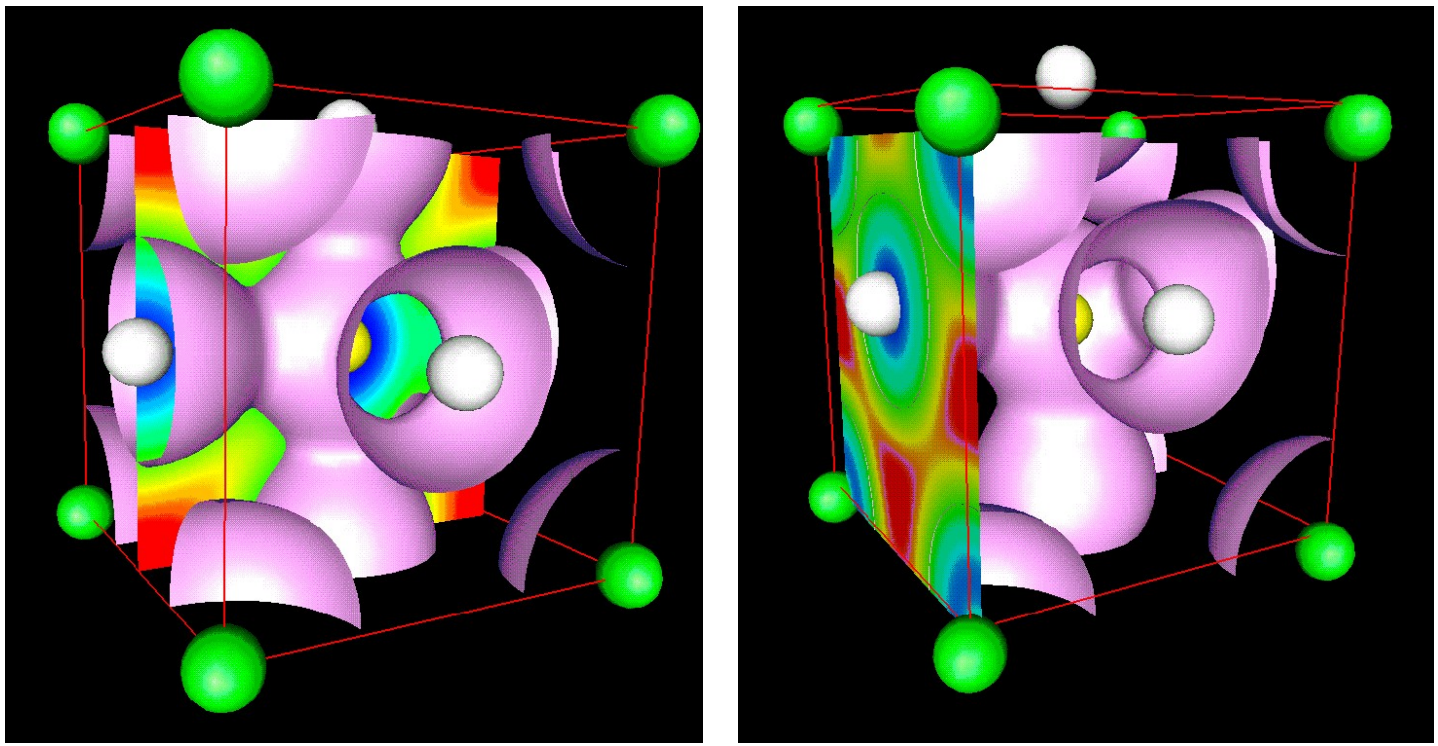
3.012 Fund of Mat Sci: Structure – Lecture 16

STRUCTURE OF SOLIDS



Charge density in paraelectric and ferroelectric $PbTiO_3$

Homework for Mon Nov 7

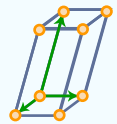
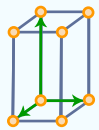
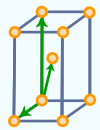
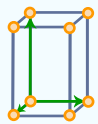
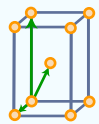
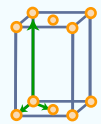
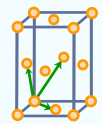
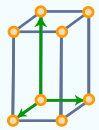
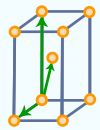
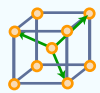
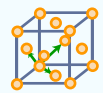
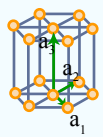
- Study: Allen and Thomas 3.2.2 up to pag. 140, and 3.4

Last time:

1. Symmetry operations: rotation, reflection, inversion, roto-inversion
2. Mirror+mirror=rotation
3. Periodicity constrains rotations (1, 2, 3, 4, 6) → ten crystallographic point groups in 2d
4. Bravais lattices
5. International tables

4 Lattice Types

7 Crystal Classes

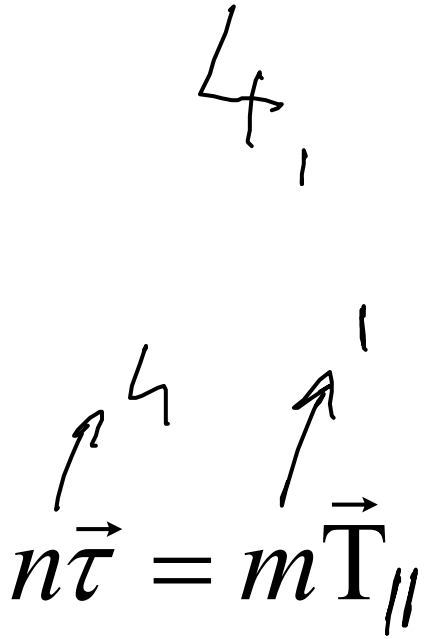
Bravais Lattice	Parameters	Simple (P)	Volume Centered (I)	Base Centered (C)	Face Centered (F)
Triclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} \neq \alpha_{23} \neq \alpha_{31}$				
Monoclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{23} = \alpha_{31} = 90^0$ $\alpha_{12} \neq 90^0$				
Orthorhombic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90^0$				
Tetragonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90^0$				
Trigonal	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} < 120^0$				
Cubic	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90^0$				
Hexagonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = 120^0$ $\alpha_{23} = \alpha_{31} = 90^0$				

Compound ops. with translations:
4) Glides

Illustration of glide symmetry removed for copyright reasons.
See p. 99, figure 3.8 in Allen, S. M., and E. L. Thomas. *The Structure of Materials*. New York, NY: J. Wiley & Sons, 1999.

Compound ops. with translations:
5) Screw (in 3 dim)

Illustration of rotation and parallel translation removed for copyright reasons.
See p. 130, figure 3.38 in Allen, S. M., and E. L. Thomas. *The Structure of Materials*. New York, NY: J. Wiley & Sons, 1999.



$$n\vec{\tau} = m\vec{\mathrm{T}}_{//}$$

Figure of object repetition removed for copyright reasons.
See p. 133, Figure 3.39 in Allen, S. M., and E. L. Thomas. *The Structure of Materials*. New York, NY: J. Wiley & Sons, 1999.

