Electronic Functional Materials and Devices

电子功能材料与元器件

QQ Group:

群名称:电子功能材料与器件
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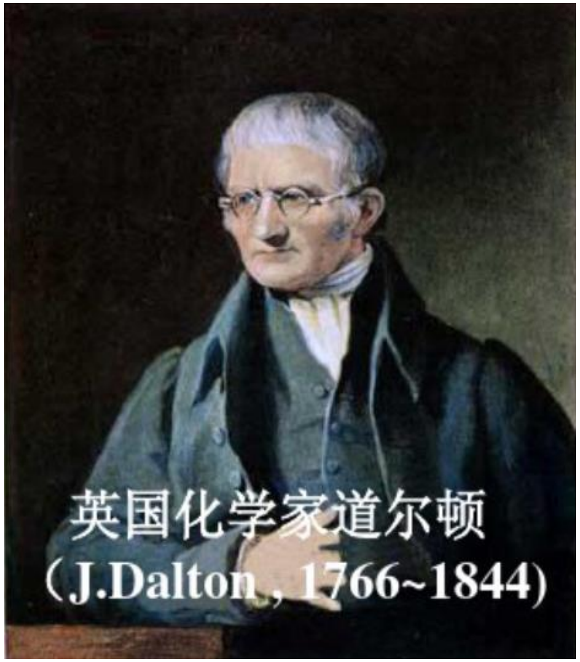
电子与电气工程系

1.1 Structure of atoms



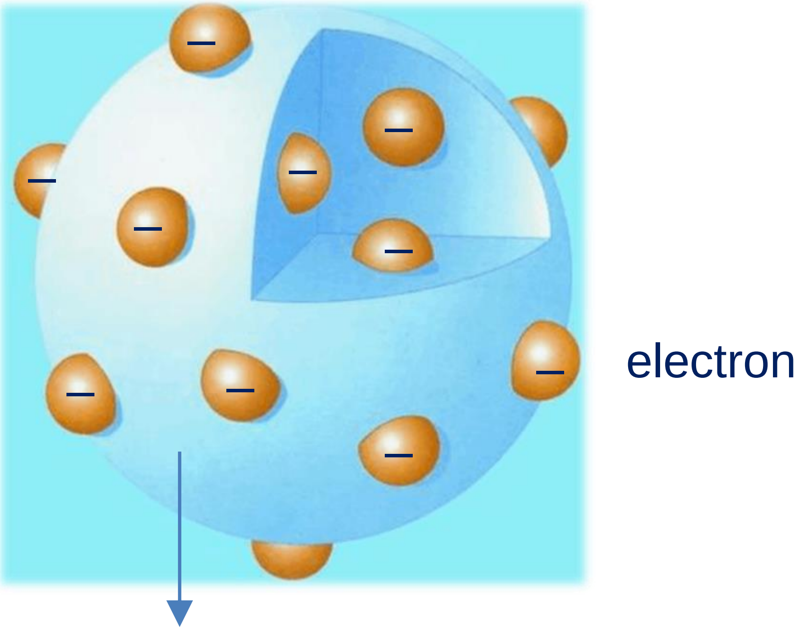
1803: J. Dalton's model

- Solid ball
- Atom is the smallest and indivisible particle

In 1897, J.J. Thomson discovered the electron.

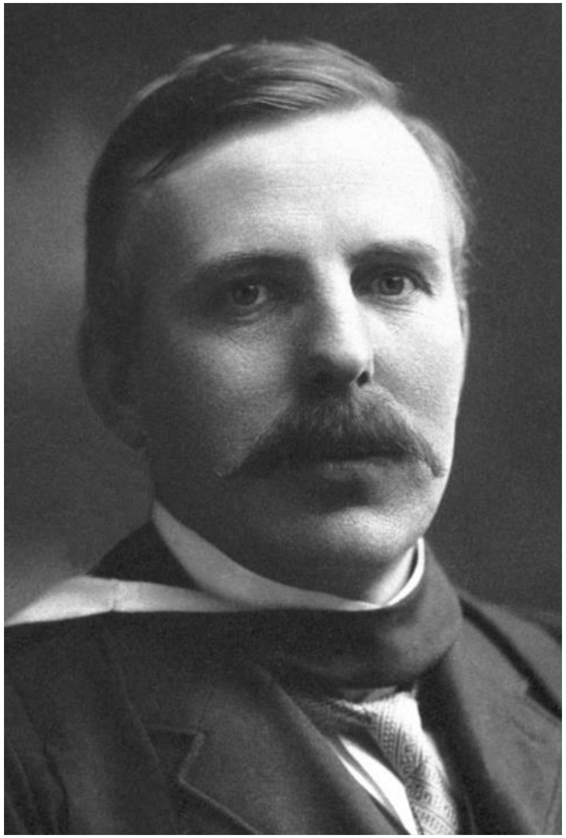
(The experiment costs **7** years)

1904 J.J. Thomson's model

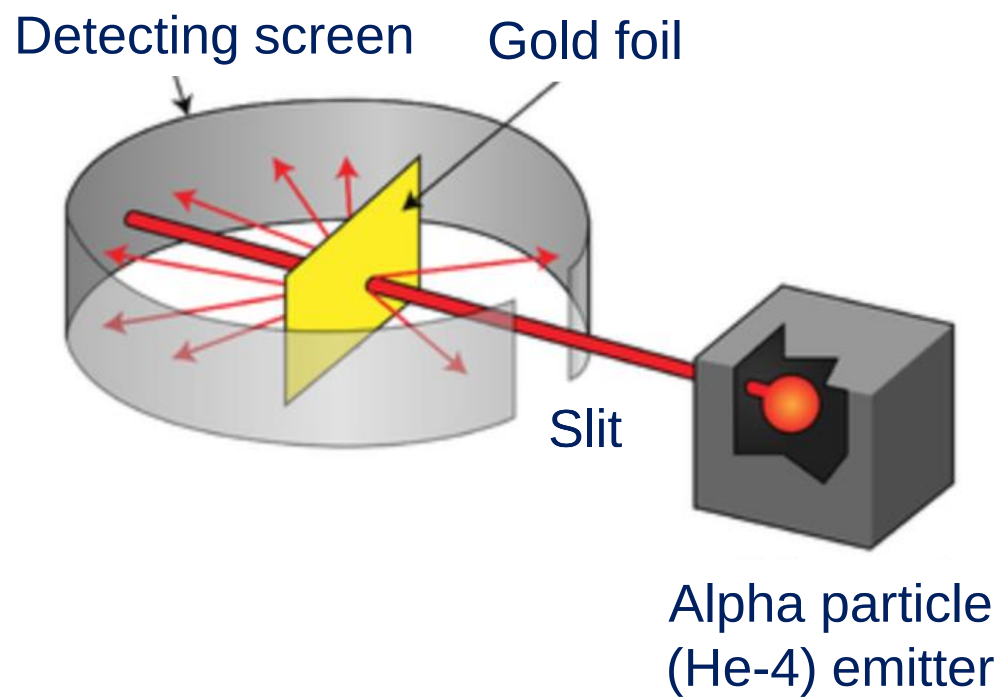


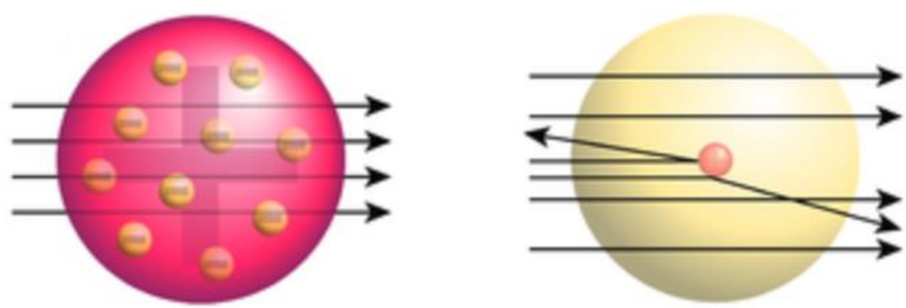
Plum pudding model

1911: Ernest Rutherford's experimental

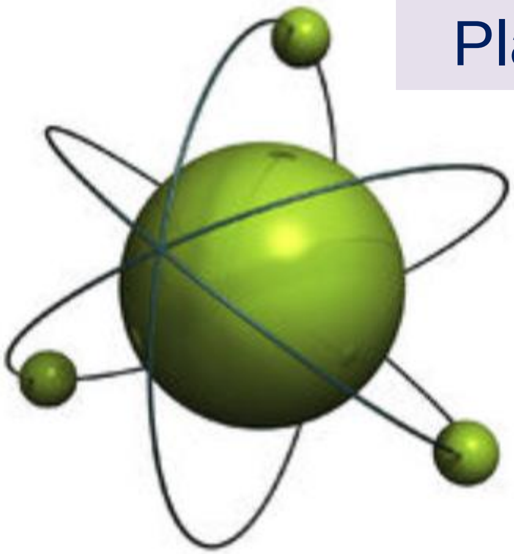


Ernest Rutherford
(British, 1871.08.30-1937.10.19)



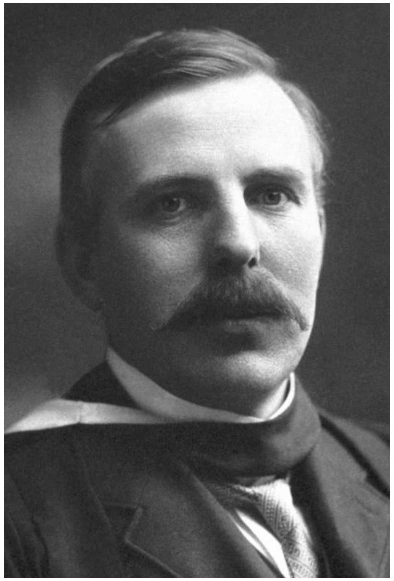


1911: Ernest Rutherford’s model



Planetary model

Nucleus is much heavier than electrons



Ernest Rutherford (1871.08.30-1937.10.19)

- Born in New Zealand in 1871.08.30
- He has 11 brothers and sisters
- 1890-1893 Bachelor degree, University of New Zealand
- 1894 Master degree, University of New Zealand
- 1895 Went to JJ Thomson's lab to purse PhD degree, Trinity College, University of Cambridge,
- 1898 Professor, McGill University

Research assistant Frederick Soddy and postdoc Otto Hahn proposed the radioactive half-life, and proved the transmutation from one element to another one.

Frederick and Otto obtained Nobel Chemistry Prize in 1921 and 1944, respectively.

- 1907 Langworthy Professor, University of Manchester

- 1908 Nobel Chemistry Prize for the study of transmutation of elements and radioactive substances

Student George de Hevesy from Hungary did the first radioactive tracer test放射性示踪剂 in 1910. He obtained the Nobel Chemistry Prize in 1943.

- 1911 Rutherford proposed the planetary model of atom

- 1913 Niels Bohr from Denmark joined Rutherford's group as a postdoc

Postdoc Bohr obtained the Nobel Physics Prize in 1922.

- 1919 Cavendish Professor, Physics Department, University of Cambridge

- 1920 Rutherford predicted that there were charge-neutral particle inside atom. Chadwick experimentally proved the existence of neutron experimentally in 1932. Chadwick obtained Nobel Physics Prize in 1935.

Assistant Charles Wilson invented the Cloud Chamber 云雾室 which could track the trajectory of particles and allowed discovery of new particles. He obtained the Nobel Physics Prize in 1927.

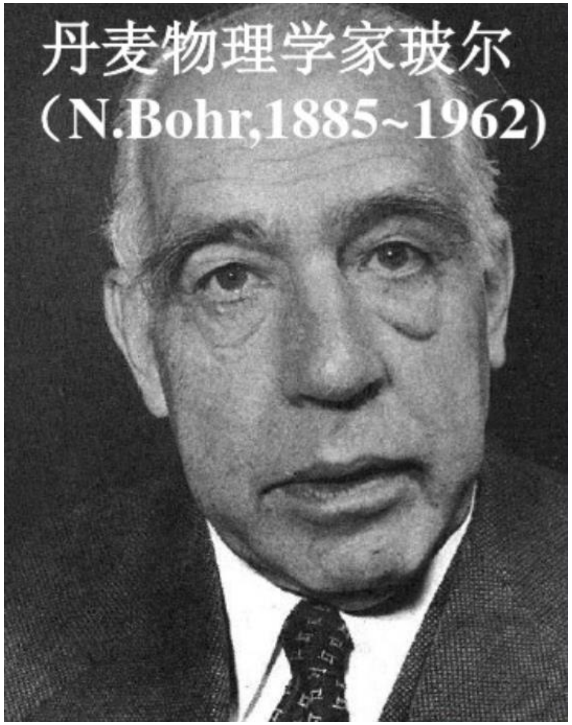
In 1924, Student Patrick Blackett improved the Cloud Chamber. He discovered that nucleus will absorb alpha-particle before the fission process. He obtained the Nobel Chemistry Prize in 1948.

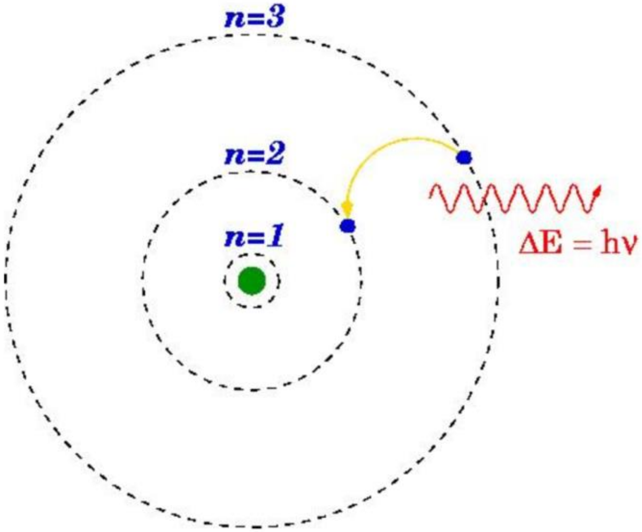
In 1932, Student John Cockcroft and Ernest Walton used the high energy accelerator to achieve the nucleus transformation. They shared the Nobel Chemistry Prize in 1951.

Student Pyotr Kapitsa discovered the superfluid behavior of liquid helium. He obtained the Nobel Physics Prize in 1978.

