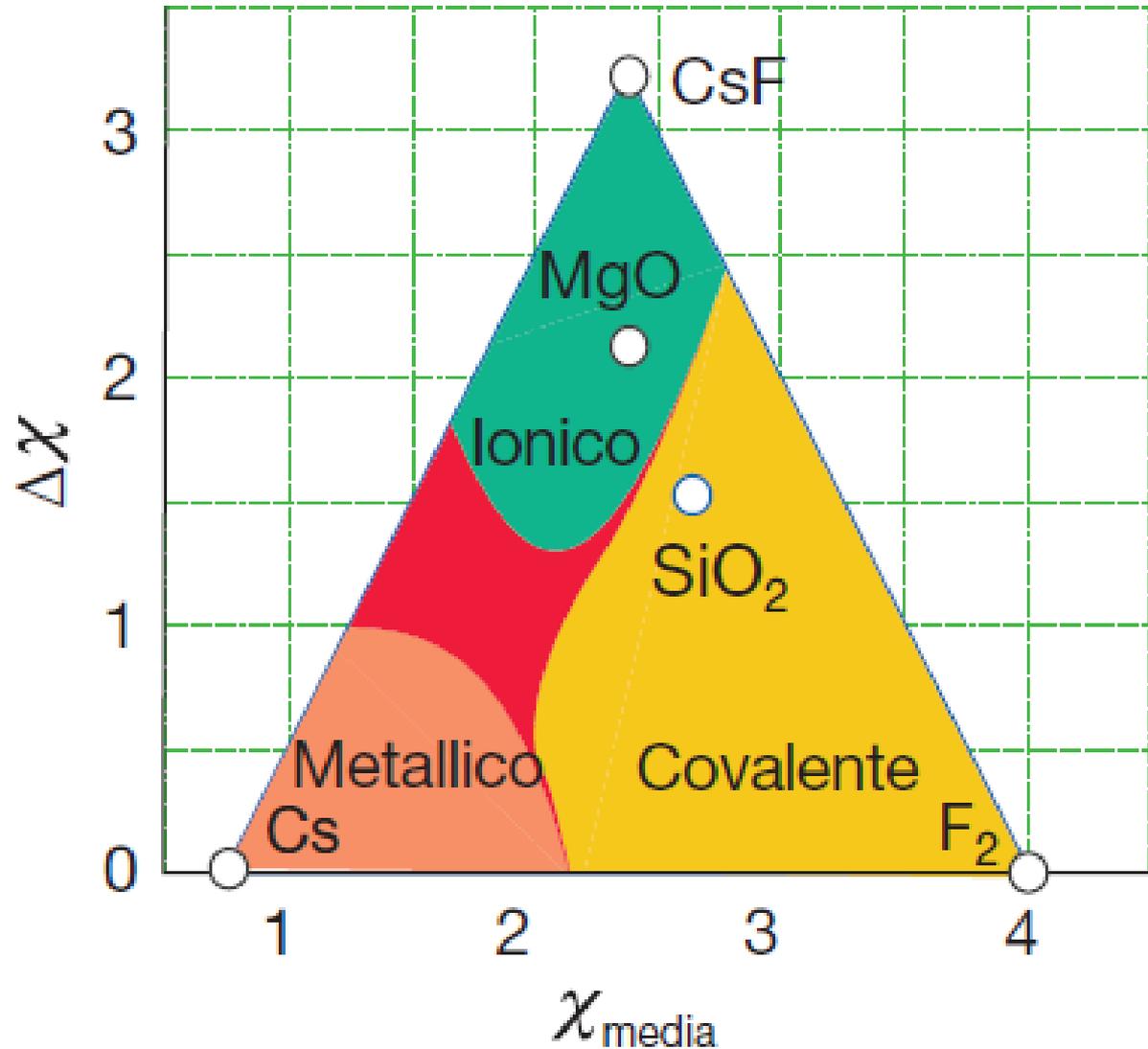


# Triangolo di Ketelaar



MgO

$$\Delta\chi = 3.44 - 1.31 = 2.13$$

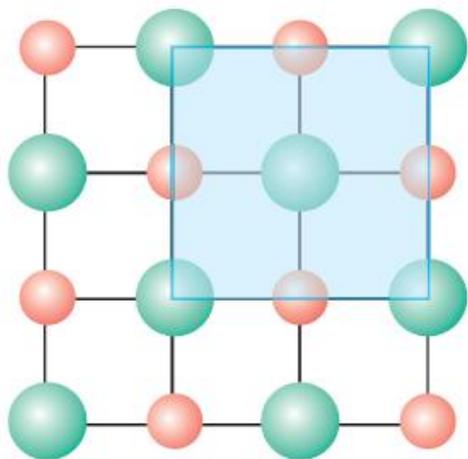
$$\chi_{\text{media}} = 2.38$$

SiO<sub>2</sub>

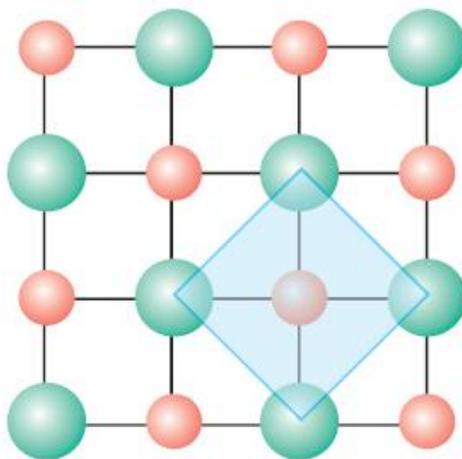