Space groups

- All possible combinations of point group symmetries with translations
- 230 in total
- We have seen 14 (Bravais lattices)
- Incorporate all possible translation with symmetries, and add screw axis and glide planes

Bravais lattices: simple cubic

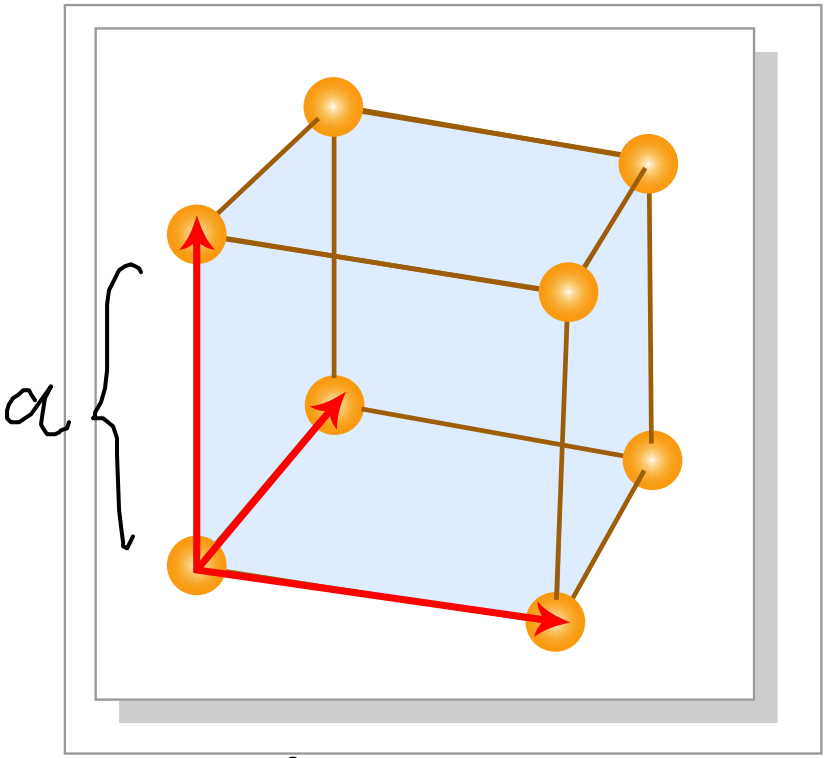


Figure by MIT OCW.

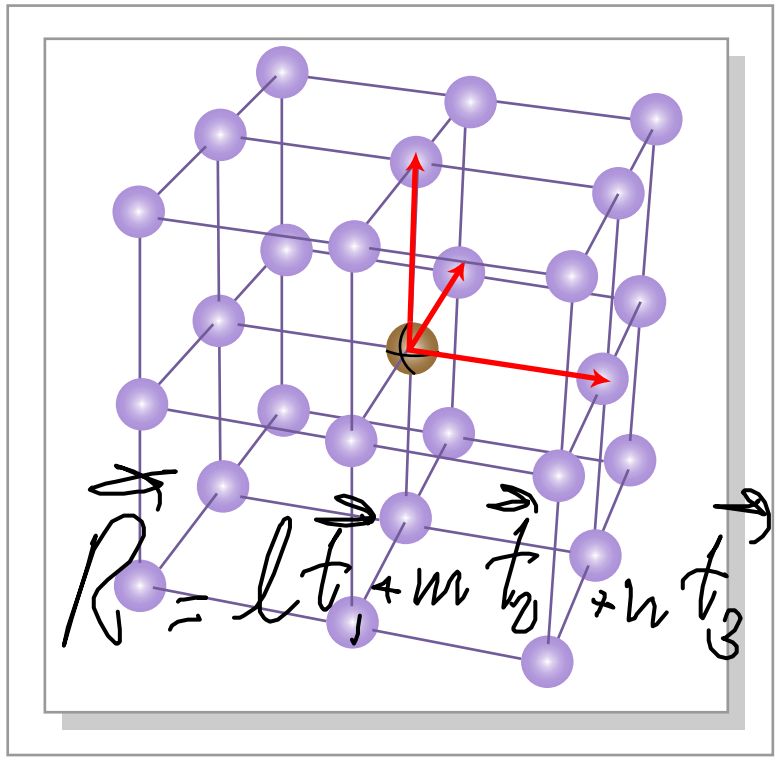


Figure by MIT OCW.

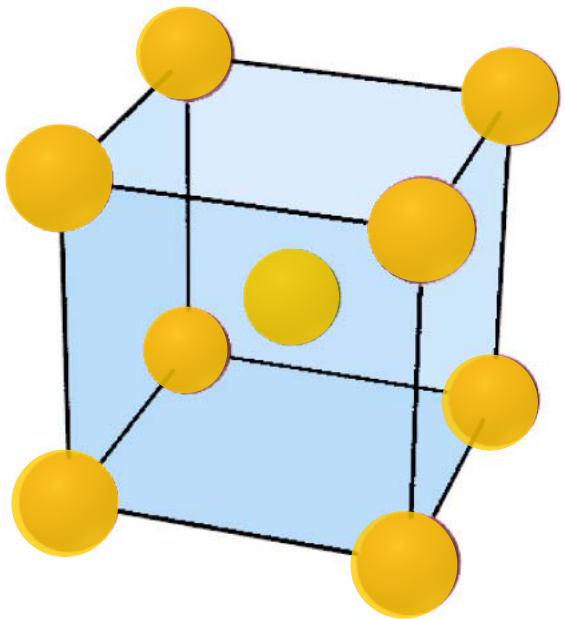
$\vec{t}_1 = a(1,0,0)$

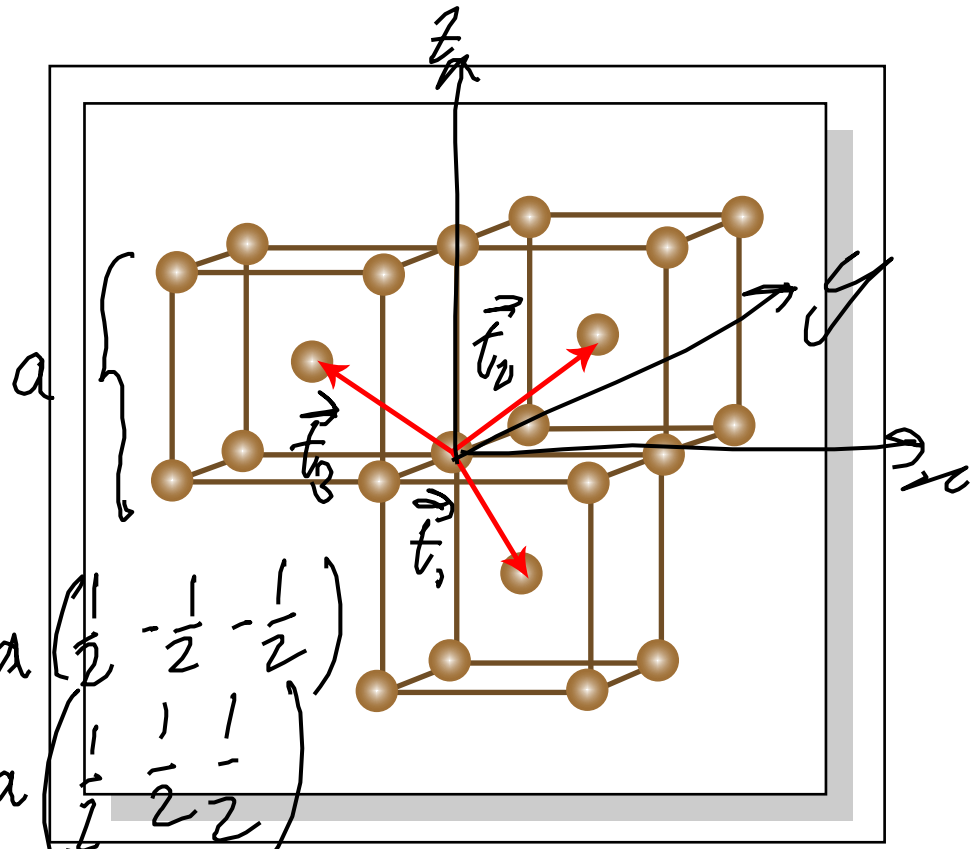
$\vec{t}_2 = a(0,1,0)$

$\vec{t}_3 = a(0,0,1)$

α-phase of polonium….