- 1977.08 International Union of Pure and Applied Chemistry (IUPAC) announced the No.104 element was called Rf (Rutherfordium) 钅卢 in memory of Rutherford

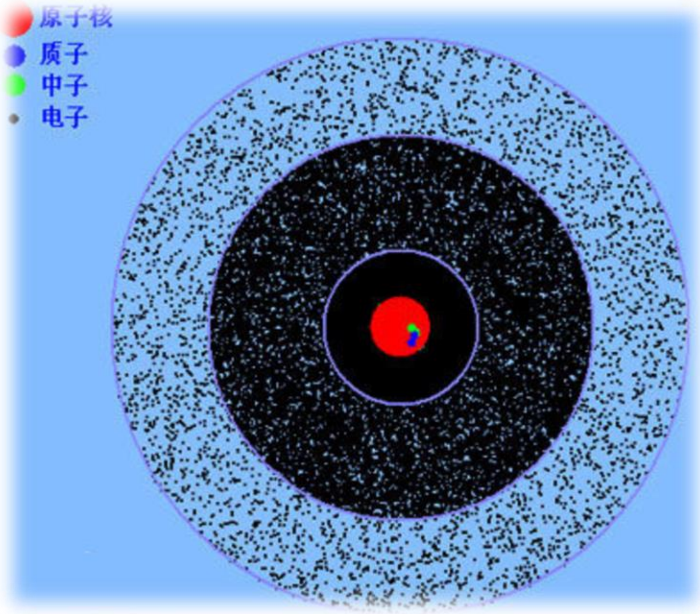
1913: Bohr’s model





Quantized model

1926: Schrodinger’s model

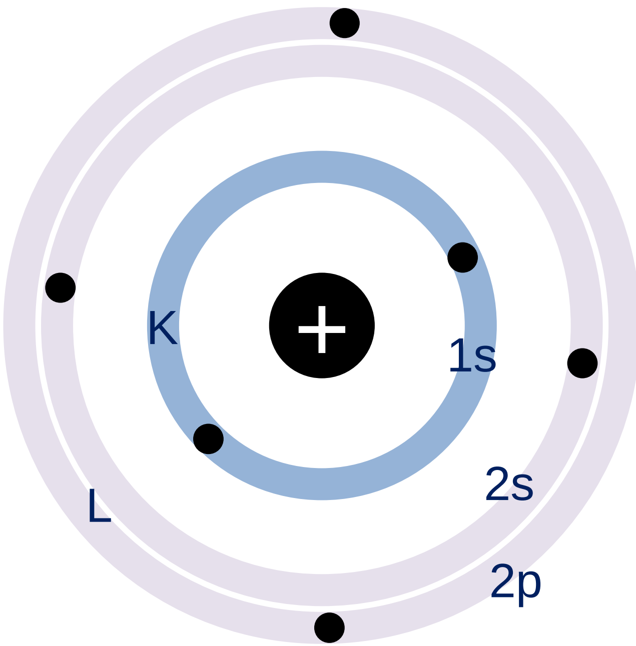


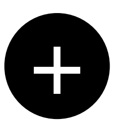
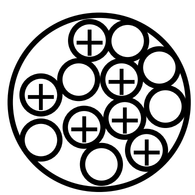
Electron cloud model

Electrons: Probability wave 几率波

Bohr’s model

Carbon atom



 : Nucleus原子核 

Nucleus: Proton (质子) and Neutron (中子)

The orbit of electrons

Principle quantum number 主量子数: n

n: 1, 2, 3, 4 …

The shell is named as K, L, M, N, …

Every shell has subshells: s, p, d, f…

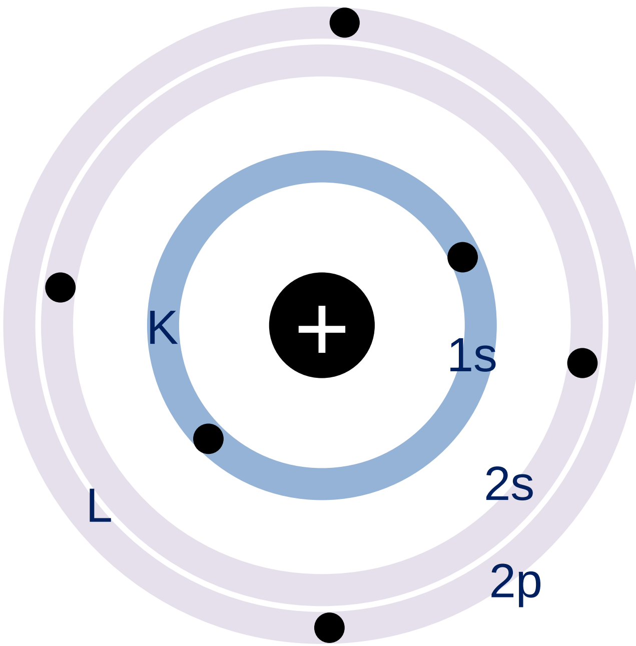
Orbital quantum number 轨道量子数: ℓ

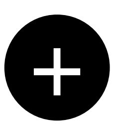
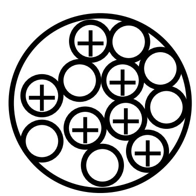
ℓ=0, 1, 2, … , n-1

The maximum electron numbers in shell and subshell

		Subshell			
		ℓ=0	1	2	3
n	Shell	s	p	d	f
1	K	2			
2	L	2	6		
3	M	2	6	10	
4	N	2	6	10	14

Carbon atom



 : Nucleus原子核 

The electronic construction of carbon atom
碳原子电子构型:

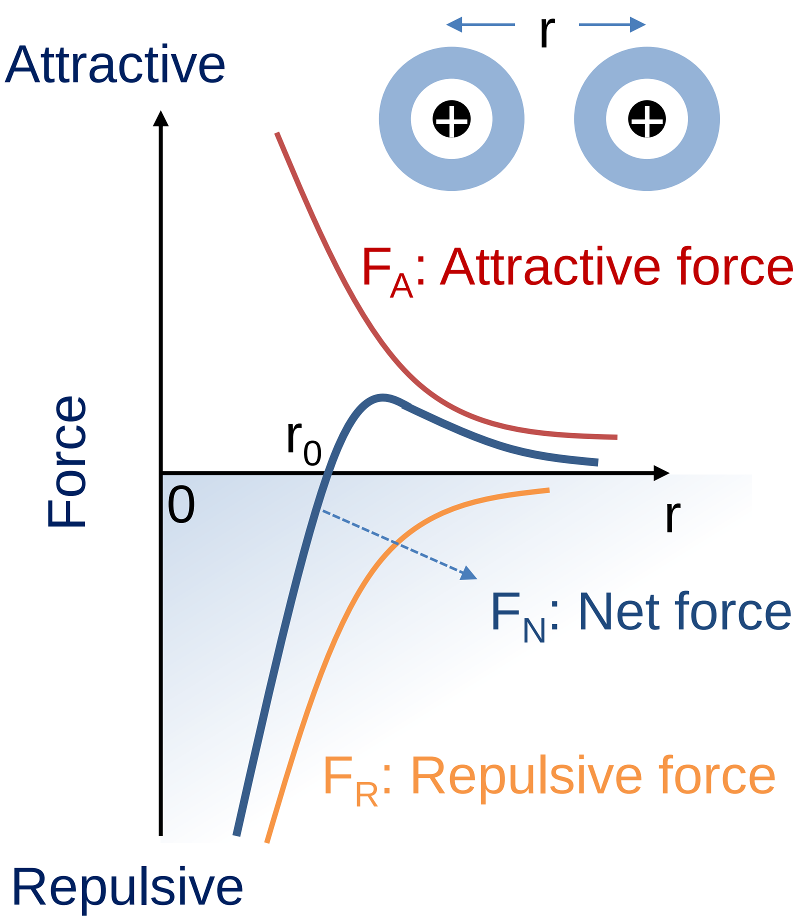
$1s^2 2s^2 2p^2$

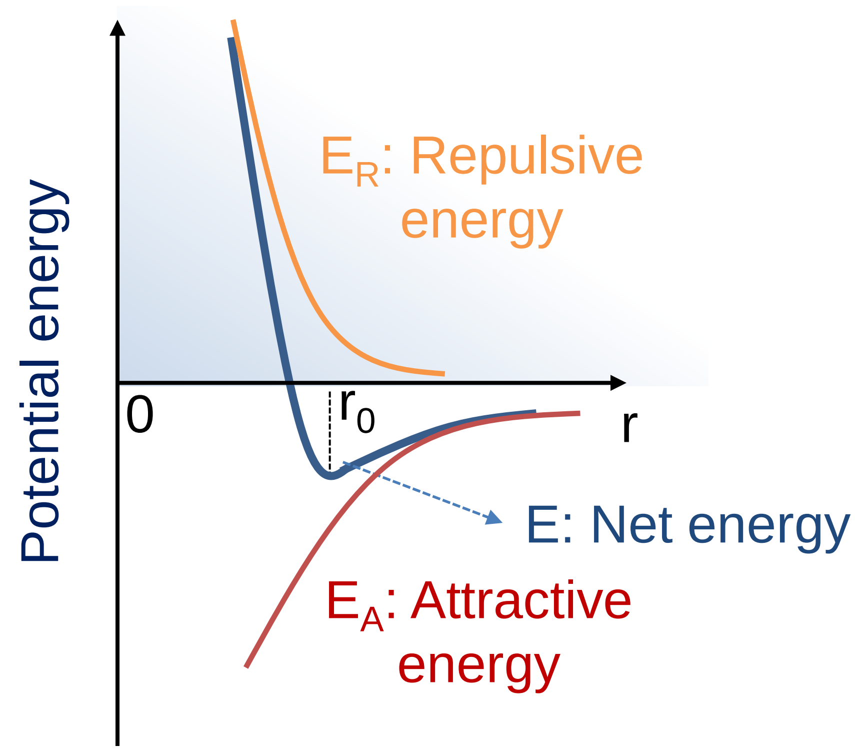
Electrons in the outermost shell:
the valence electron 价电子

For carbon atom:
4 valence electron in L shell

The most stable atom:
the outmost shell is fully filled

1.2 Atomic bond

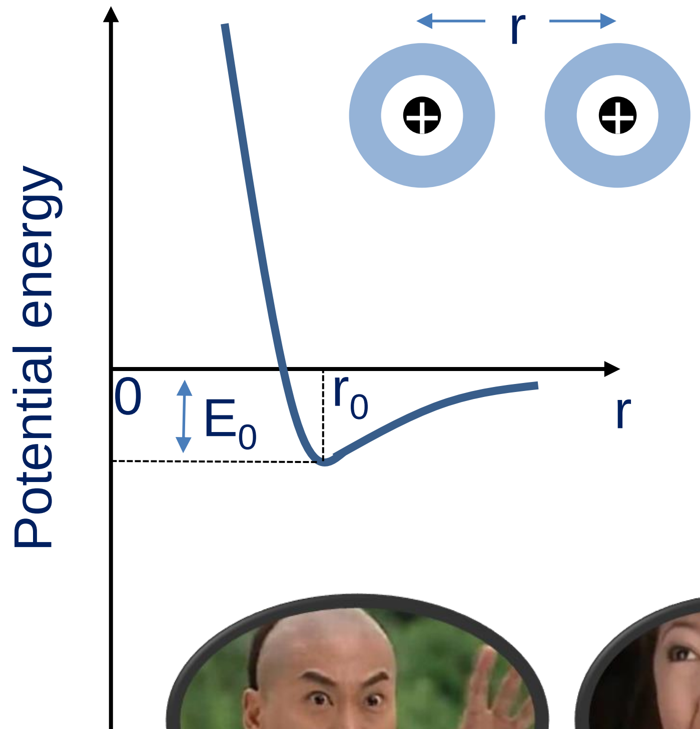




$F_N = F_A + F_R$

$$F_N = \frac{\mathrm{d}E}{\mathrm{d}r}$$

Bond/Binding energy 键能



Binding energy E_0:

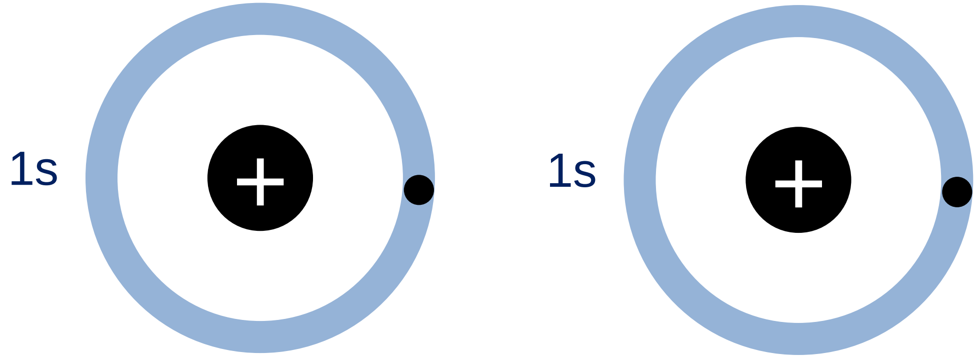
The energy required to separate two atoms

The types of atomic bond

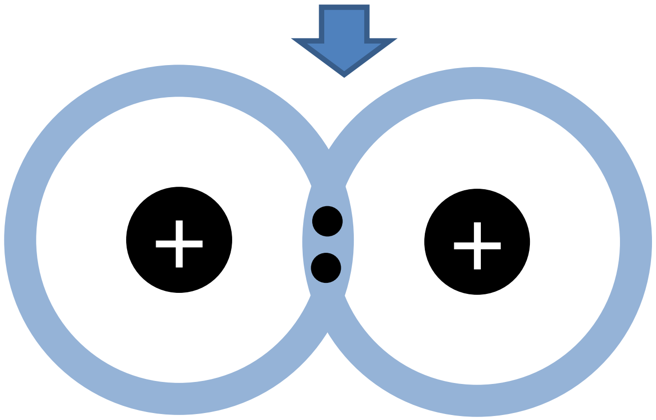
- Covalent bond
- Metallic bond
- Ionic bond
- Secondary bond: van der Waals bond
- Hybrid bond 混合键

Covalent bond

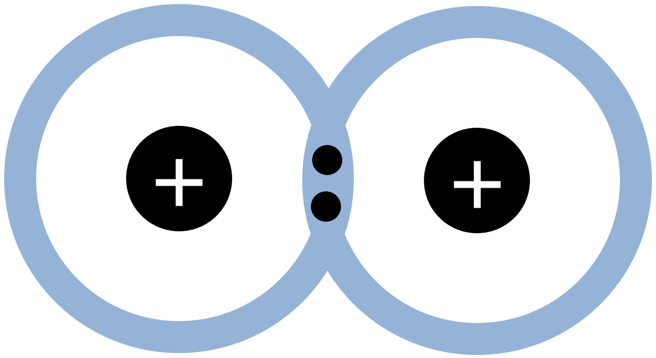
Hydrogen atom



Atoms share the valence electrons and make subshell fully filled

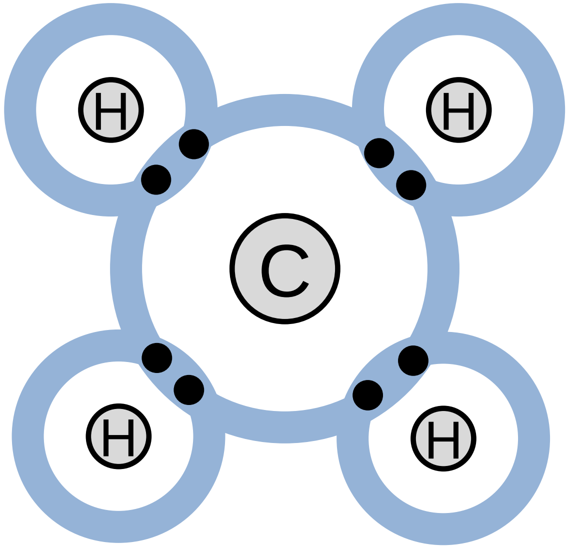


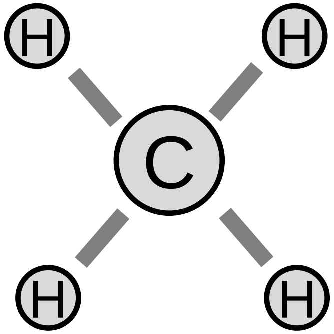
Covalent bond



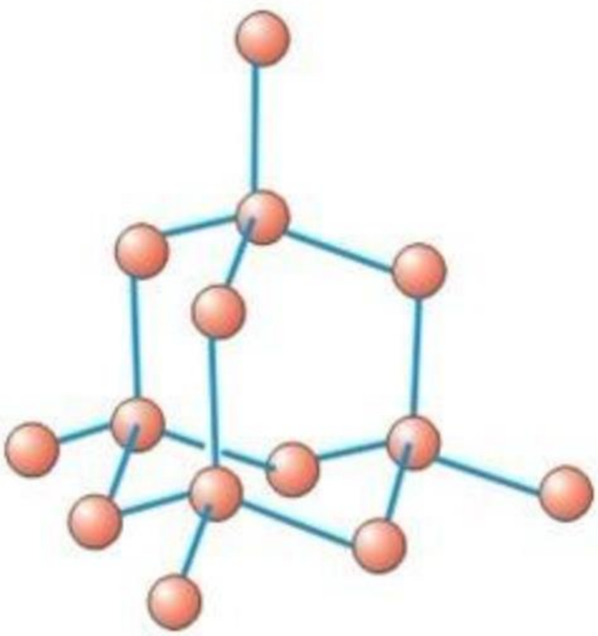
Q1: Which region has the highest electron cloud density?