$$\Delta\chi = 3.44 - 1.90 = 1.54$$

$$\chi_{\text{media}} = 2.67$$

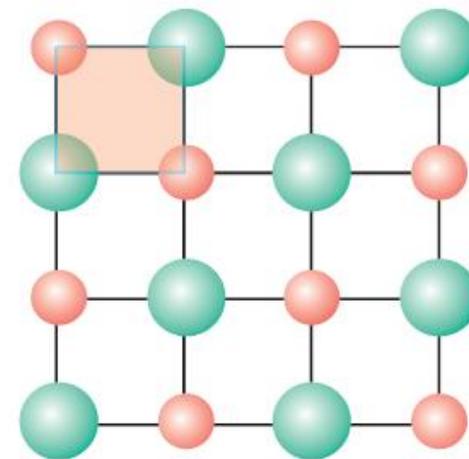
# Celle unitarie bidimensionali



(a) Possibile cella unitaria



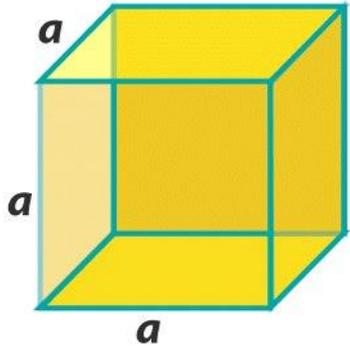
(b) Scelta preferita per la cella unitaria