Bravais lattices: body-centered cubic





$\vec{t}_1 = a\left(\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}\right)$

$\vec{t}_2 = a\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$

$\vec{t}_3 = a\left(-\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right)$

Figure by MIT OCW.

Ba, Cr, Cs, Fe, K, Li, Mo, Na, Nb, Rb, Ta, Tl, V, W…

Bravais lattices: body-centered cubic

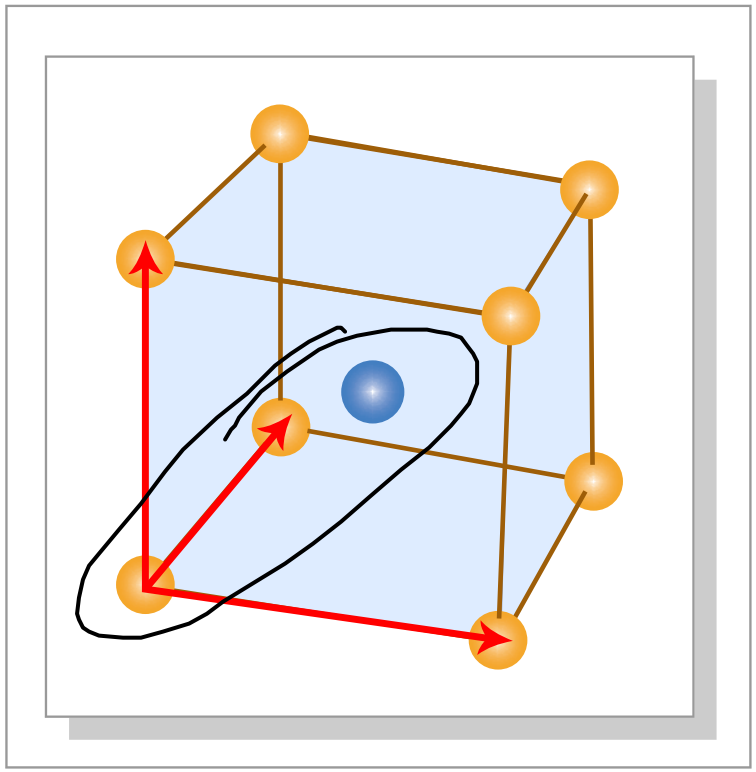


Figure by MIT OCW.

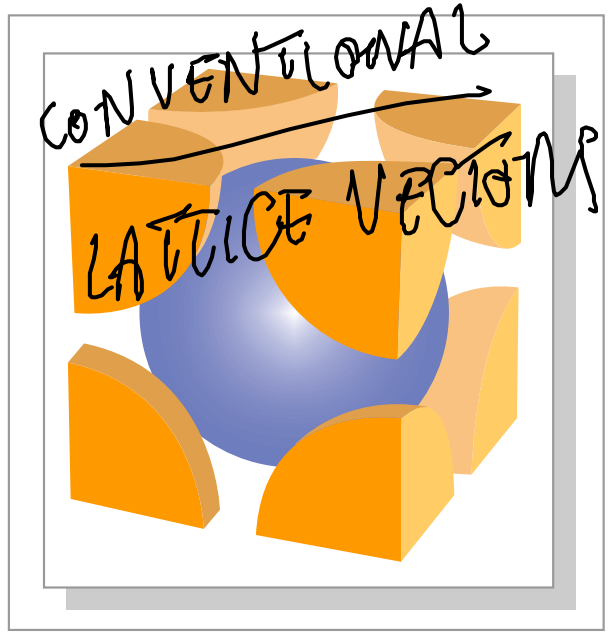
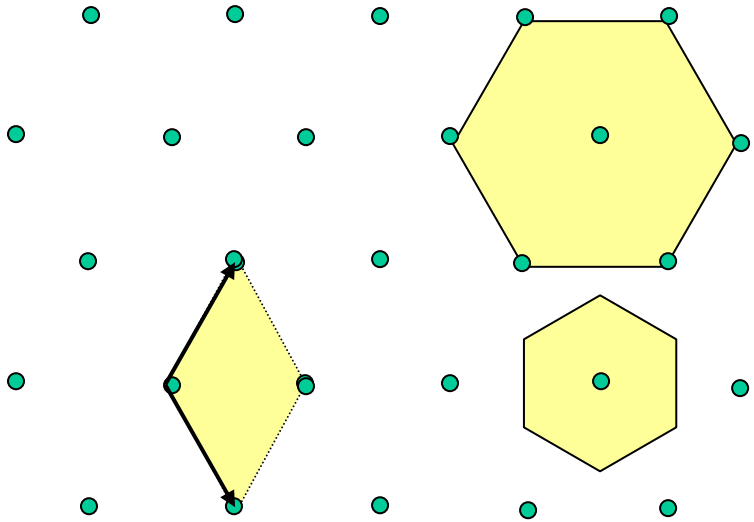


Figure by MIT OCW.