Distribution of valence electrons in **methane CH_4**





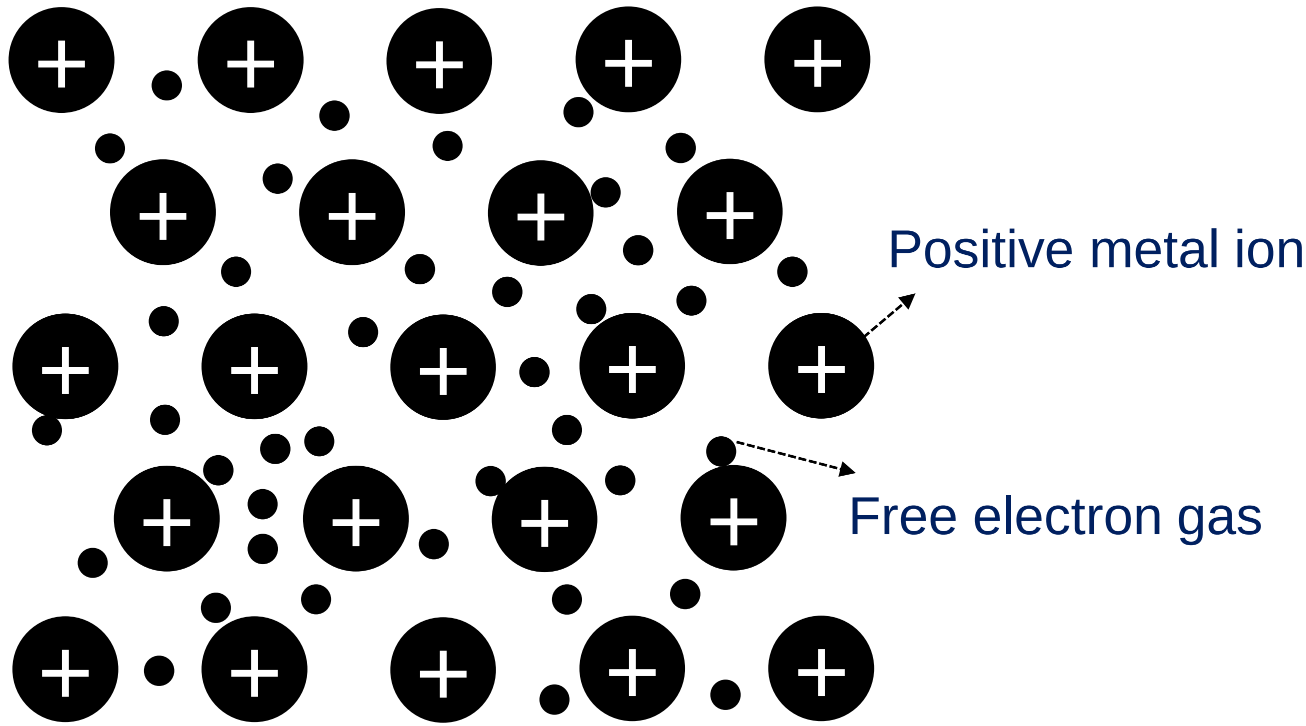
Crystalline structure of silicon and diamond



Q: Draw the distribution of valence electrons.

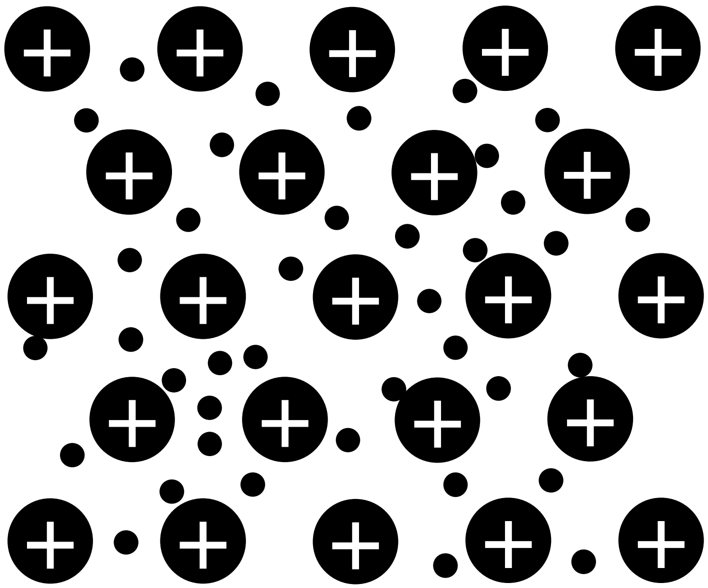
Metallic bond

Metal atom only has few valence electrons, electrons can easily move around



In metals, the metal ions tends to be as close to each other as possible, and form the **close-packed structure 密堆积结构**

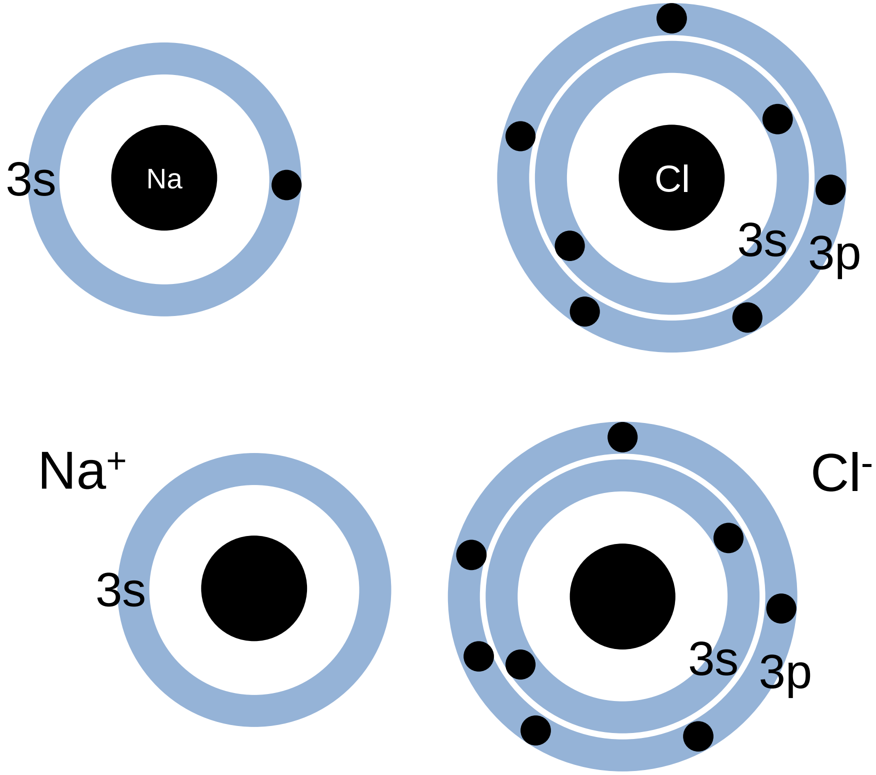
Metal

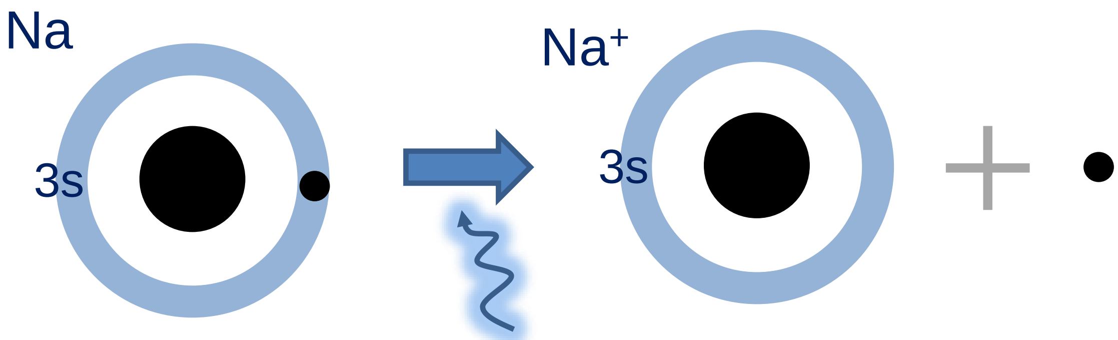


- High electronic conductivity
- High thermal conductivity

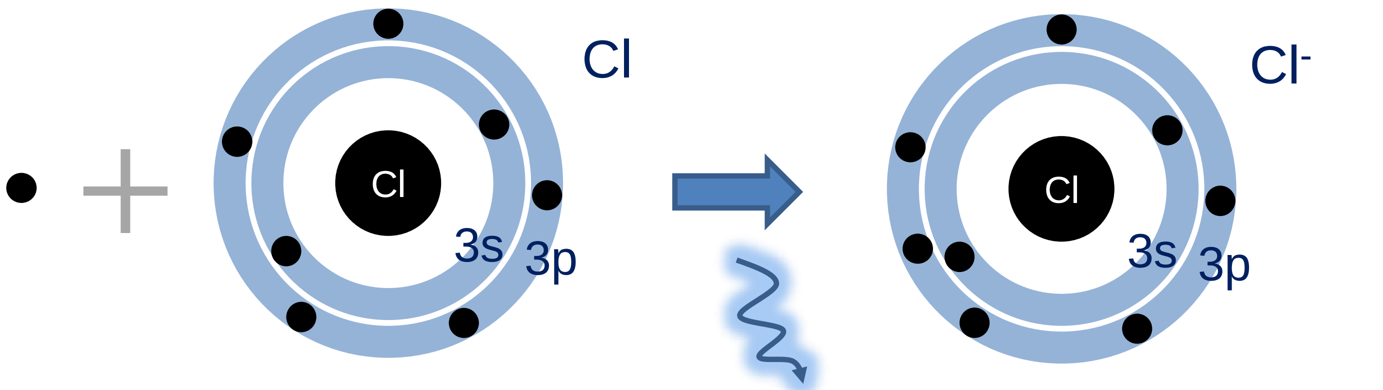
Ionic bond

NaCl is a typical ionic crystal



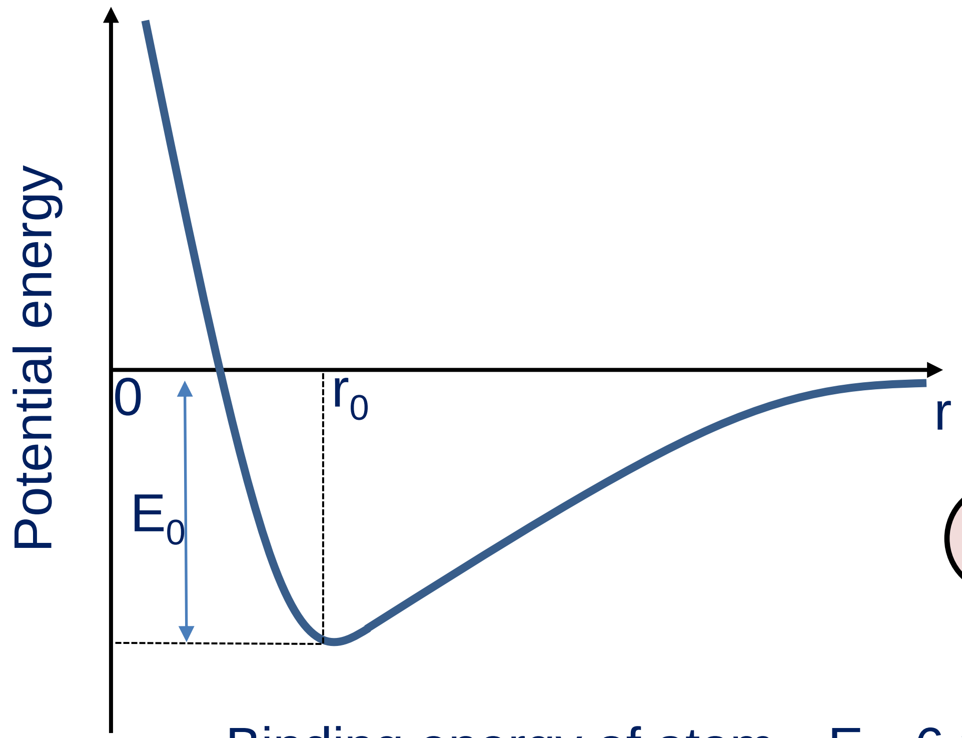


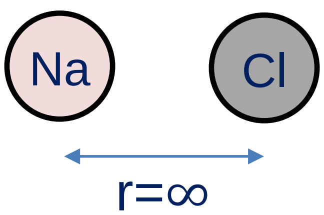
Provide energy: **ionization energy 电离能** 5.1 eV



Release energy: **electron affinity energy 电子亲和能** 3.6 eV

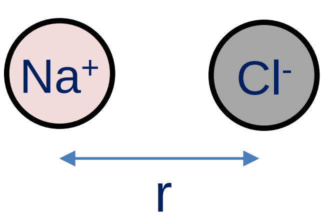
Potential energy of atom pair





Binding energy of atom： E_0=6.3 eV

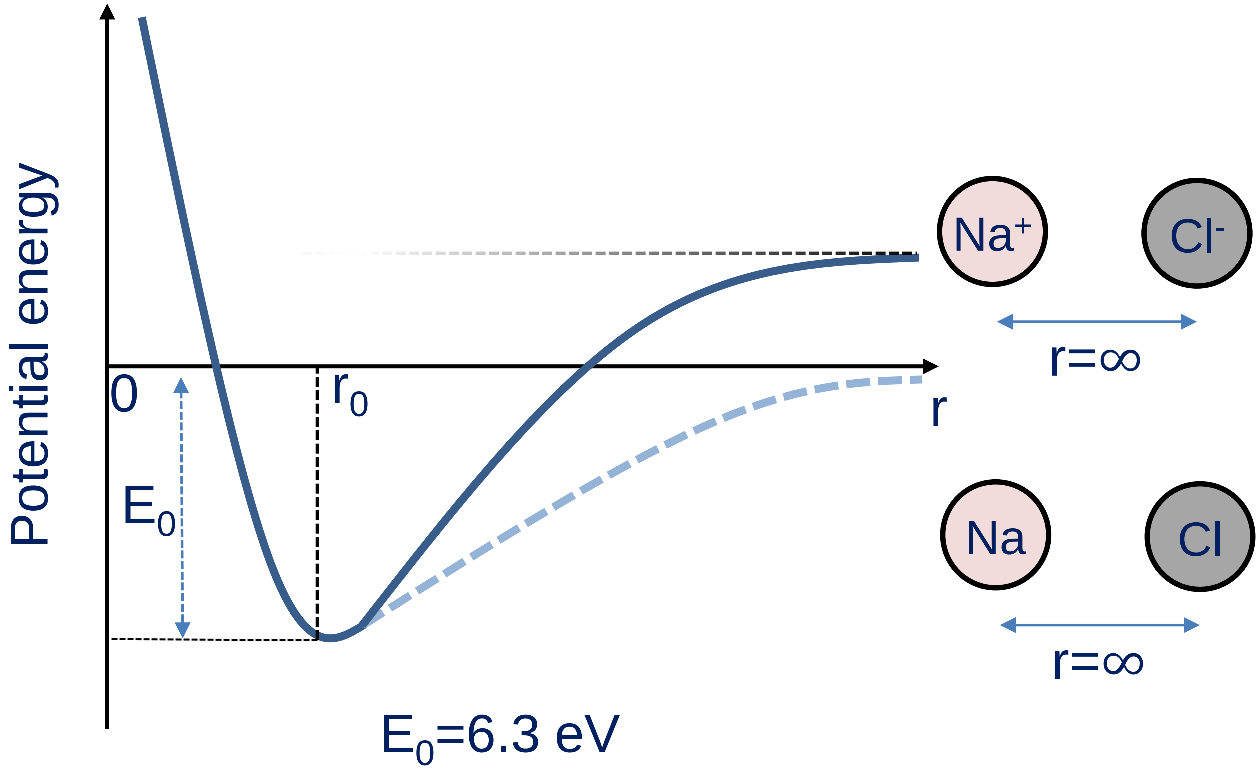
Potential energy of ion pair?