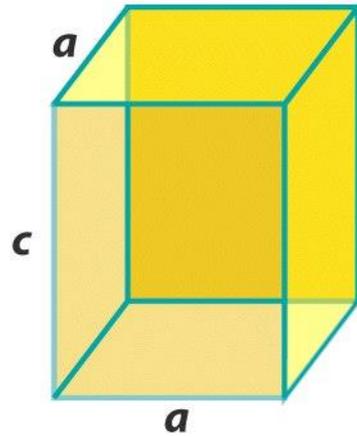
(c) Non è una cella unitaria

Preferita

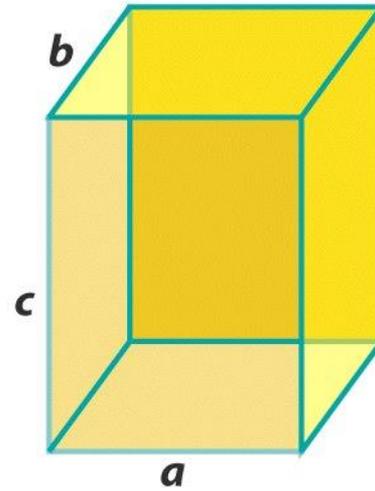
# I 7 sistemi cristallini



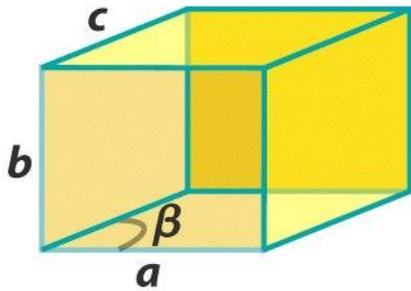
**Cubic**



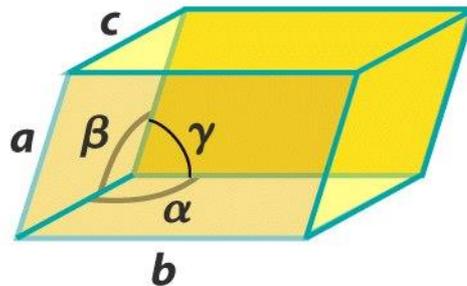