Primitive unit cell and conventional unit cell



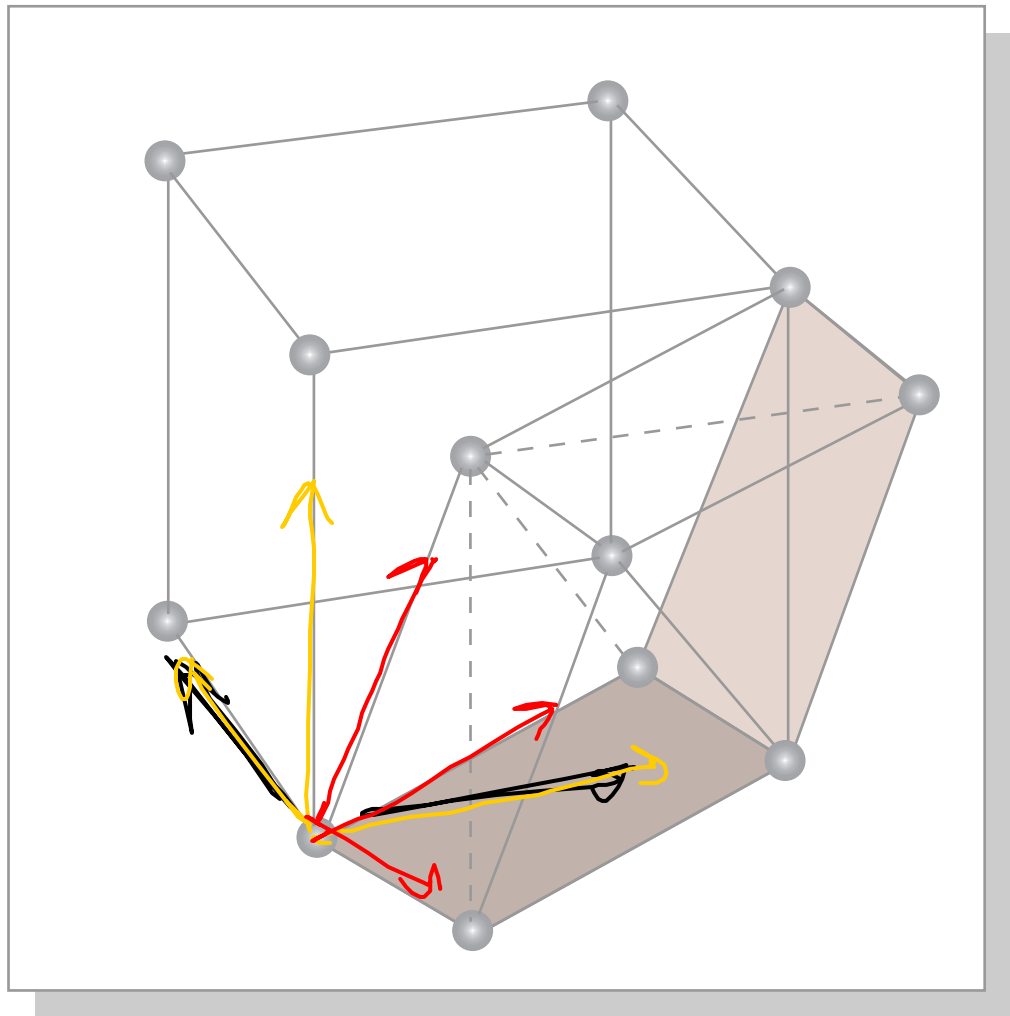
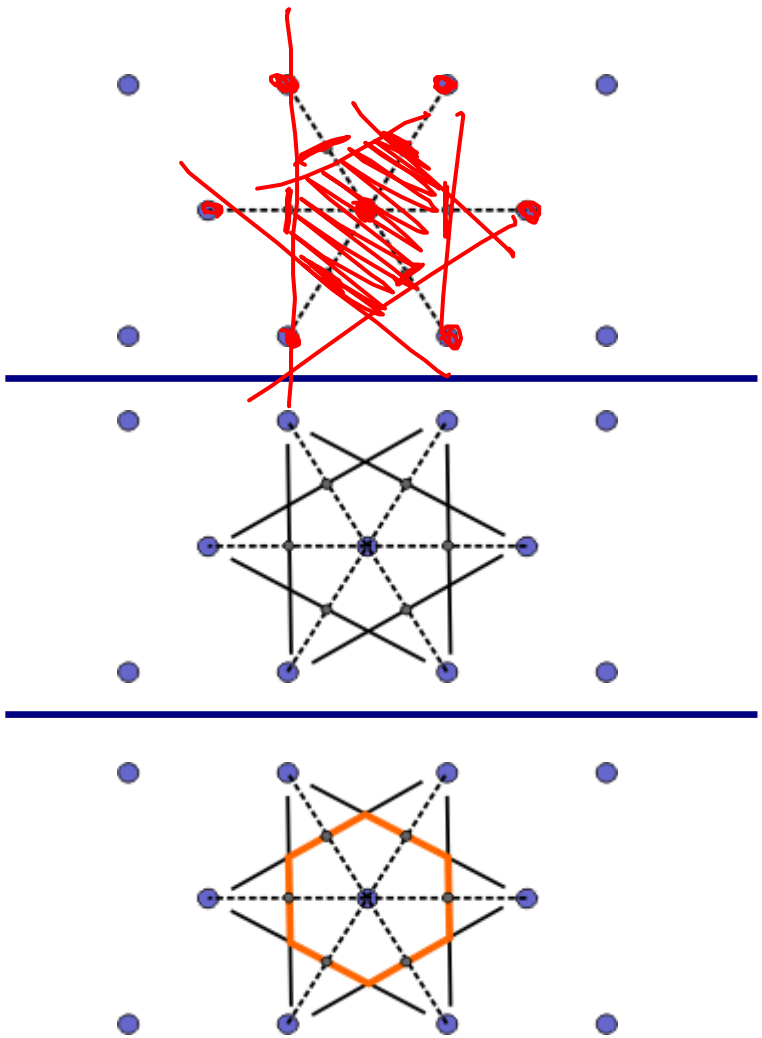


Figure by MIT OCW.

Wigner-Seitz cell



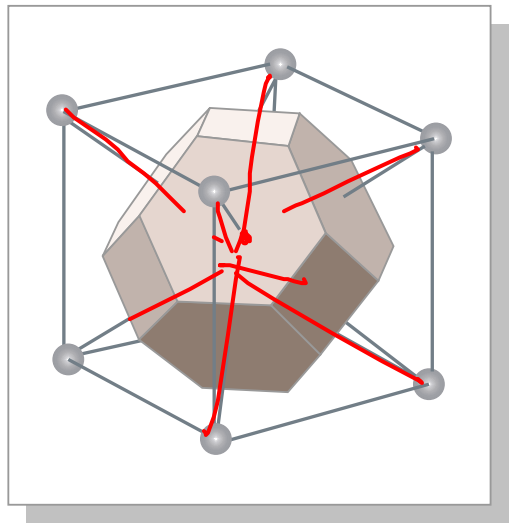


Figure by MIT OCW.

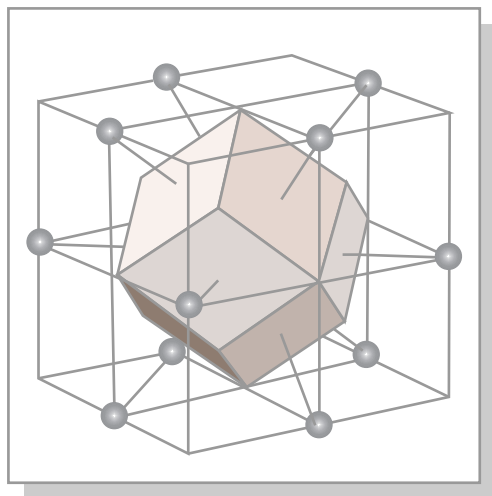
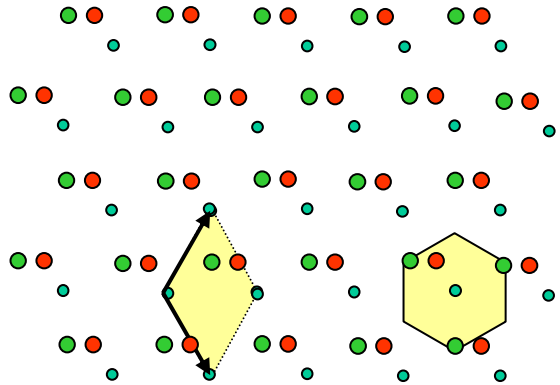
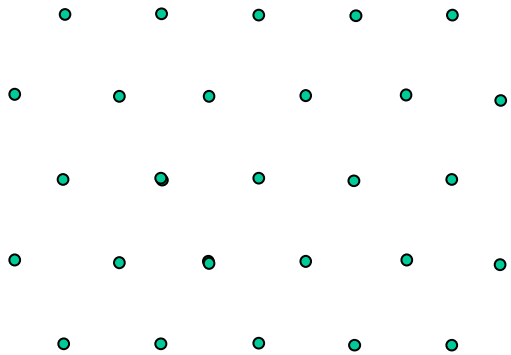


Figure by MIT OCW.