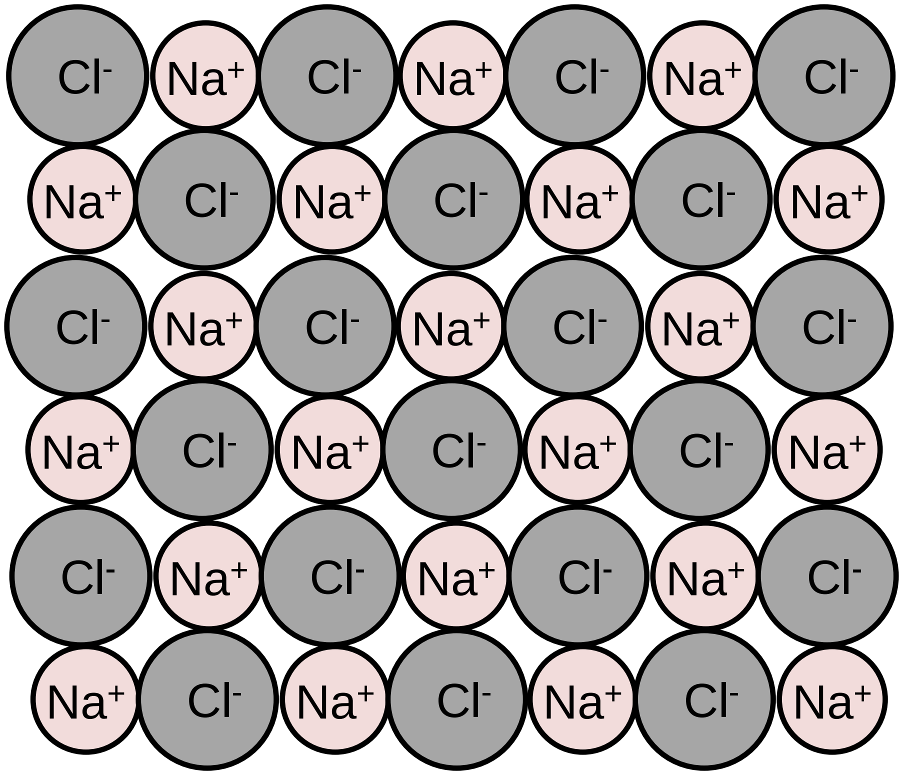
Potential energy of ion pair?

Ionization energy of Na: 5.1 eV

Electron affinity energy of Cl: 3.6 eV



Binding energy of ion 离子结合能：6.3 + 5.1 - 3.6=7.8 eV

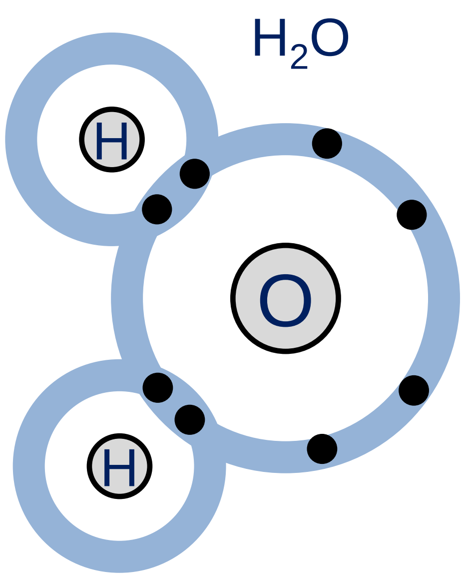


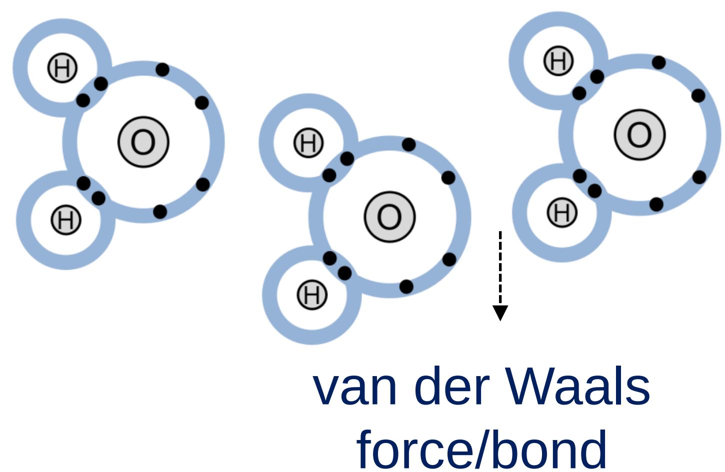
Cl- Na+ Cl- Na+ Cl- Na+ Cl-
Na+ Cl- Na+ Cl- Na+ Cl- Na+
Cl- Na+ Cl- Na+ Cl- Na+ Cl-
Na+ Cl- Na+ Cl- Na+ Cl- Na+
Cl- Na+ Cl- Na+ Cl- Na+ Cl-
Na+ Cl- Na+ Cl- Na+ Cl- Na+

Van der Waals bond 范德华键

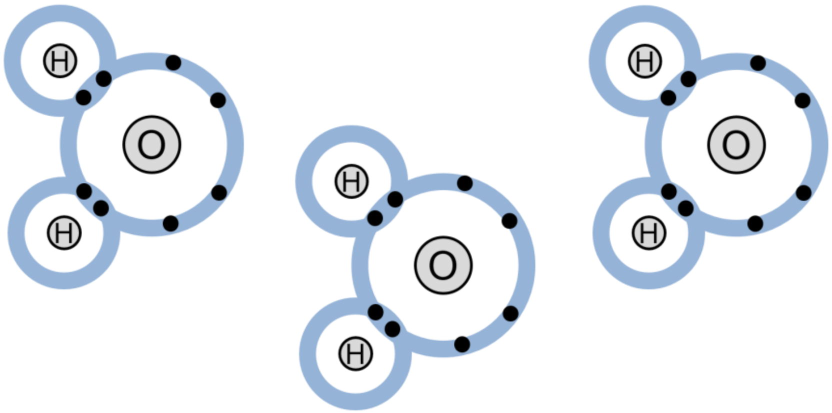
Molecular crystals 分子晶体: ice, dry ice (CO_2), solid state of other gas

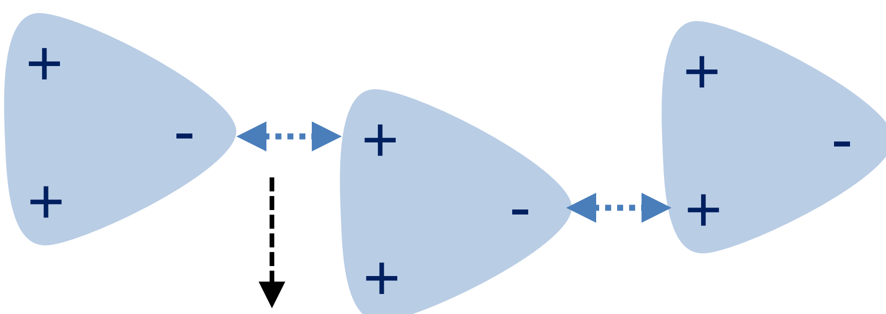
Gas will become solid when temperature is low enough. The force between gas molecular is van der Waals force.





The H_2O molecule is polar and has a net permanent dipole moment





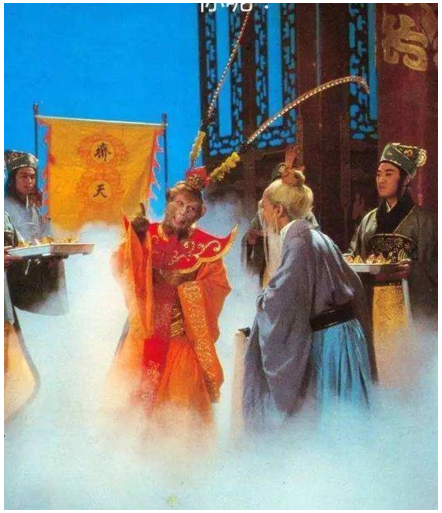
van der Waals
force/bond

Dry ice (solid CO_2)

Density: 1.560 g/cm^3 (-78℃)

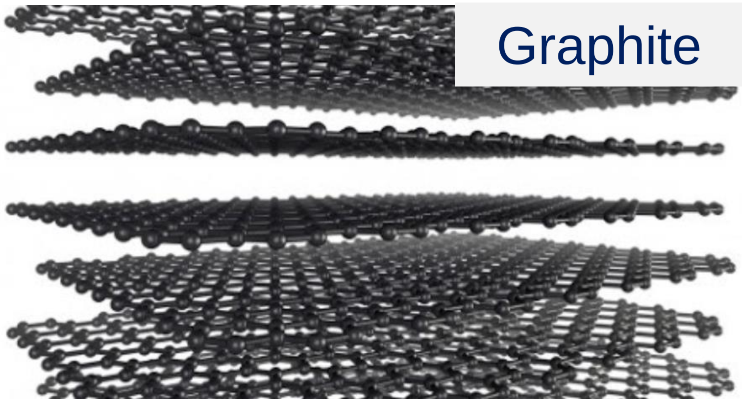
Melting point: -57℃

Ice point: -78.5℃

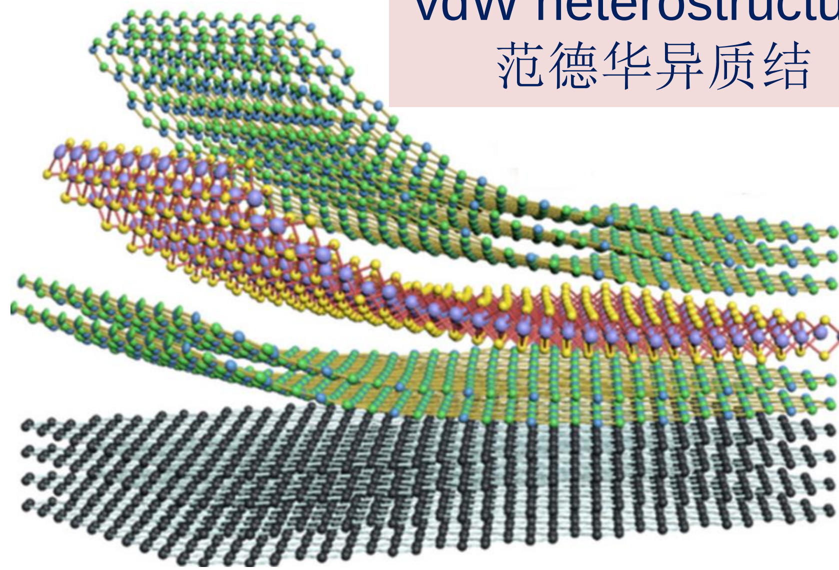


van der Waals layered material

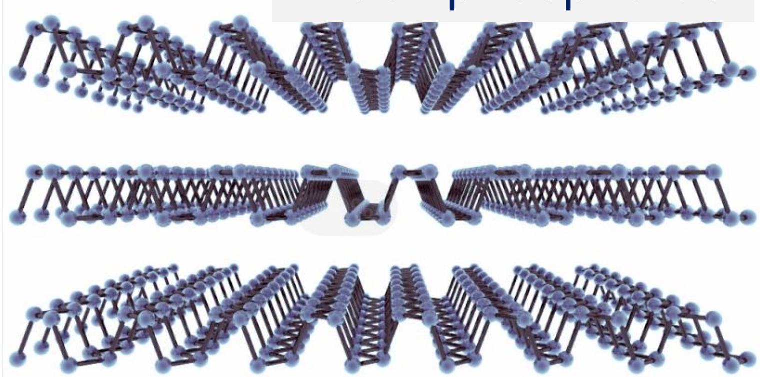
Graphite

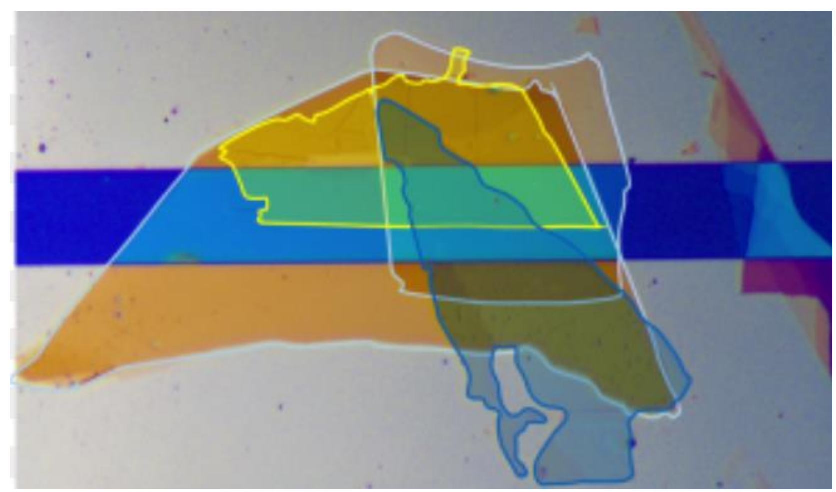


vdW heterostructure
范德华异质结



Black phosphorus





van der Waals bond is very weak compared with covalent, metallic and ionic bond

Bond	Material	Binding energy (eV/atom)
Ionic	NaCl	3.2
Metallic	Mg	3.1
Covalent	Si	4
vdWs	Ice	0.52

- Primary bond 强键: ionic, metallic, and covalent bond
- Secondary bond 弱键: vdWs bond

The potential energy of vdWs bond

Lennard – Jones 6-12 formula:

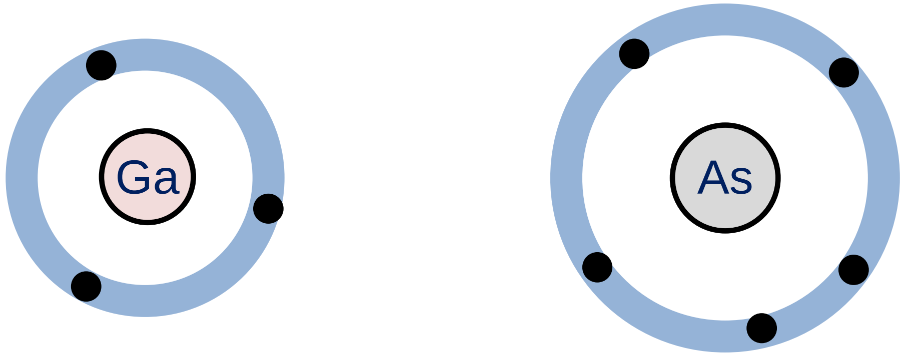
$$E(r) = -Ar^{-6} + Br^{-12}$$

Q: The average distance between atoms/molecules?