**Tetragonal**



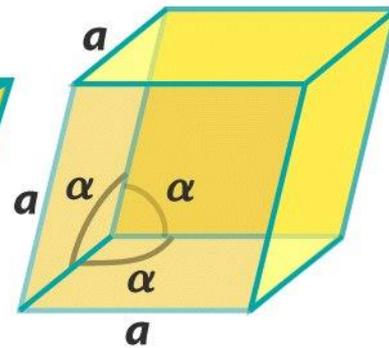
**Orthorhombic**



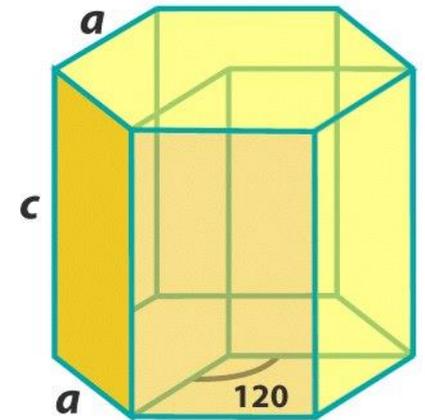
**Monoclinic**



**Triclinic**

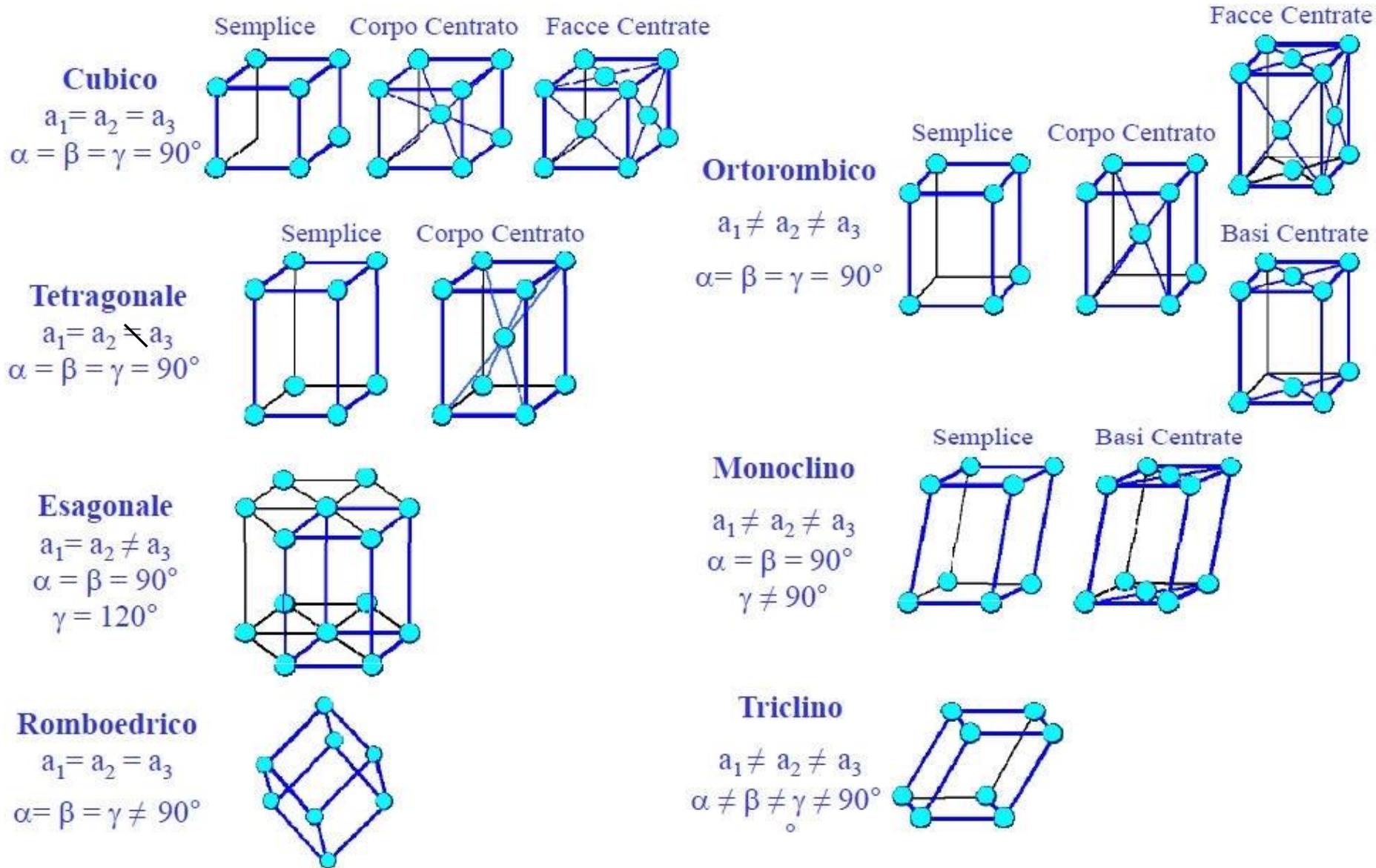


**Trigonal**

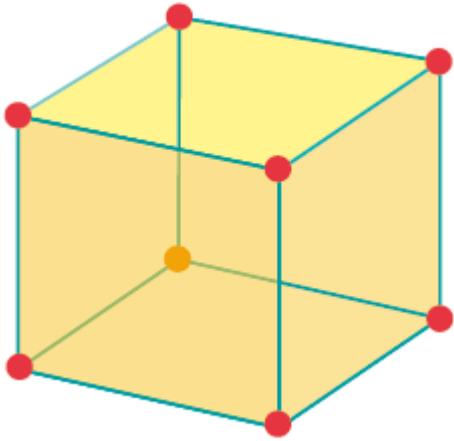


**Hexagonal**

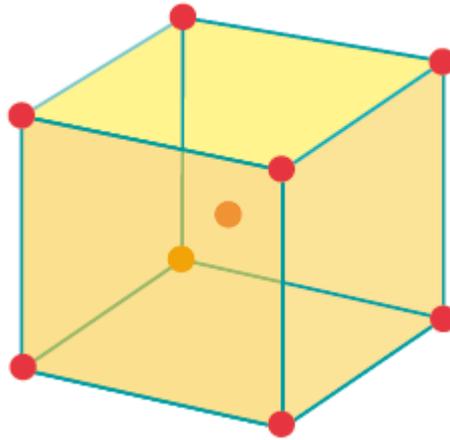