Crystal Structure = Lattice + Basis



Crystal Structure = Lattice + basis



Lattice

Basis

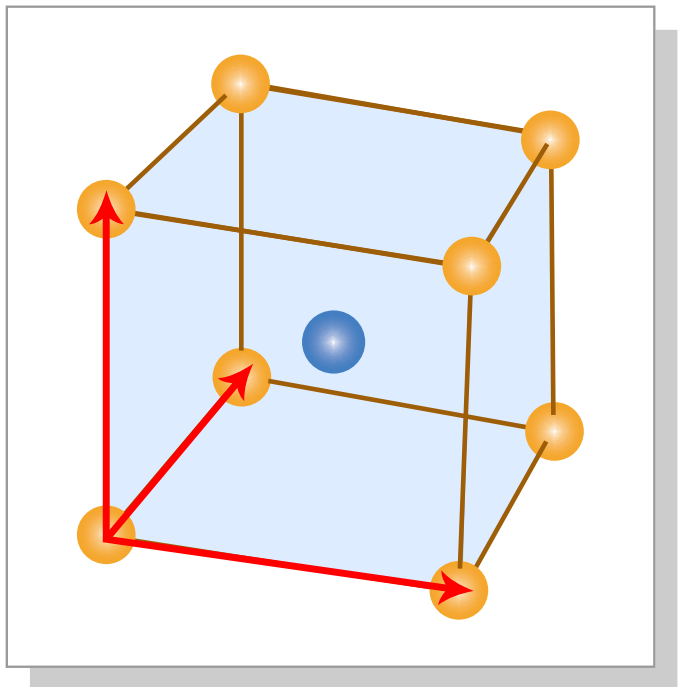
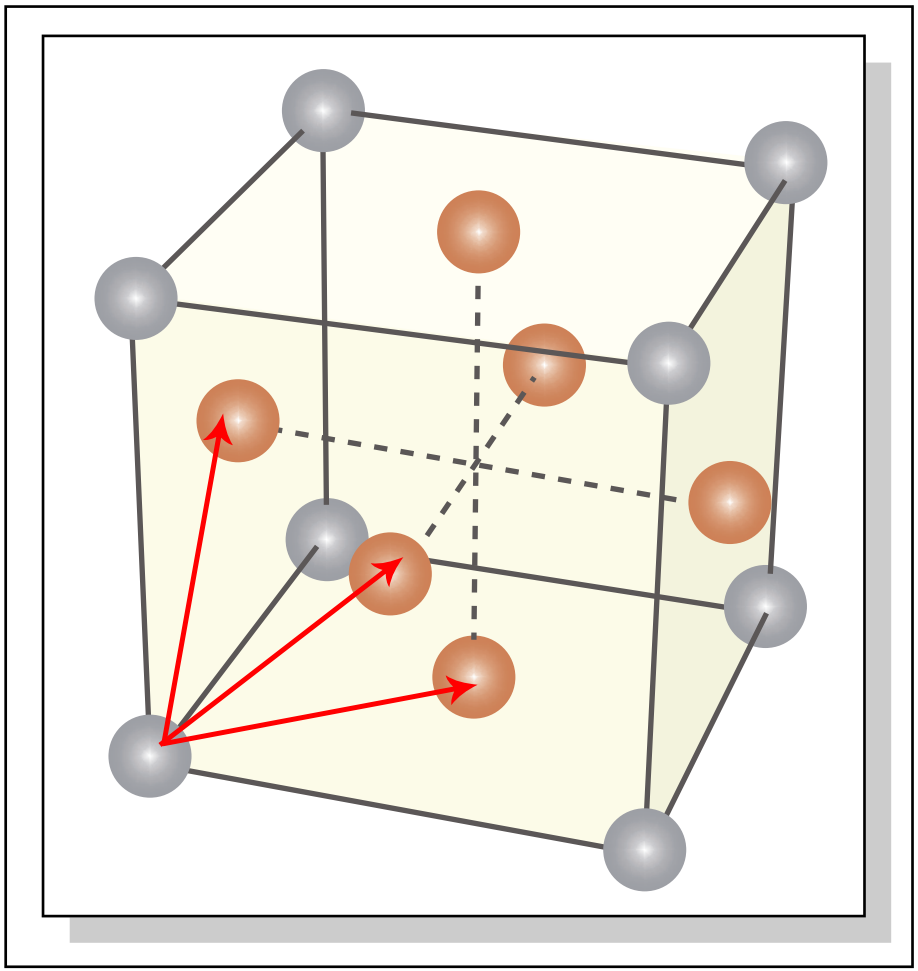


Figure by MIT OCW.

Bravais lattices: face-centered cubic



$\vec{t}_1 = \frac{a}{2}(110)$

$\vec{t}_2 = \frac{a}{2}(101)$

$\vec{t}_3 = \frac{a}{2}(011)$

Figure by MIT OCW.