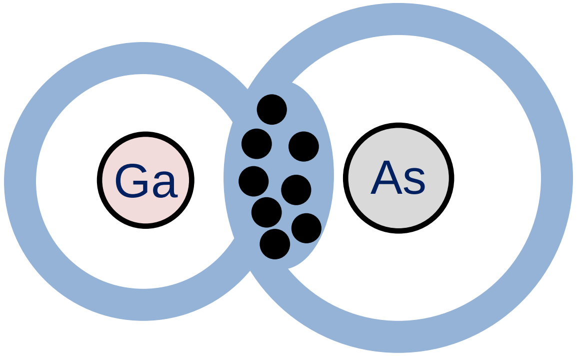
$$\frac{\mathrm{d}E}{\mathrm{d}r} = 0$$

Hybrid bond

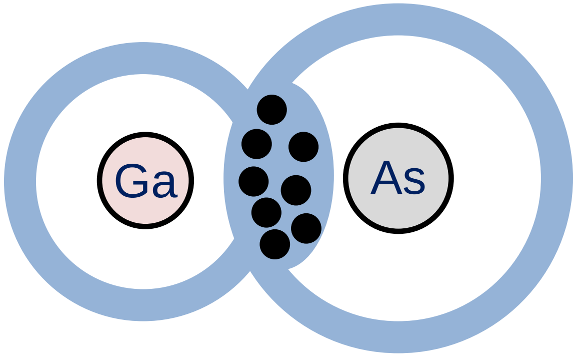
III-V compound: GaAs



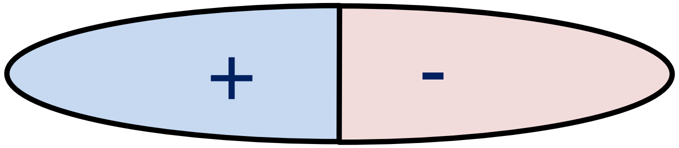
The electron cloud density is higher near As^{5+} nucleus



The bond has properties of both covalent bond and ionic bond



The bond is also called polar bond 极性键

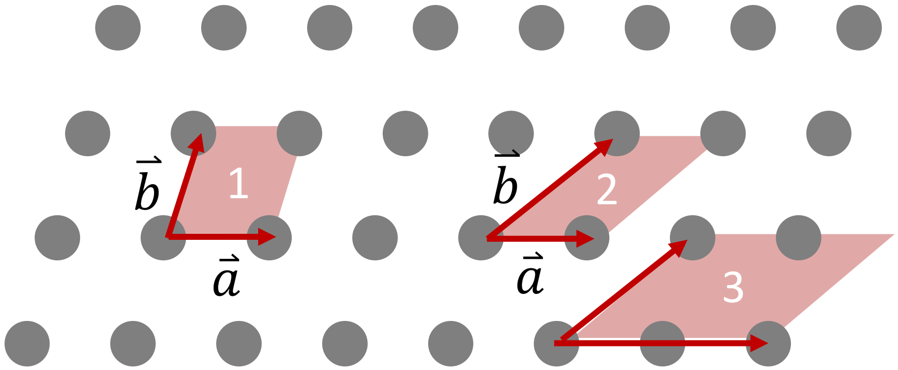


The bond has properties of both covalent bond and ionic bond

1.3 Crystal structure

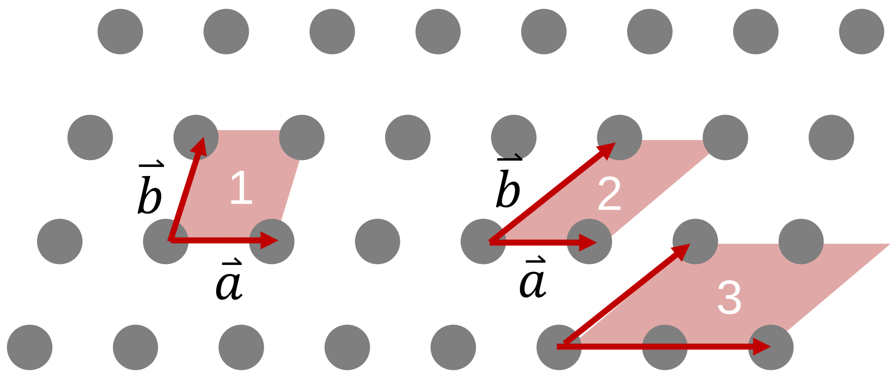
Crystal 晶体: periodic array of atoms

Lattice 晶格 is an infinite periodic array of geometric points in space



The position of atoms: $\vec{r} = n\vec{a} + m\vec{b}$

$\vec{a}, \vec{b}$ are called the **basis**



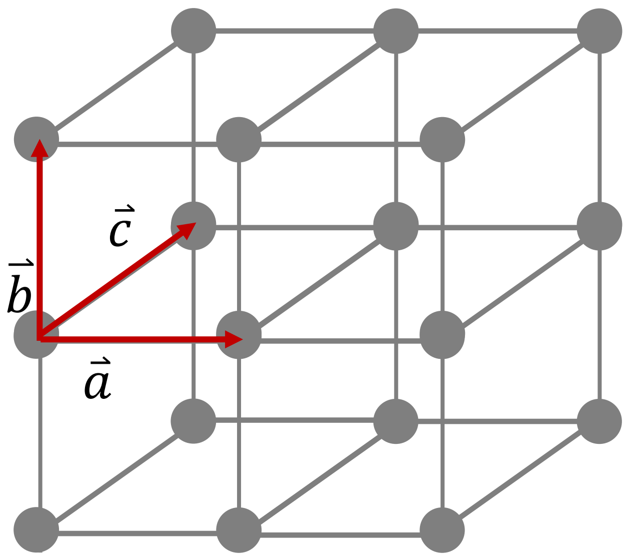
$\vec{a}, \vec{b}$ are called the **basis**

The **unit cell 晶胞** is the most convenient small cell in the crystal structure that carriers the properties of the crystal.

The smallest repeating cell called the **primitive cell 原胞**

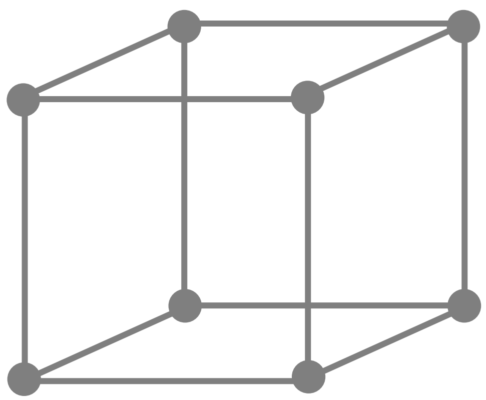
Area 1,2 and 3 are primitive cell?

Basis and primitive cell of cubic lattice

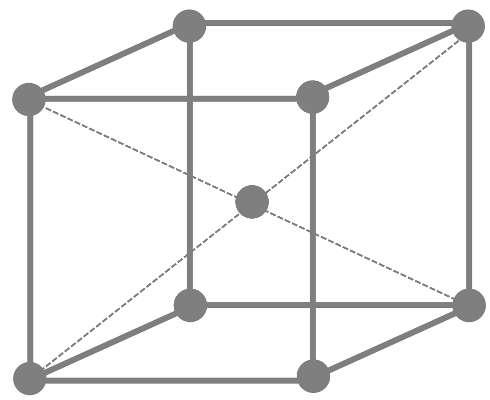


Cubic lattice立方格子: sc, bcc, fcc,

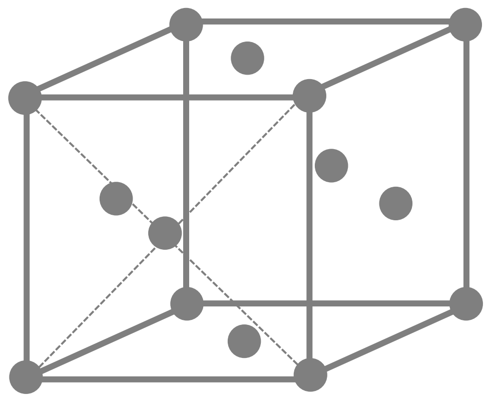
sc: simple cube



bcc: body-centered cube



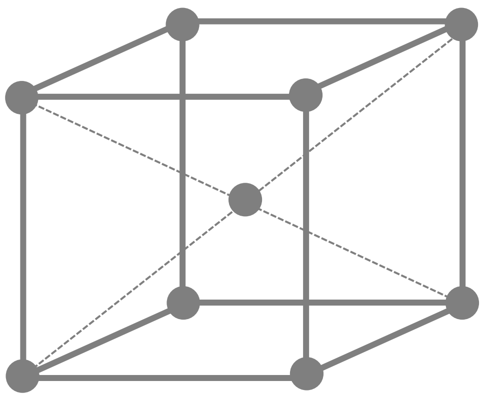
fcc: face-centered cube



Unit cell or primitive cell?

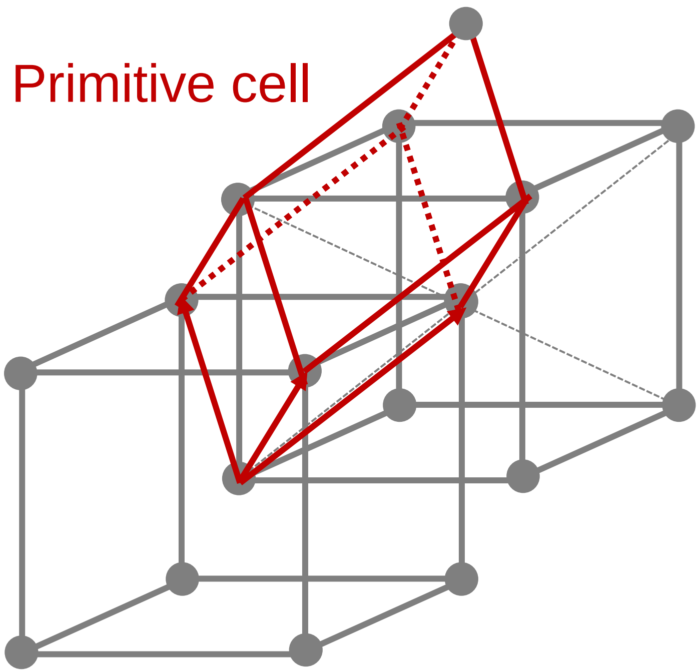
bcc: body-centered cube

Unit cell



2 atoms in unit cell

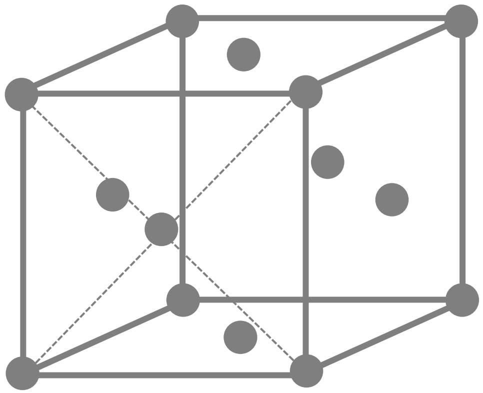
Primitive cell



1 atoms in primitive cell

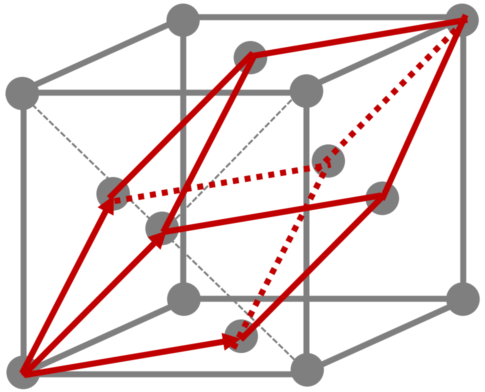
fcc: face-centered cube

Unit cell



4 atoms in unit cell

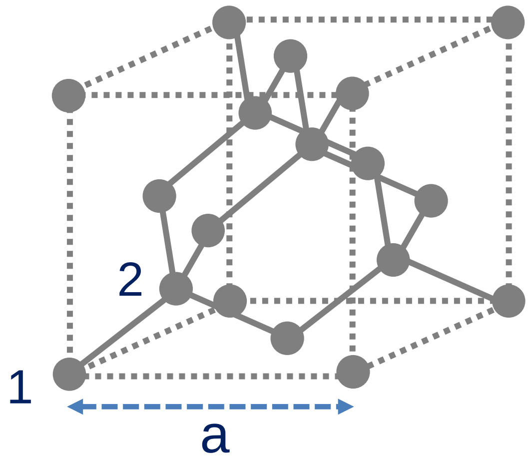
Primitive cell



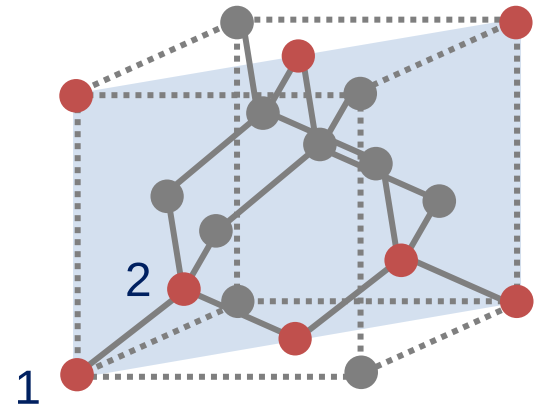
1 atoms in primitive cell

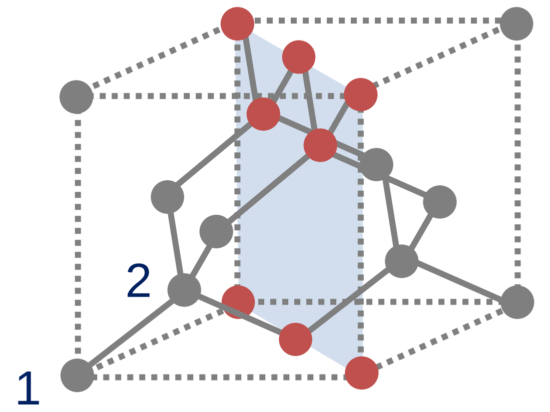
Crystal structure of silicon/germanium/diamond

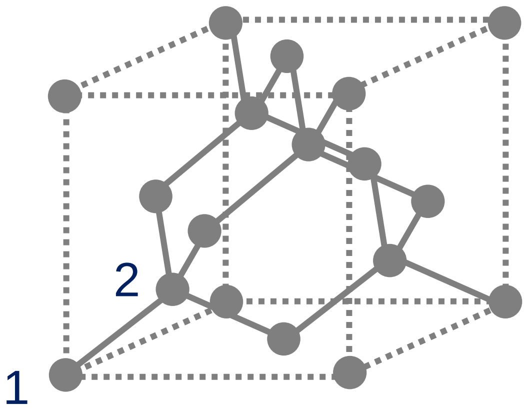
Unit cell



Atom 2 is shifted by (a/4, a/4, a/4) respect to atom 1





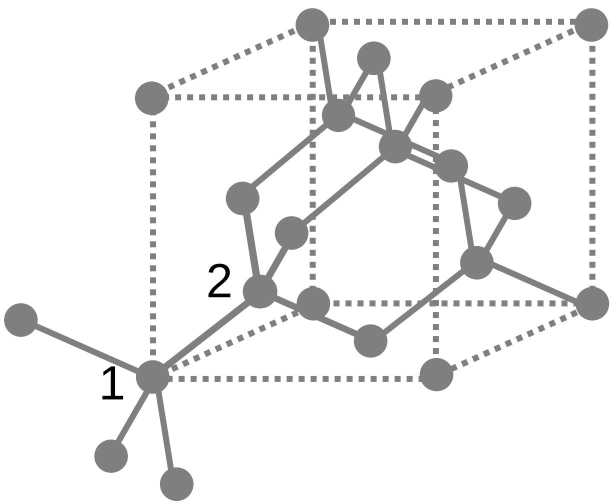


Q1: How many atoms in unit cell ?