# I 14 reticoli di Bravais



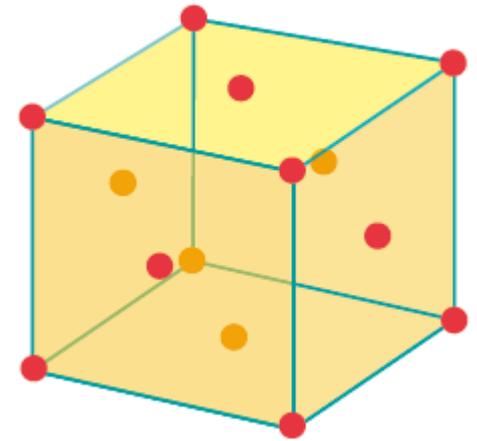
# Celle unitarie cubiche



Cubica primitiva, P

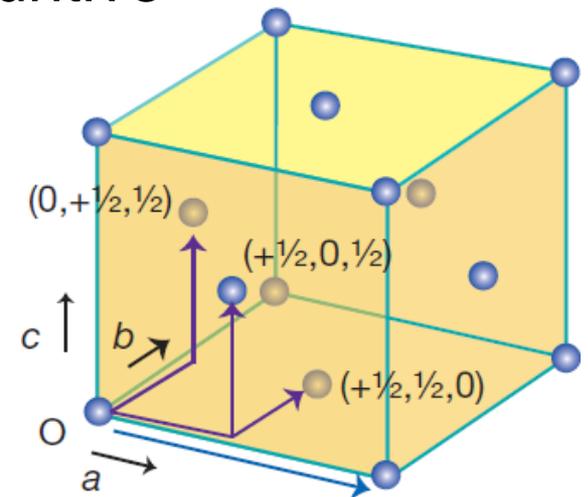
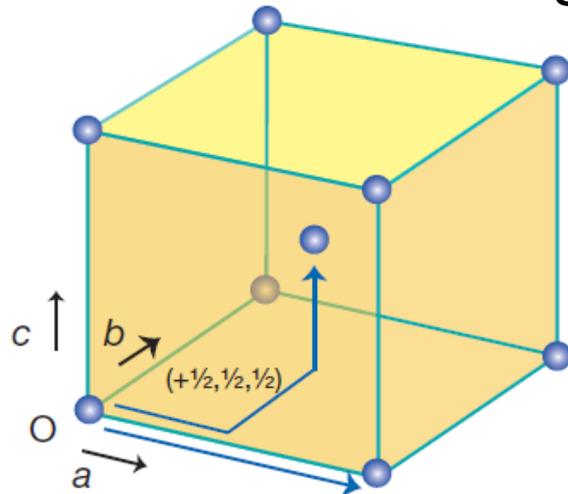
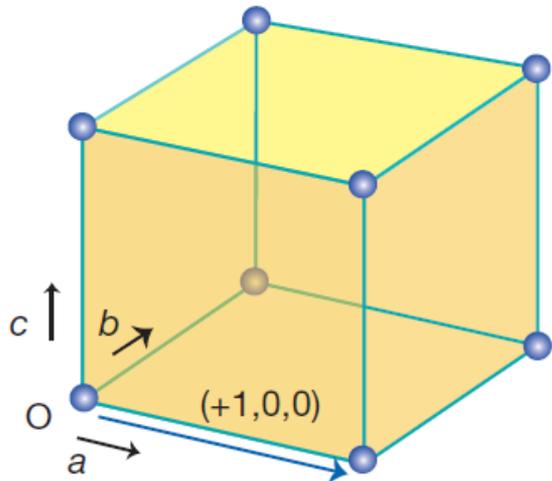


