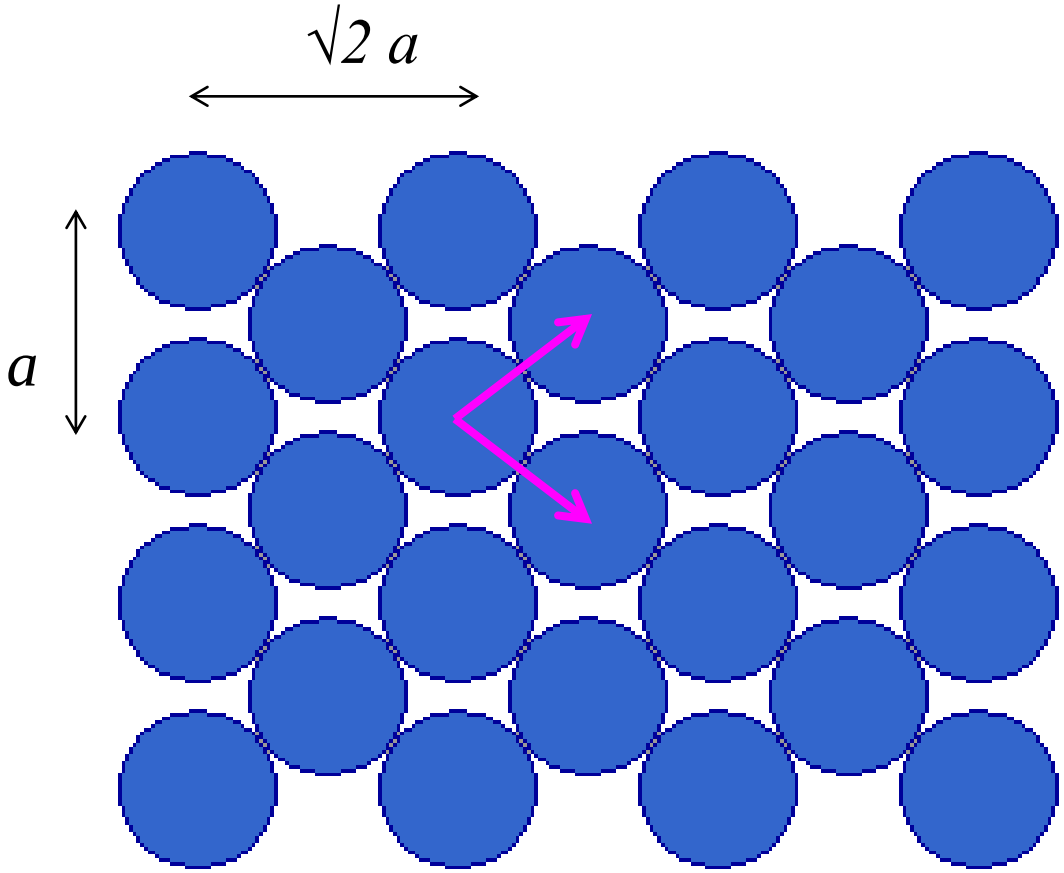


Topmost (surface) layer



Chegg

WORKSHEET 3

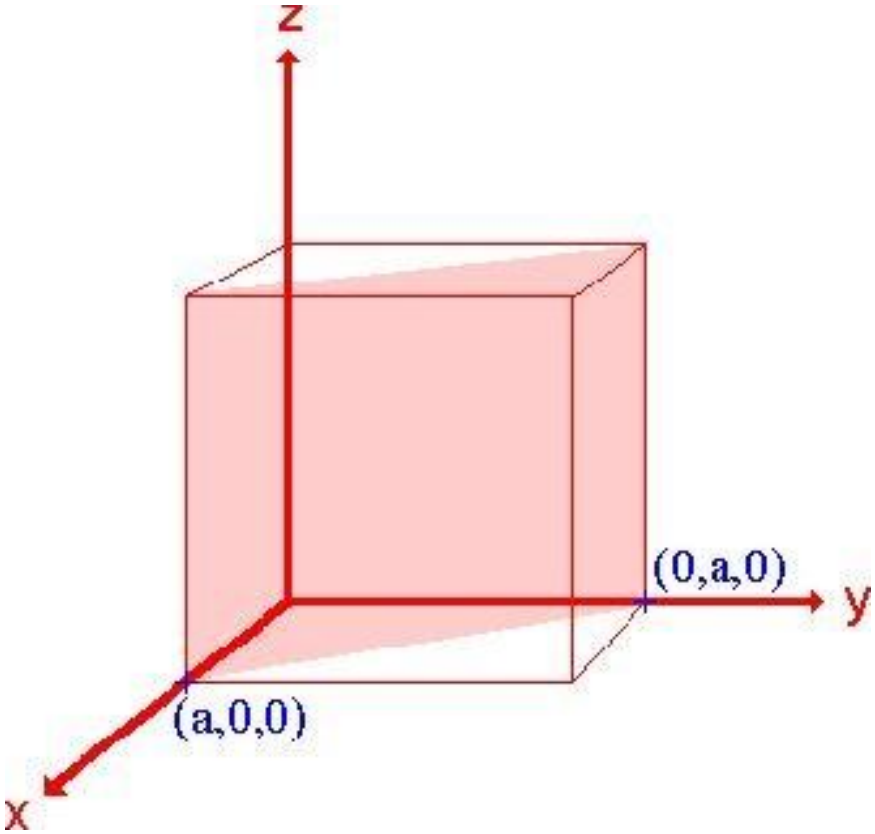


Topmost (surface) layer

R. Nix

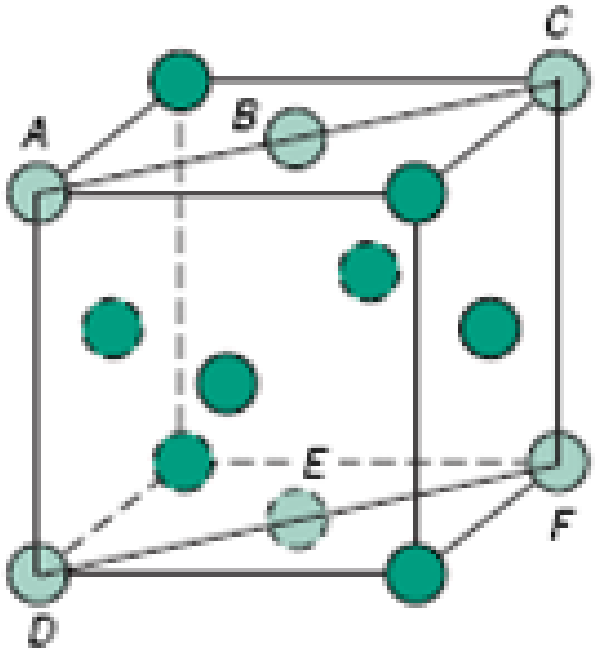
WORKSHEET 3

FCC (110) Surface



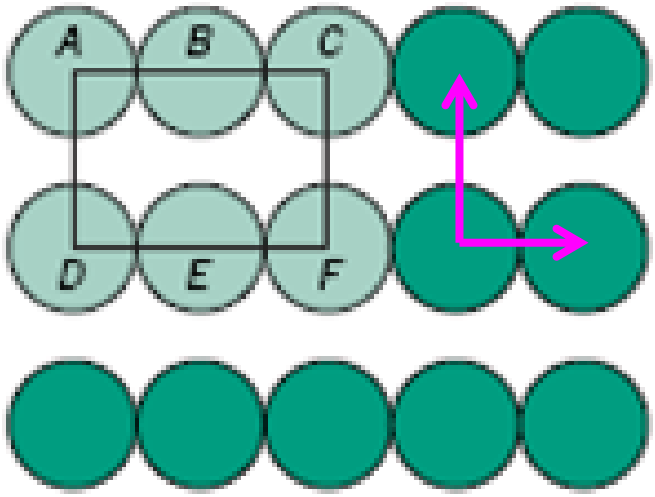
- Draw the 2D arrangement of atoms on a FCC(110) surface.
- Make sure you mark lengths in units of a (side of conventional cubic unit cell of FCC)
- Draw two PLVs.
- Draw the boundaries of a primitive unit cell.
- To do later: get the (x,y,z) coordinates of atoms in the first three layers.

WORKSHEET 3



(a)

Topmost (surface) layer



(b)

Chegg