Q2: Are atom 1 and atom 2 identical?

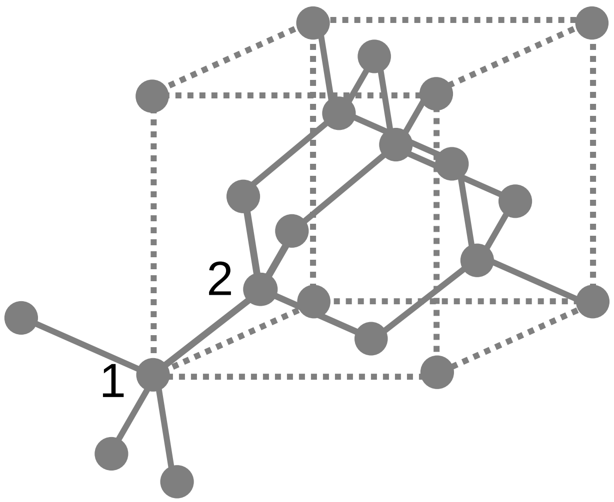
Q3: Which lattice type?

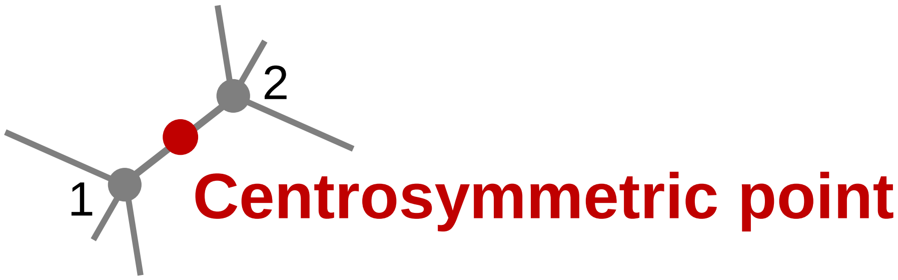
Q2: Are atom 1 and atom 2 identical?



在一个克隆的世界，怎么判断原子是等价还是不等价的呢?

看走位！！

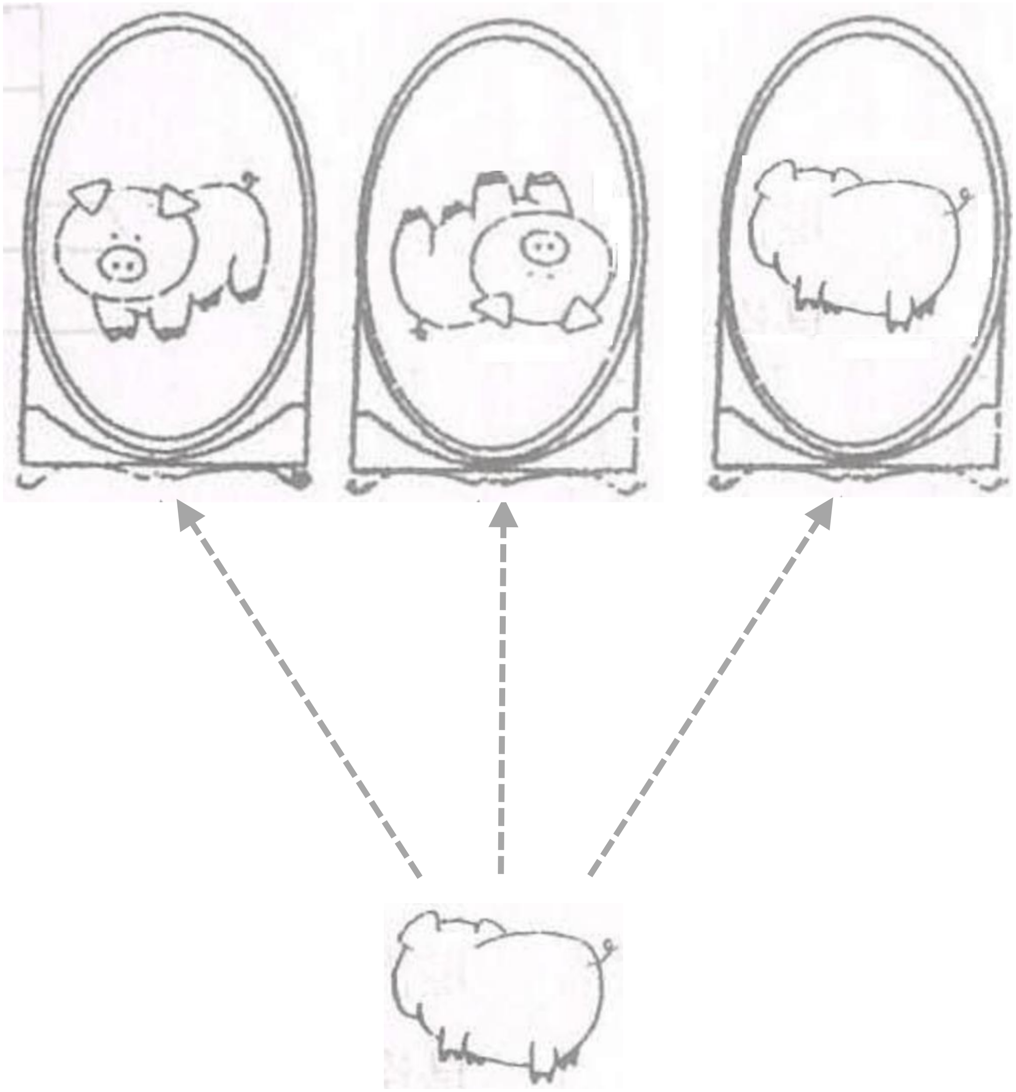




Atom 1 and 2 are **not identical**!

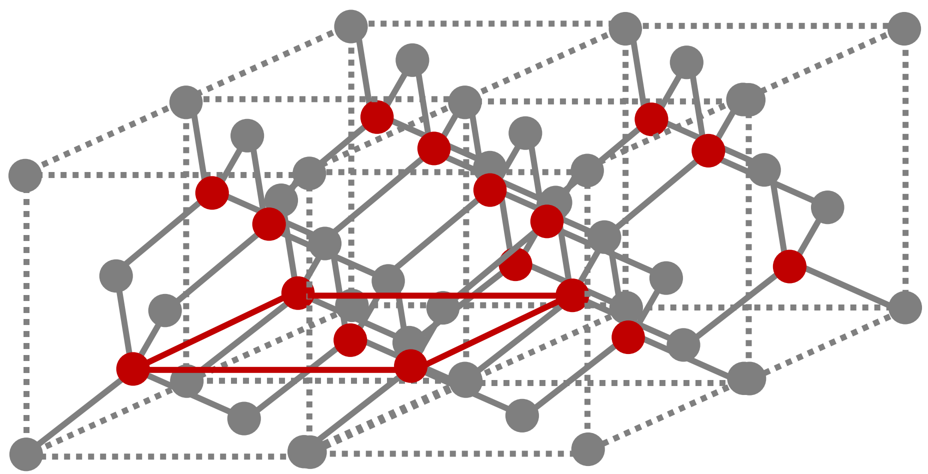
There are two arrays of atoms in unit cell.

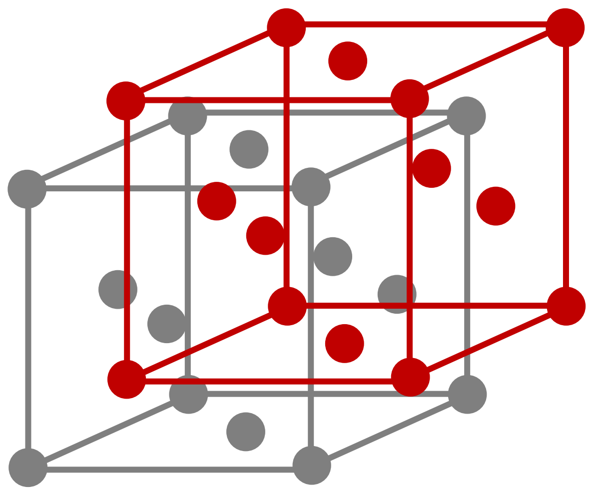
Mirror-symmetry **Centro-symmetry** **Identical**



Crystal structure of silicon/germanium/diamond

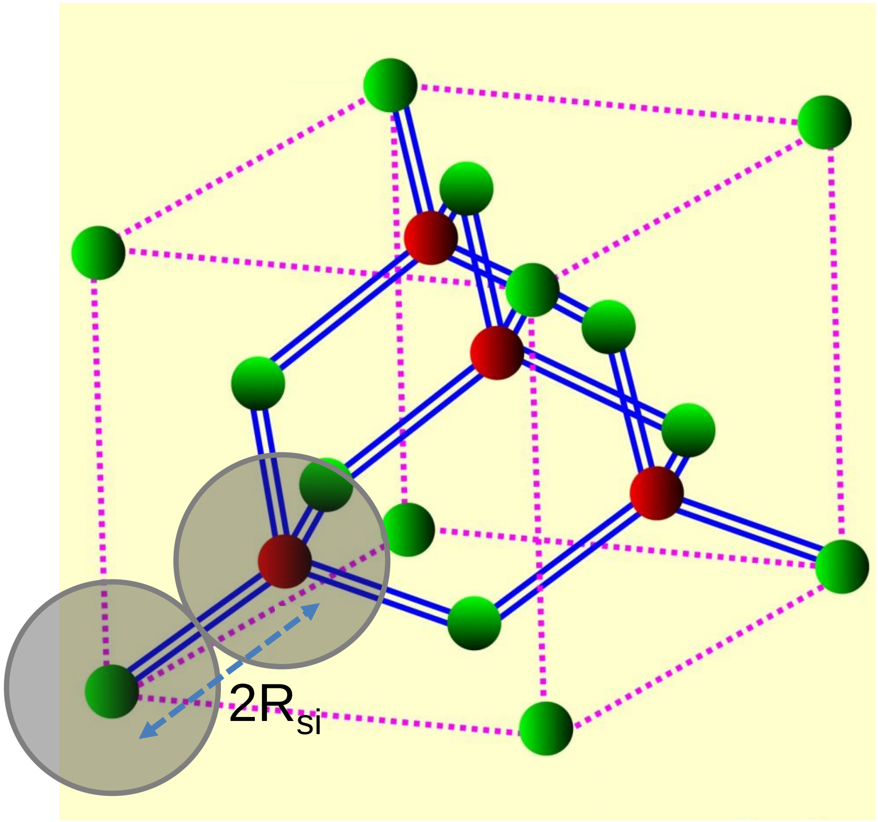
Q3: Which lattice type?





Constructed by 2 fcc lattice

Q: Which two atoms are closest? **Q: The radius of Si atom R_{si}?**

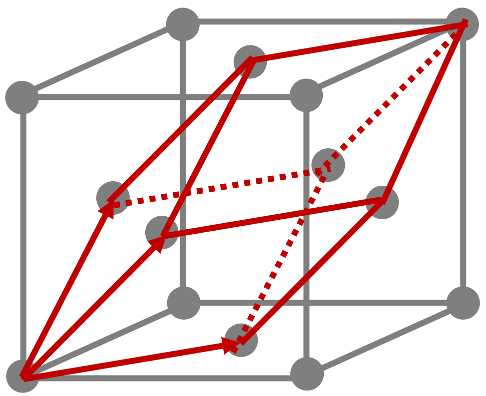


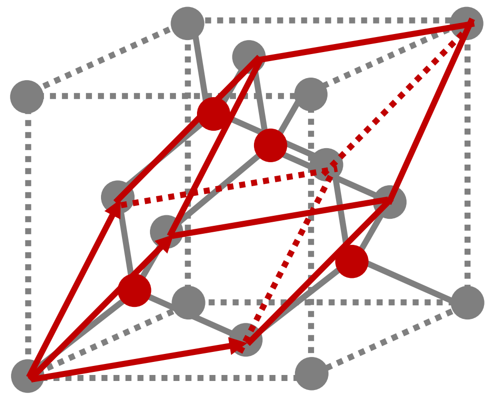
- Radius of atom can be calculated as the half of the distance of two nearest atoms in the lattice.

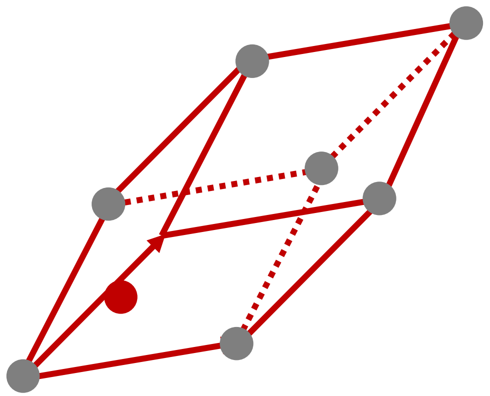
Q4: Primitive cell?

Primitive cell of fcc

Primitive cell of Si







◆ Find three identical nearest atoms and draw three vectors

Q5: How many atoms in primitive cell?

2 atoms in primitive cell

If primitive cell contain 1 atom:

- Every atom in lattice are identical.

If primitive cell contain 2 atoms:

- There are two array of atoms which are not identical.

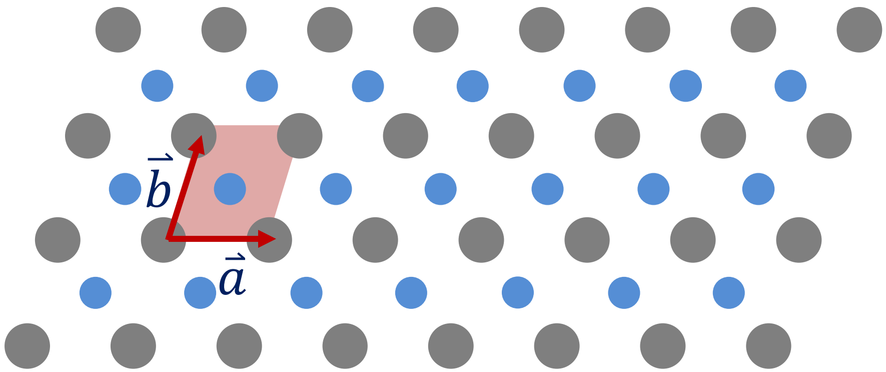
If primitive cell contain N atoms:

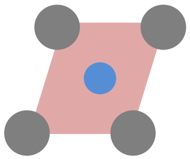
- There are N array of atoms which are not identical.