Cubica a corpo  
centrato, I

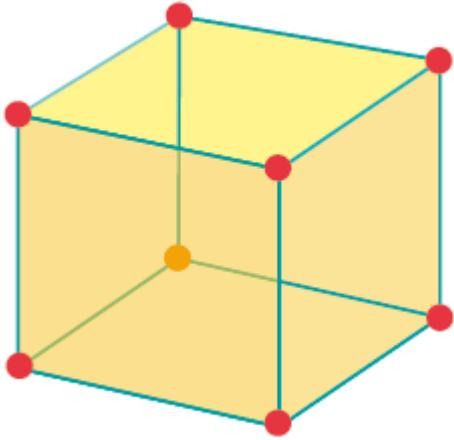


Cubica a facce  
centrate, F

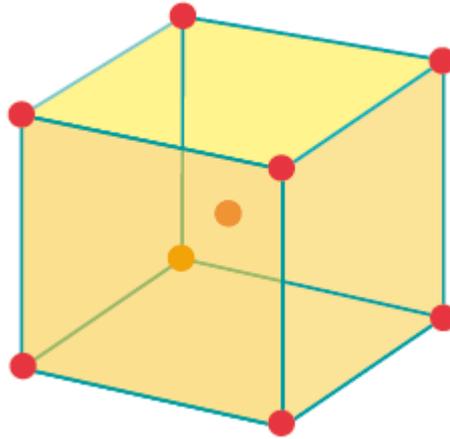
## Simmetrie traslazionali aggiuntive



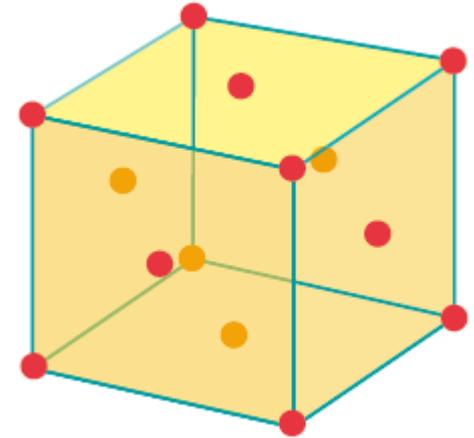
# Proiezioni di celle unitarie cubiche



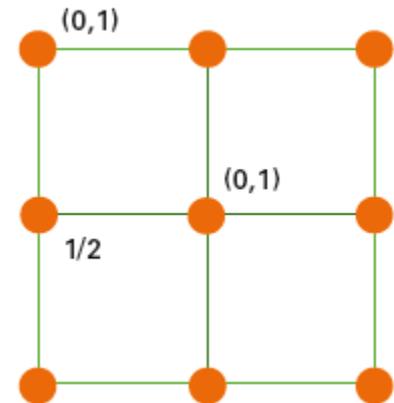
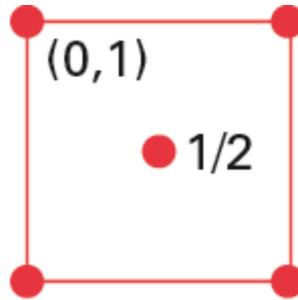
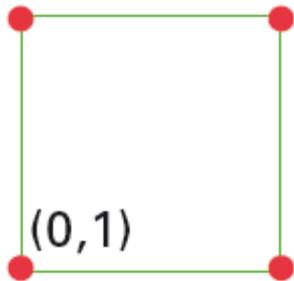
Cubica primitiva, P