Ag, Al, Au, Ca, Cu, Ir, Ni, Pb, Pd, Pt, Sc, Sr…

Close-Packed Structures

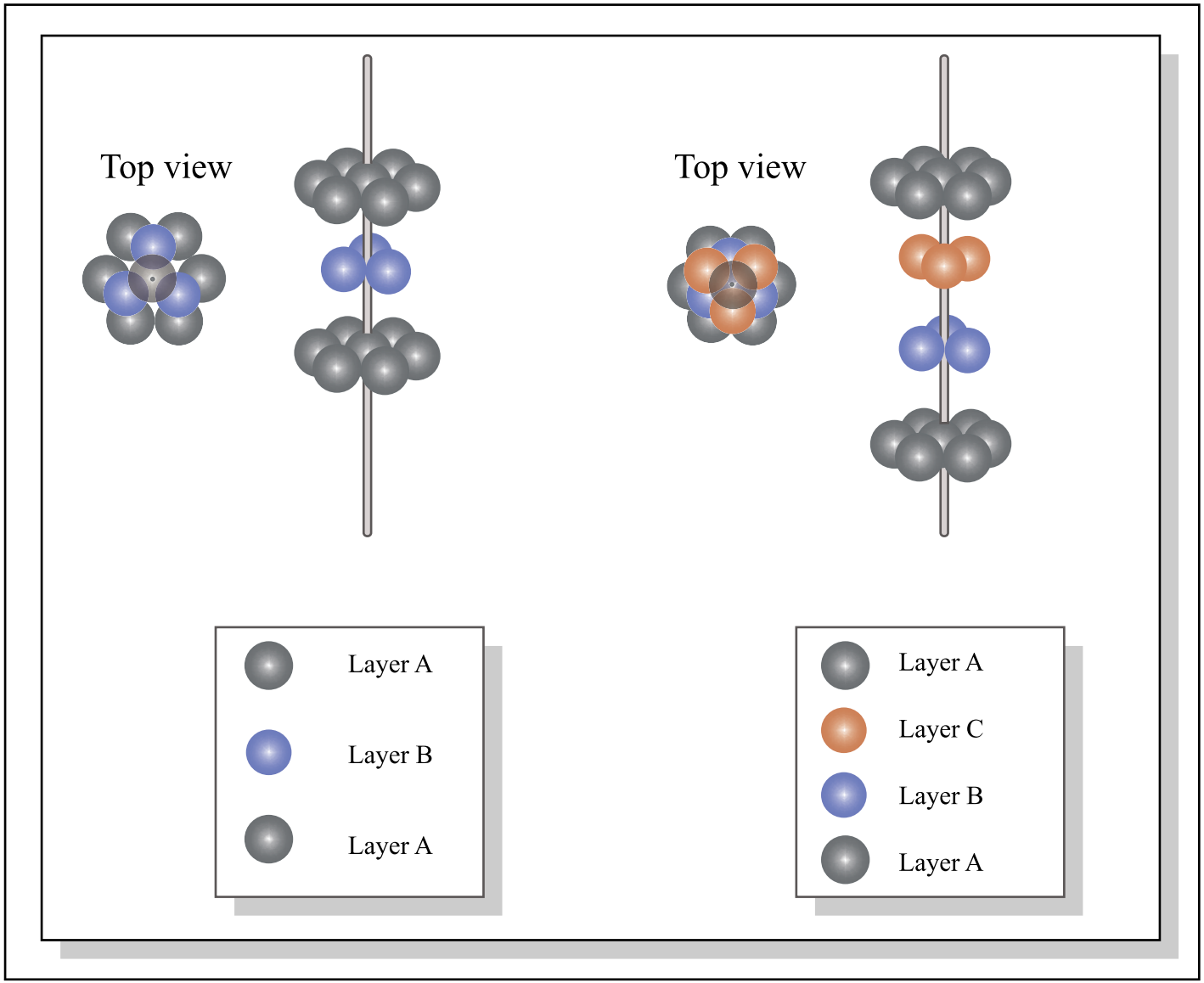


Figure by MIT OCW.

Interstitials in Close-Packed

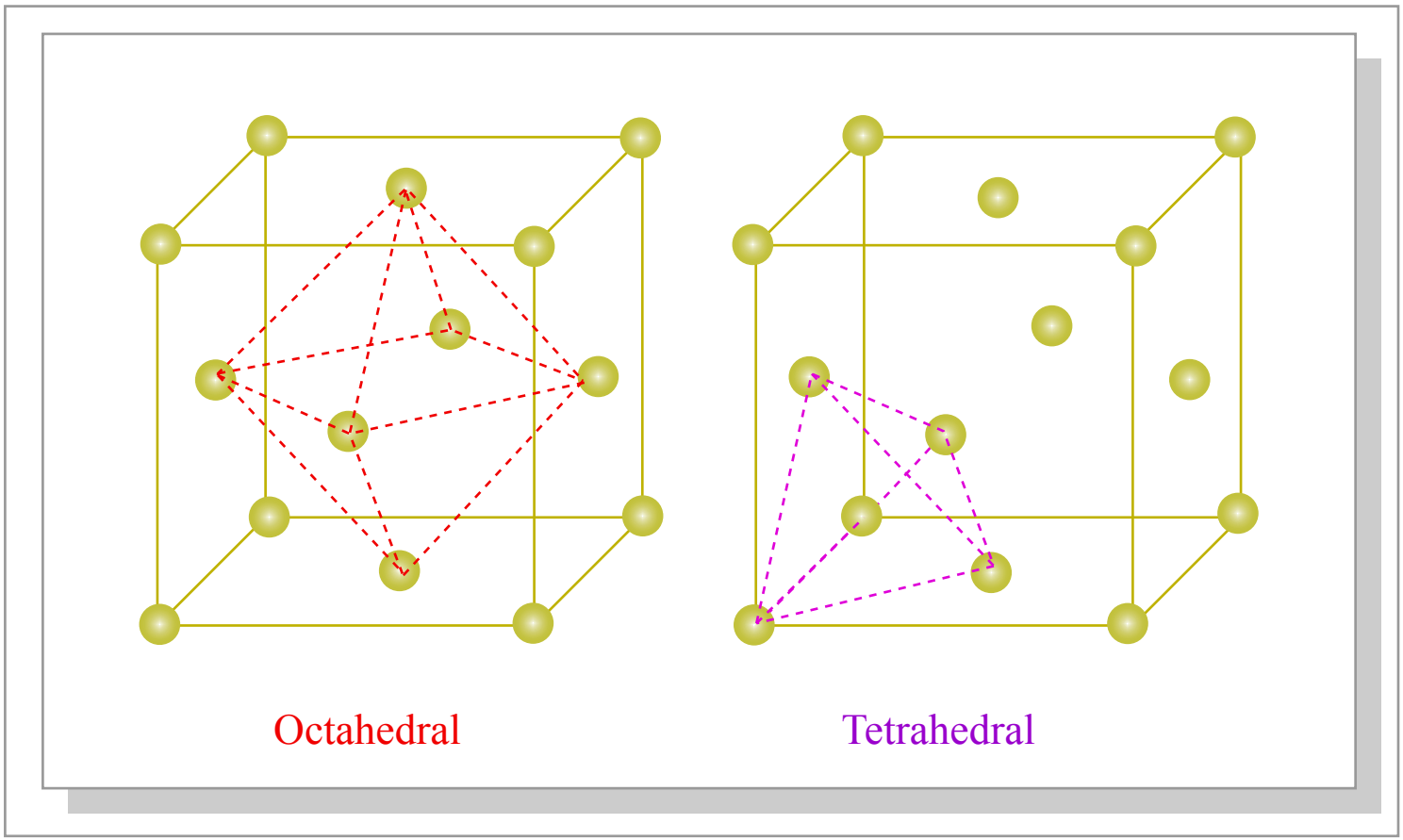
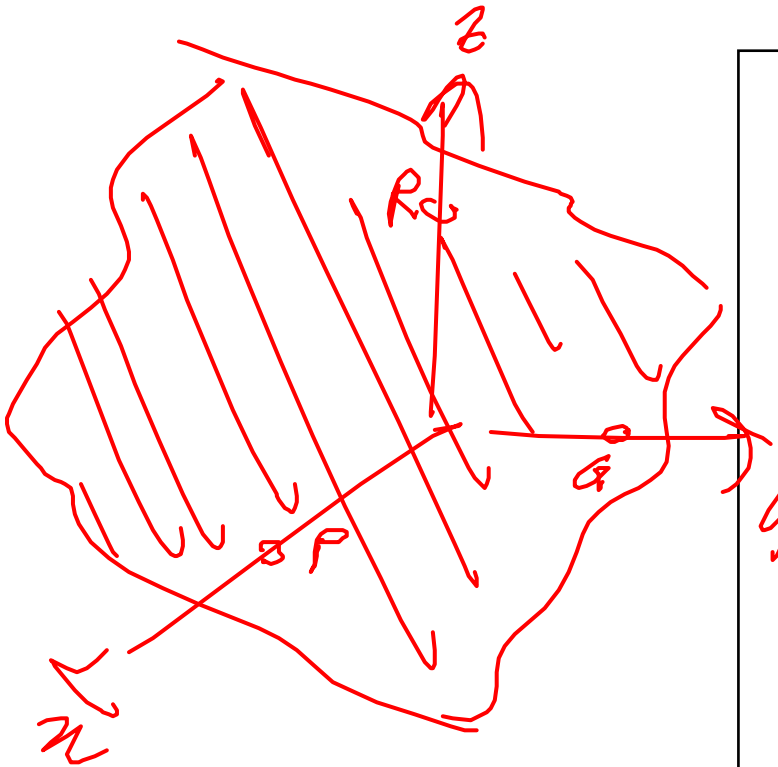


Figure by MIT OCW.