We call it the compound lattice 复式晶格

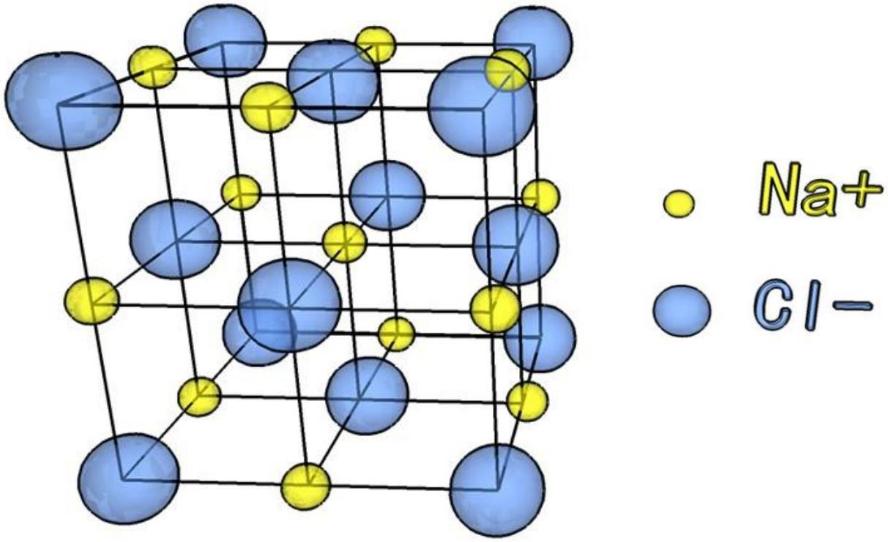
Compound lattice 复式晶格

Contains multiple arrays of periodic atoms which are not identical.



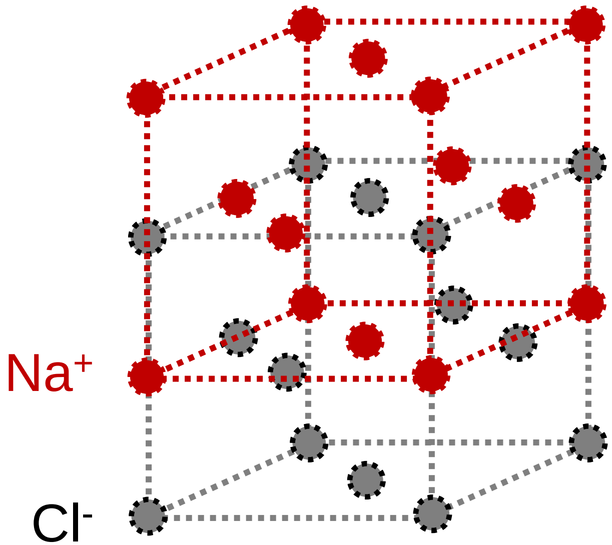
Primitive/unit cell 

The crystal structure of NaCl



Q: Which lattice type?

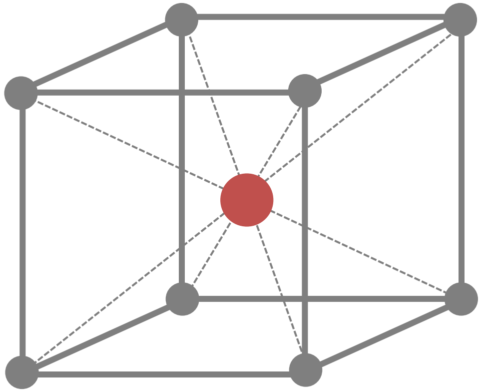
The crystal structure of NaCl



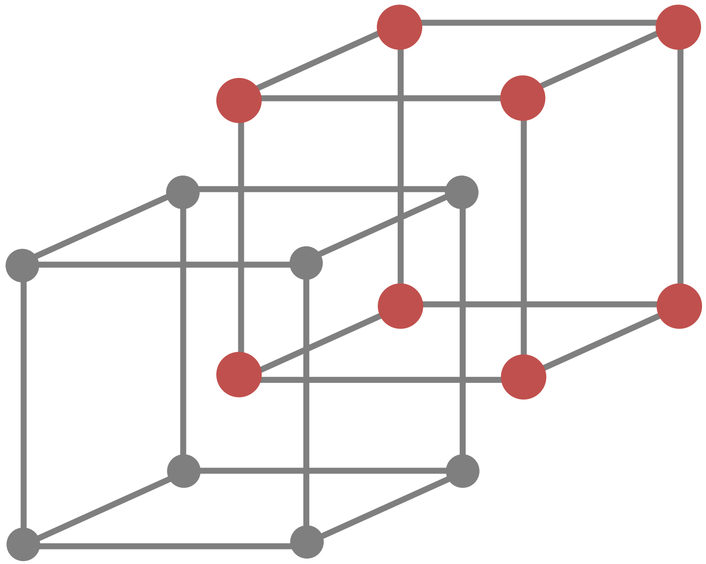
Two interpenetrating fcc unit cell!

The crystal structure of CsCl

Unit cell



Q: Which lattice type?



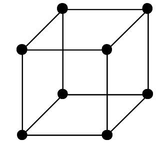
Two interpenetrating sc unit cell!

立方晶系

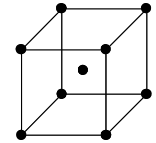
CUBIC SYSTEM

$a = b = c \quad \alpha = \beta = \gamma = 90°$

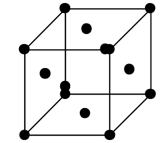
Many metals, Al, Cu, Fe, Pb. Many ceramics and semiconductors, NaCl, CsCl, LiF, Si, GaAs



Simple cubic



Body centered cubic



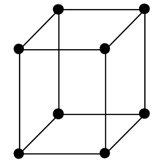
Face centered cubic

四方晶系

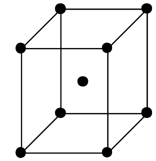
TETRAGONAL SYSTEM

$a = b \neq c \quad \alpha = \beta = \gamma = 90°$

In, Sn, Barium Titanate, TiO_2



Simple tetragonal
简单四方



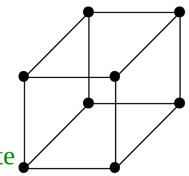
Body centered tetragonal
体心四方

正交晶系

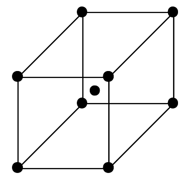
ORTHORHOMBIC SYSTEM

$a \neq b \neq c \quad \alpha = \beta = \gamma = 90°$

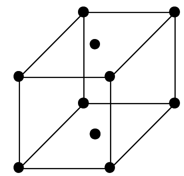
S, U, Pl, Ga (<30°C), Iodine, Cementite (Fe_3C), Sodium Sulfate



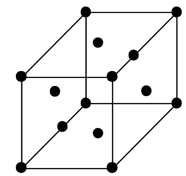
Simple orthorhombic
简单正交



Body centered orthorhombic
体心正交



Base centered orthorhombic
底心正交



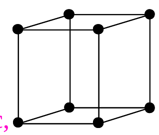
Face centered orthorhombic
面心正交

六方晶系

HEXAGONAL SYSTEM

$a = b \neq c \quad \alpha = \beta = 90°\ ;\ \gamma = 120°$

Cadmium, Magnesium, Zinc, Graphite



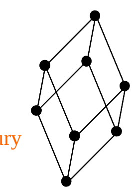
Hexagonal
六方

三方晶系

RHOMBOHEDRAL SYSTEM

$a = b = c \quad \alpha = \beta = \gamma \neq 90°$

Arsenic, Boron, Bismuth, Antimony, Mercury (<-39°C)



菱形

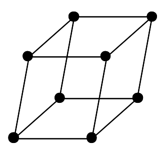
Rhombohedral

单斜晶系

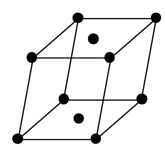
MONOCLINIC SYSTEM

$a \neq b \neq c \quad \alpha = \beta = 90°\ ;\ \gamma \neq 90°$

α–Selenium, Phosphorus
Lithium Sulfate
Tin Fluoride



Simple monoclinic
简单单斜



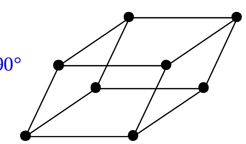
Base centered monoclinic
底心单斜

三斜晶系

TRICLINIC SYSTEM

$a \neq b \neq c \quad \alpha \neq \beta \neq \gamma \neq 90°$

Potassium dicromate



Triclinic
三斜

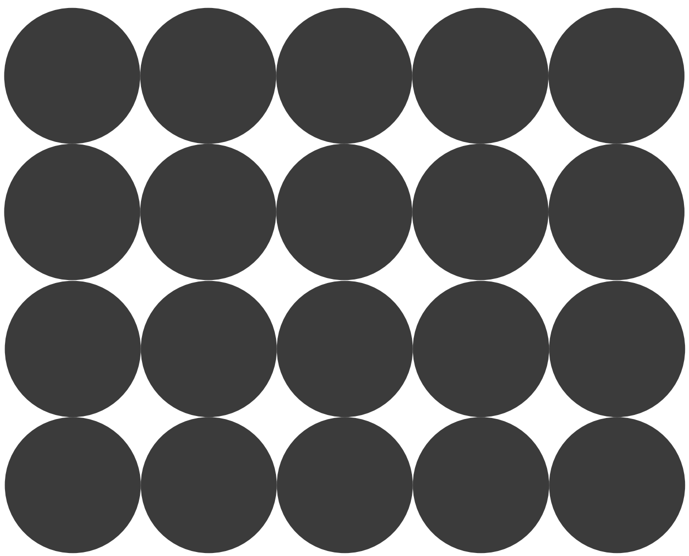
The seven crystal systems (unit cell geometries) and fourteen Bravais lattices.

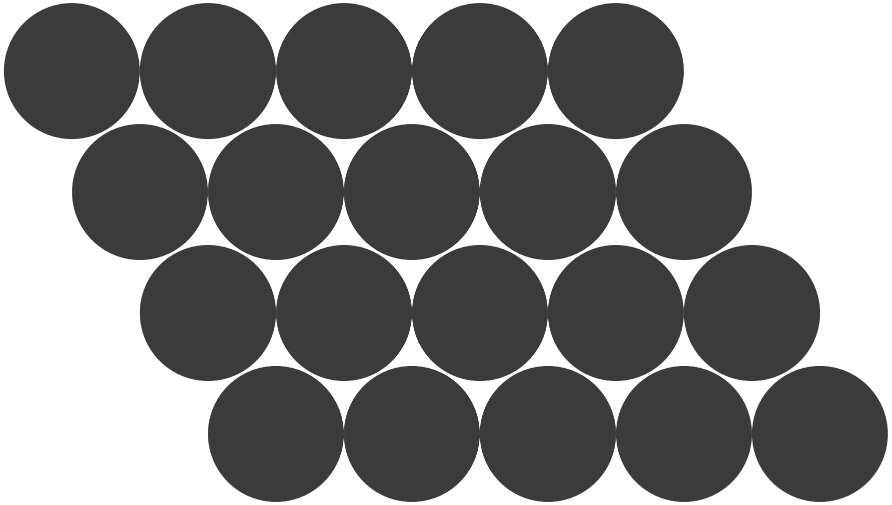
Close-packed structure密堆积结构

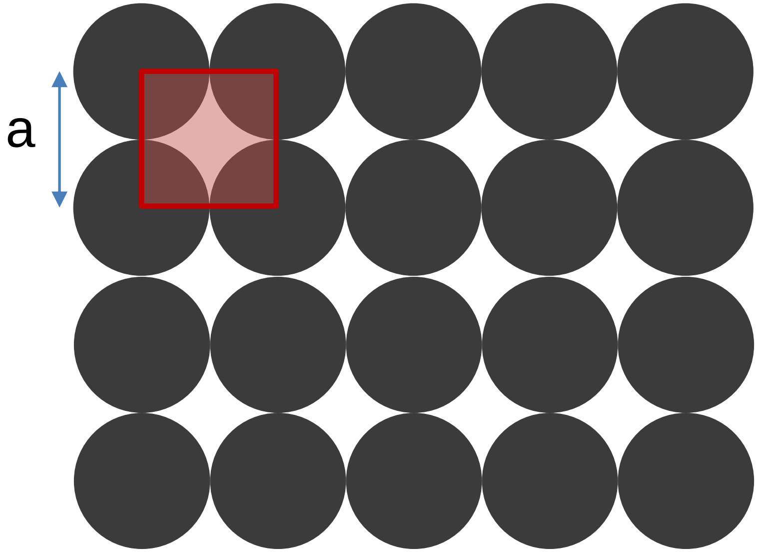
The structure with highest volume of atoms in unit cell.

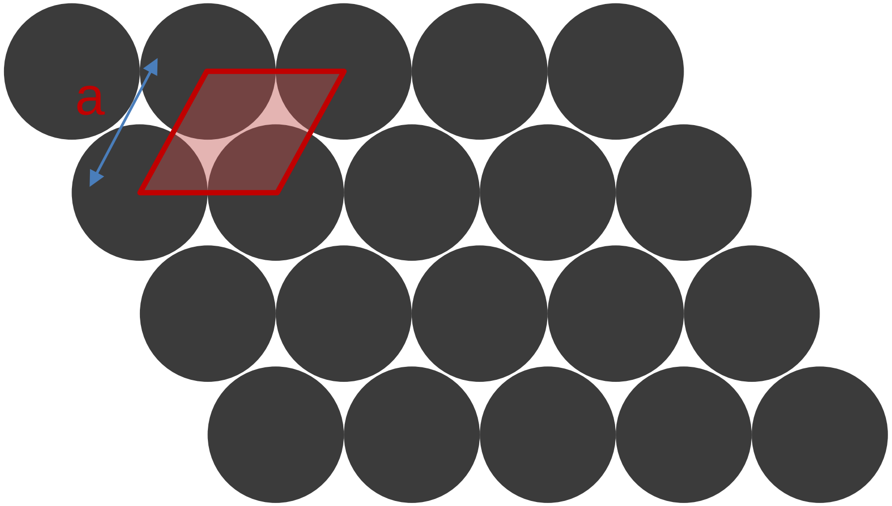
Close-packed structure密堆积结构

For two-dimensional lattice, what’s the close-packed structure?