Miller Indices



$$\frac{x}{P} + \frac{y}{Q} + \frac{z}{R} = 1$$

$$xQR + yPR + zPQ = PQR$$

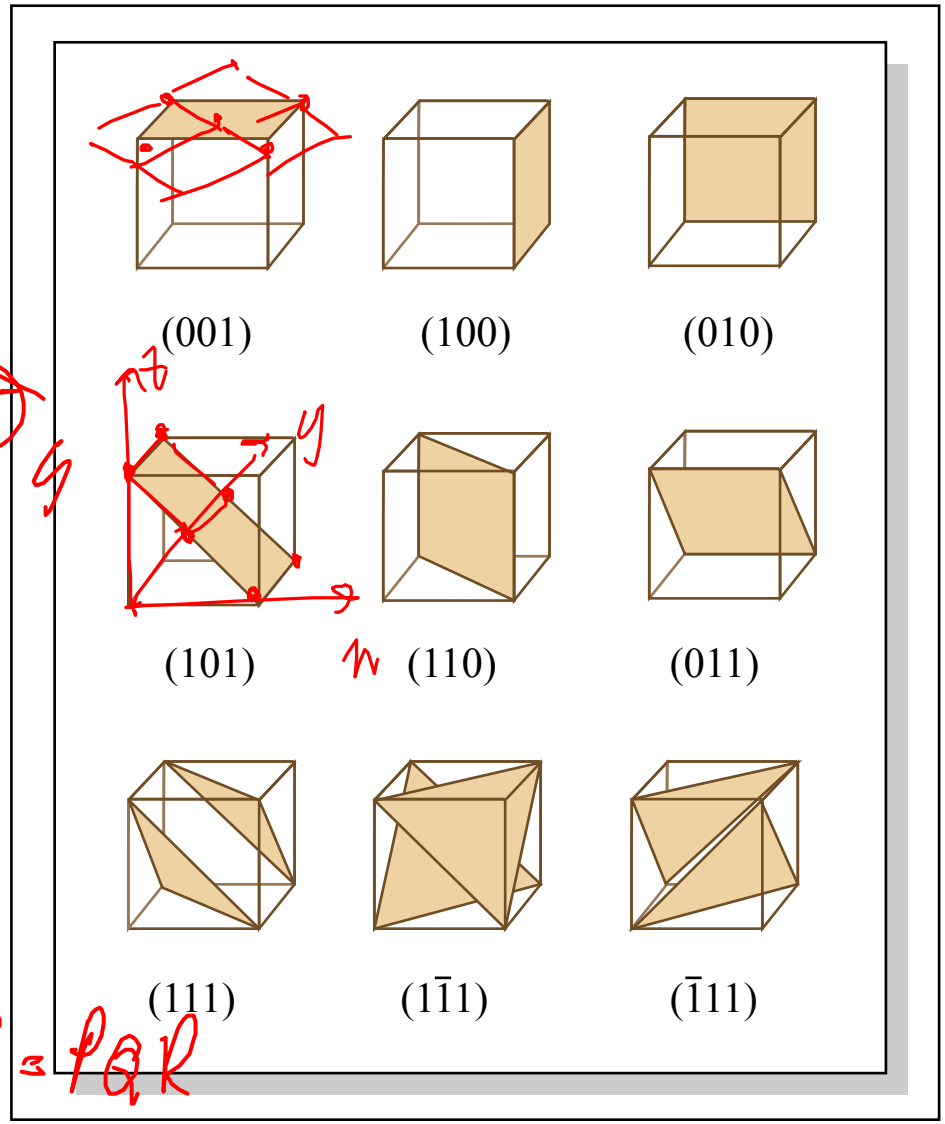
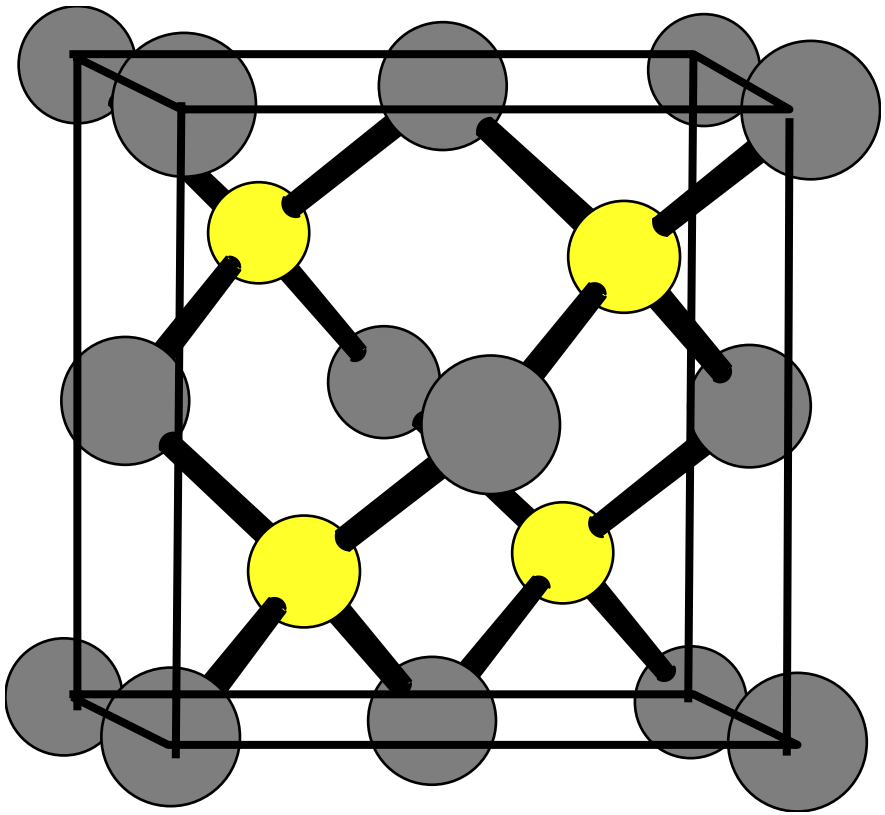
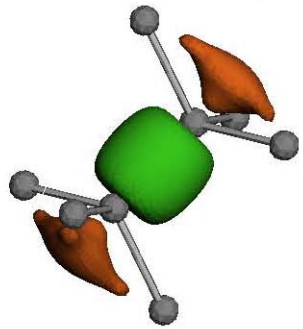


Figure by MIT OCW.

Diamond and Zincblend

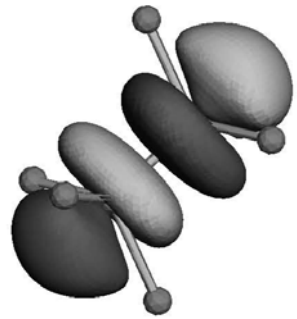


Bonding



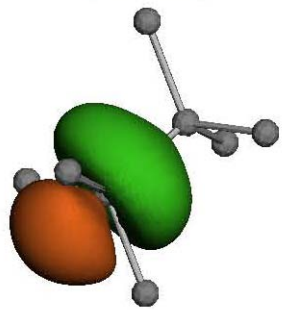
7.53 bohr^2

Antibonding



24.37 bohr^2

sp^3



spread=10.68 bohr^2

Perovskites

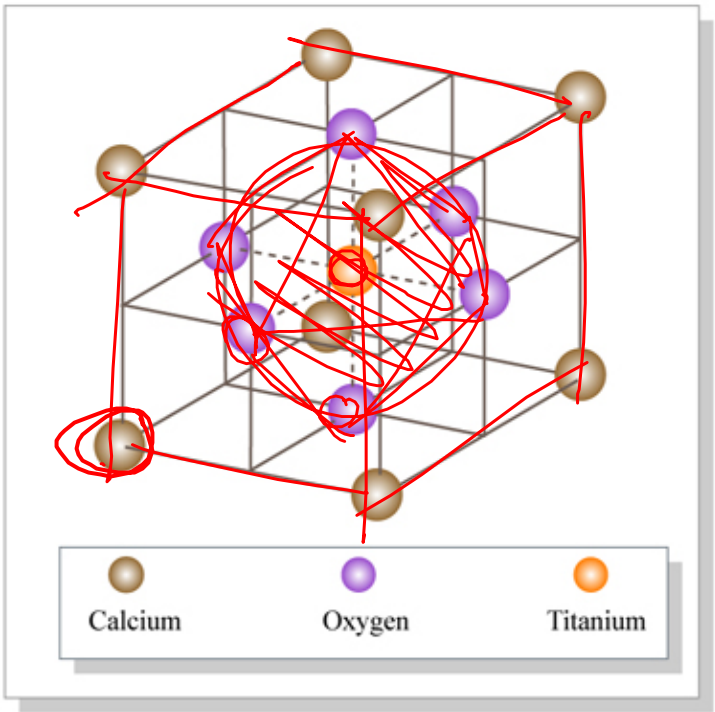


Figure by MIT OCW.

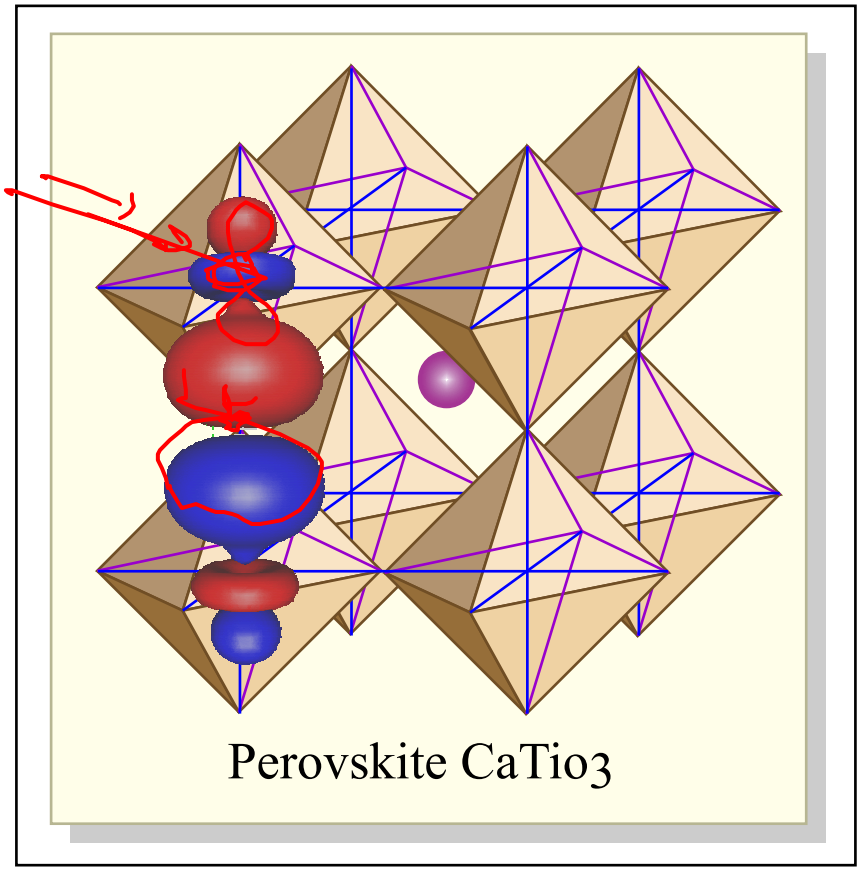
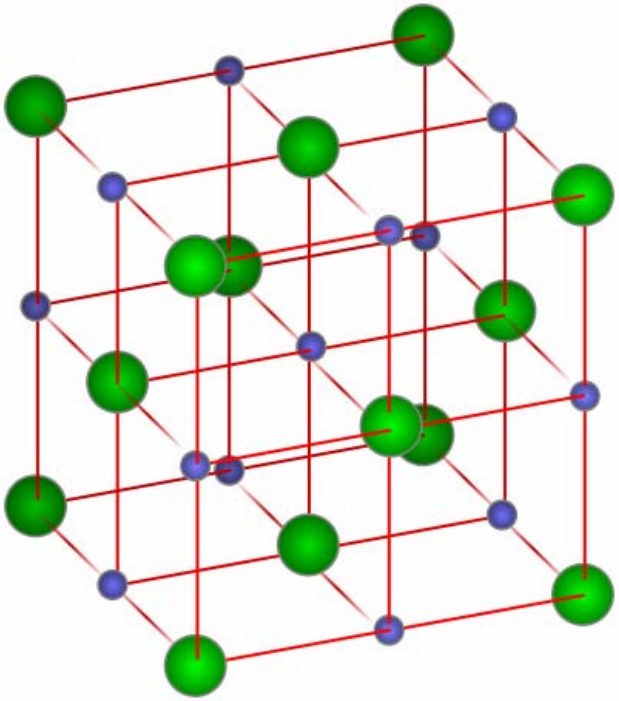
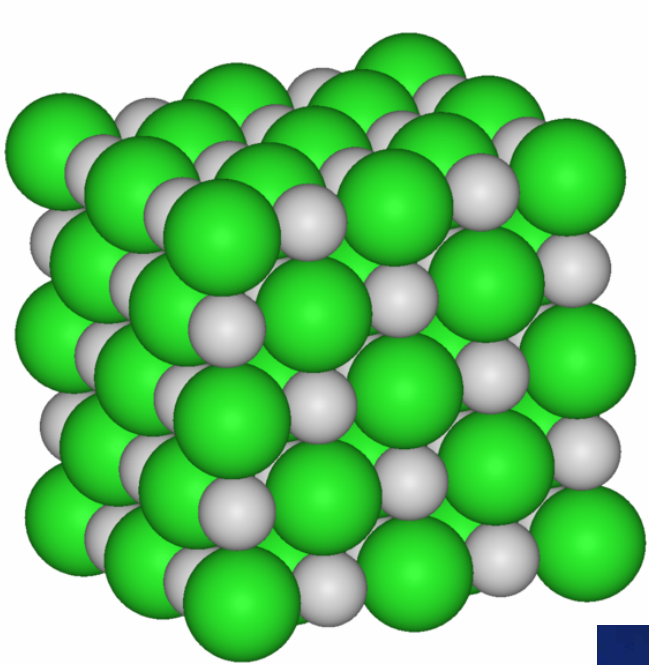


Figure by MIT OCW.

Sodium Chloride (rocksalt)





Source: Wikipedia

Cesium Chloride

Image of the structure of Cesium Chloride removed for copyright reasons.