Area of unit cell: $S = a^2$

Area of atom: $S = \pi(\frac{a}{2})^2$

The fraction of total area occupied by the spheres:

$$\frac{\pi}{4} = 0.79$$

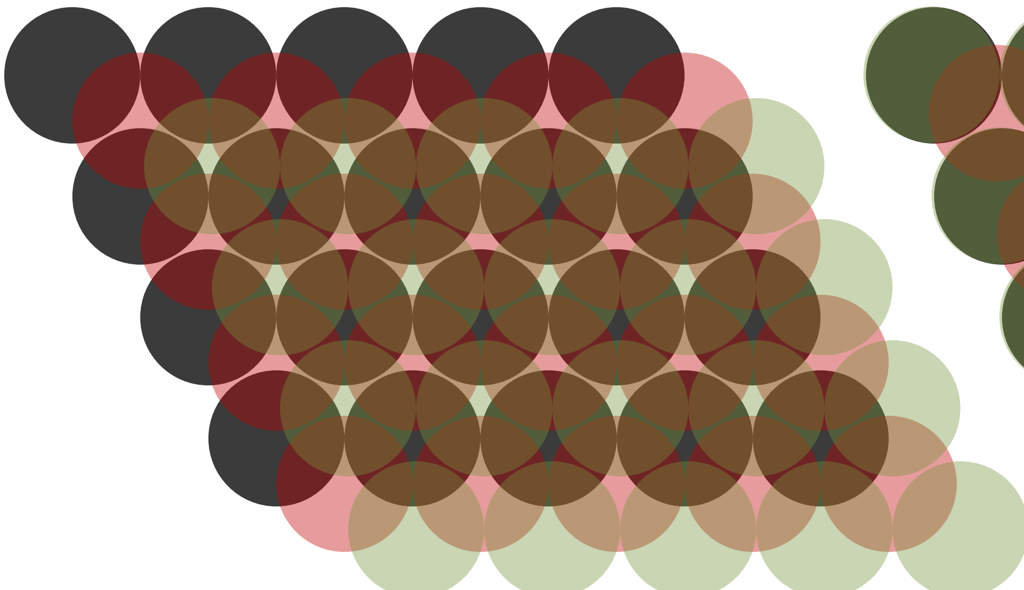
Area of unit cell: $S = \frac{\sqrt{3}}{2}a^2$

Area of atom: $S = \pi(\frac{a}{2})^2$

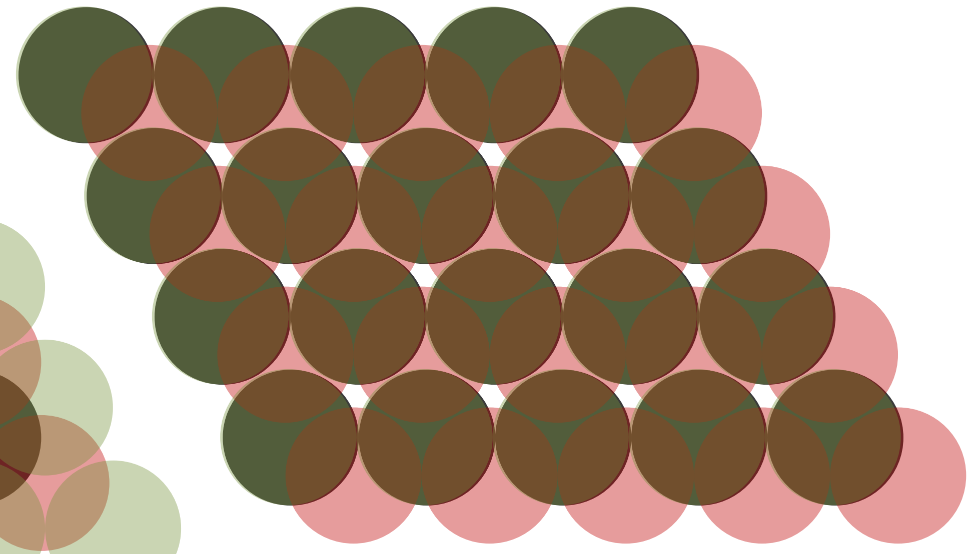
The fraction of total area occupied by the spheres:

$$\frac{\pi}{2\sqrt{3}} = 0.91$$

For three-dimensional lattice, what's the close-packed structure?

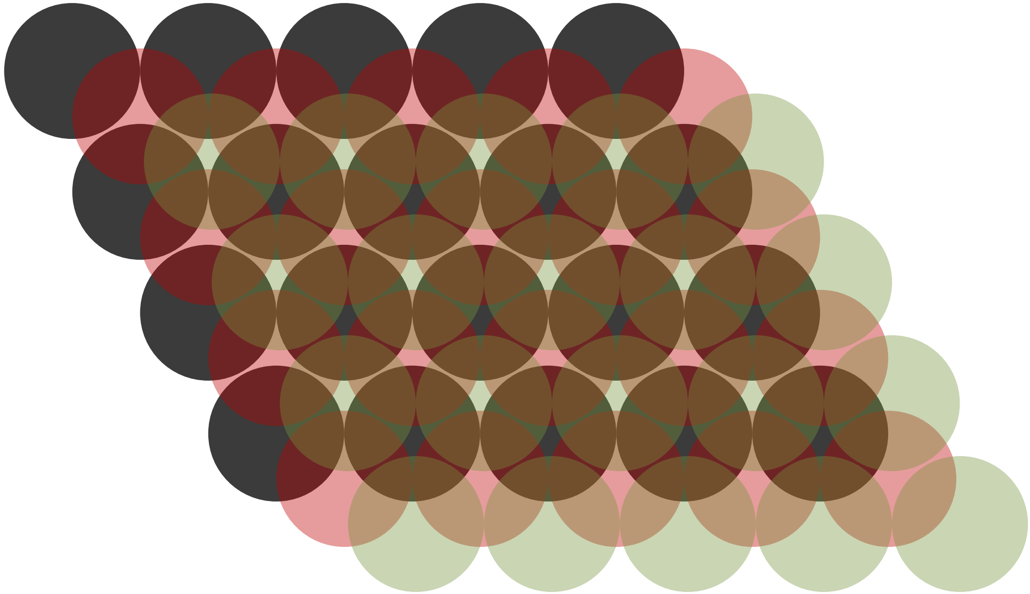


ABCABC…

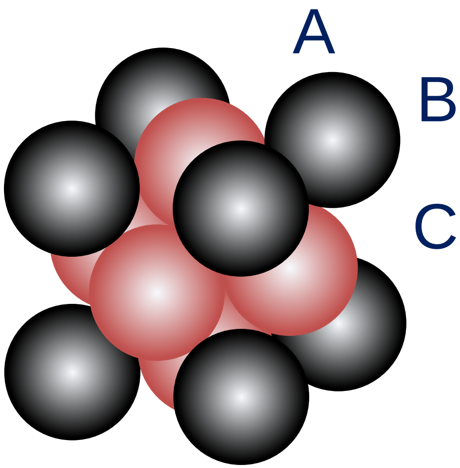


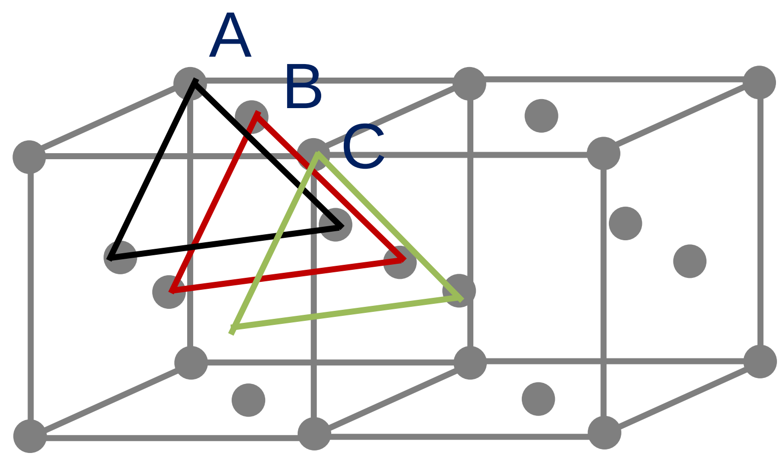
ABABAB…

Which lattice type ?



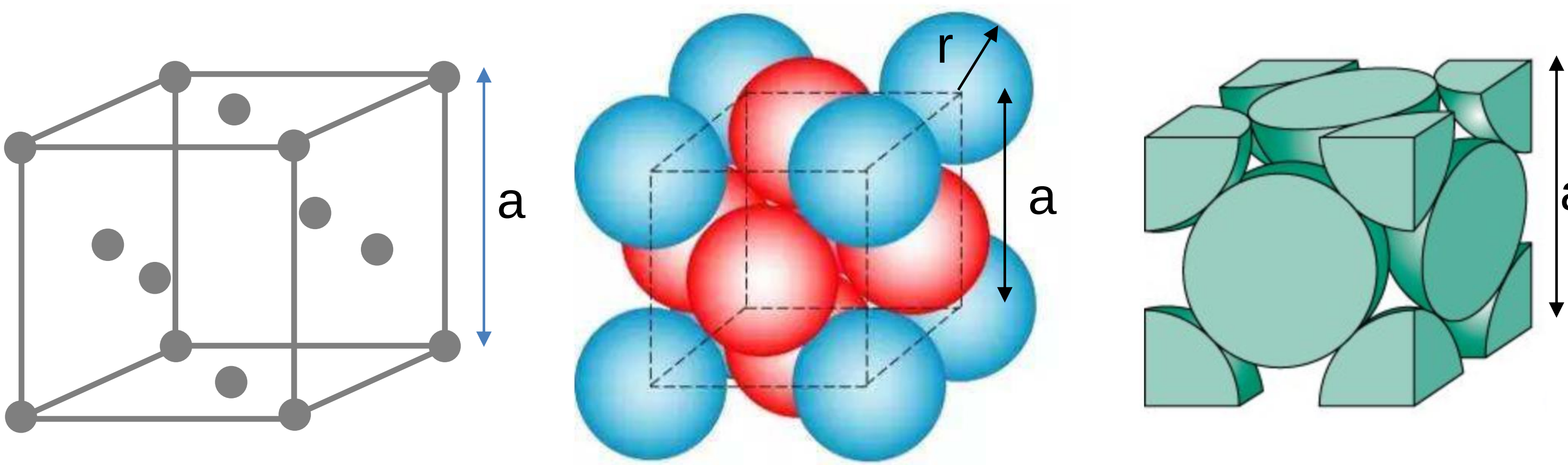
ABC





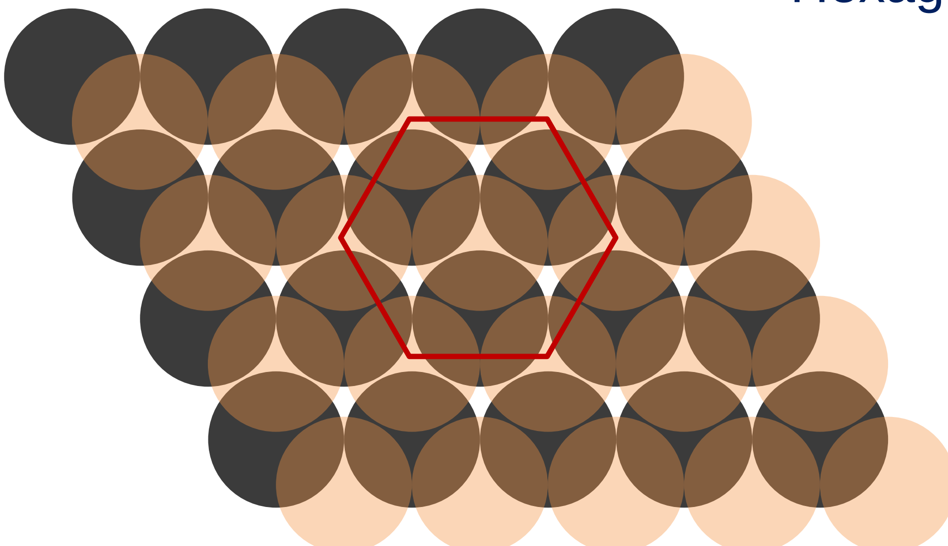
fcc!!

Atomic packing factor: the fraction of total volume occupied by the spheres:

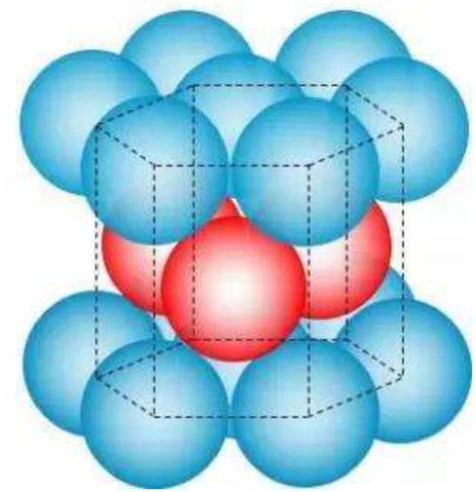


- Volume of unit cell: $V = a^3$
- Volume of atom: $V = 4 \times \frac{4}{3}\pi r^3$
- Relationship between *r* and *a*: $4r = \sqrt{2}a$
- Atomic packing factor: $\frac{\sqrt{2}}{6}\pi = 0.74$

Which lattice type for ABAB…



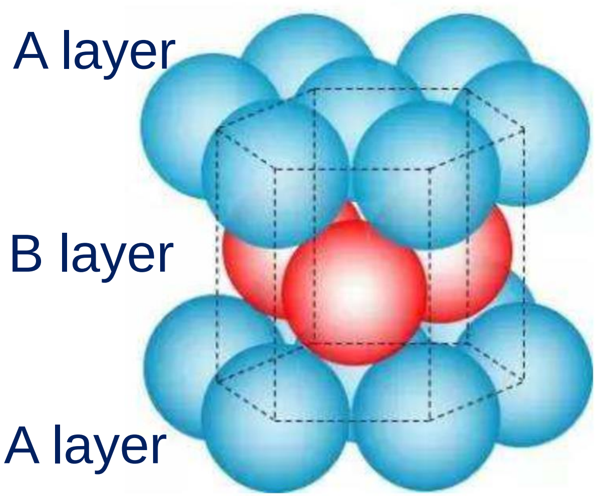
Hexagonal close-packed (hcp) structure

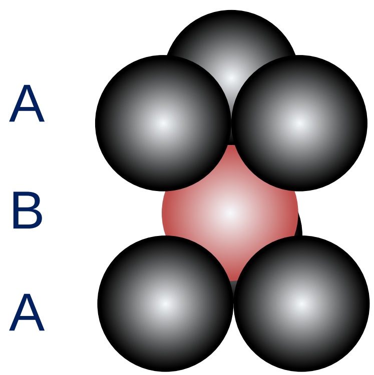


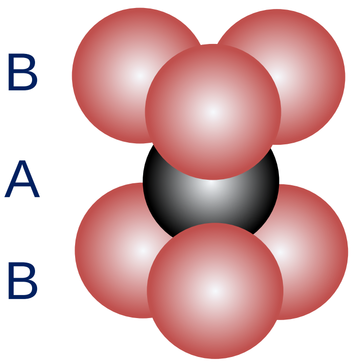
Q: How many atoms in hcp unit cell?

$$\frac{1}{6} \times 12 + \frac{1}{2} \times 2 + 3 = 6$$

Which lattice type for ABAB…







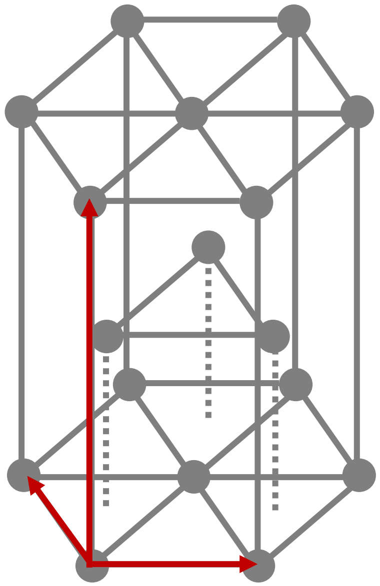
Primitive cell for hcp structure

Unit cell

A layer

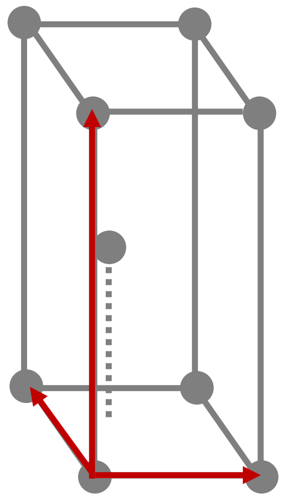
B layer

A layer



Atoms in A and B layer
are not identical!

Primitive cell



2 atoms in primitive cell

Atomic packing factor?