Cubica a corpo  
centrato, I

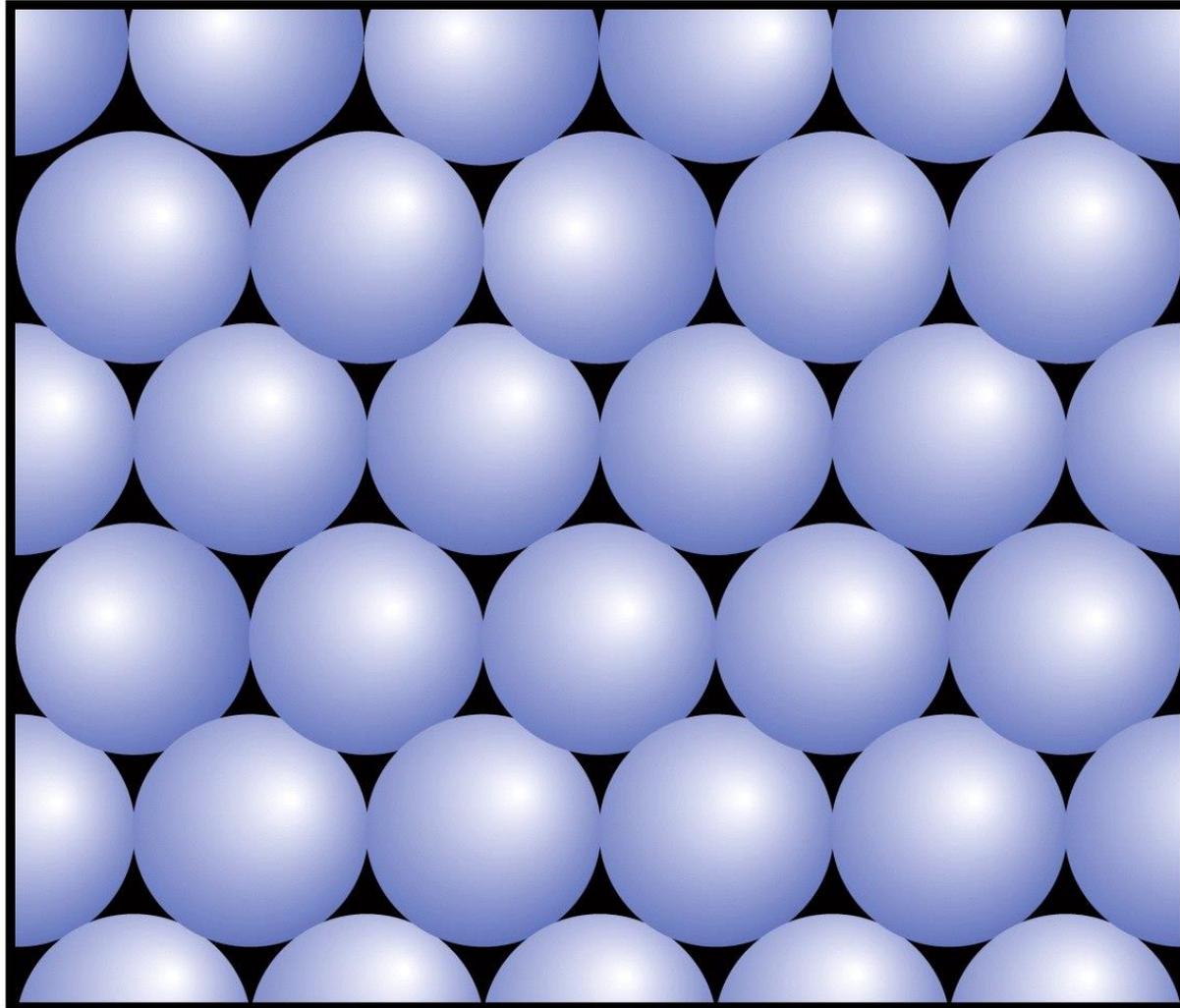


Cubica a facce  
centrate, F

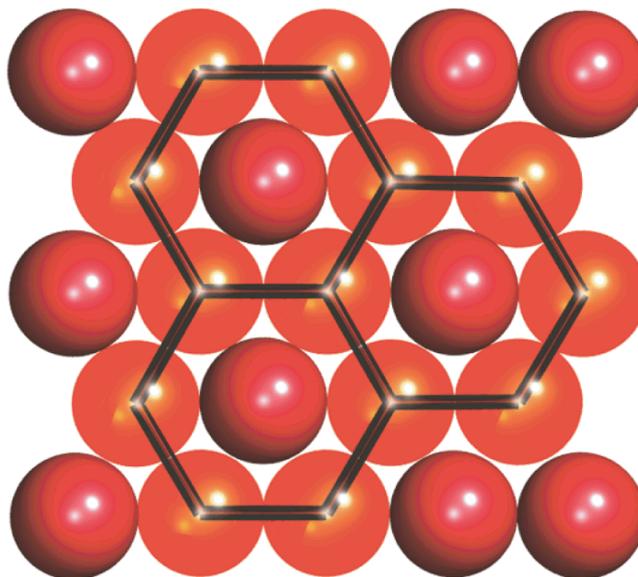


Coordinate frazionarie

# Impaccamento compatto di sfere rigide

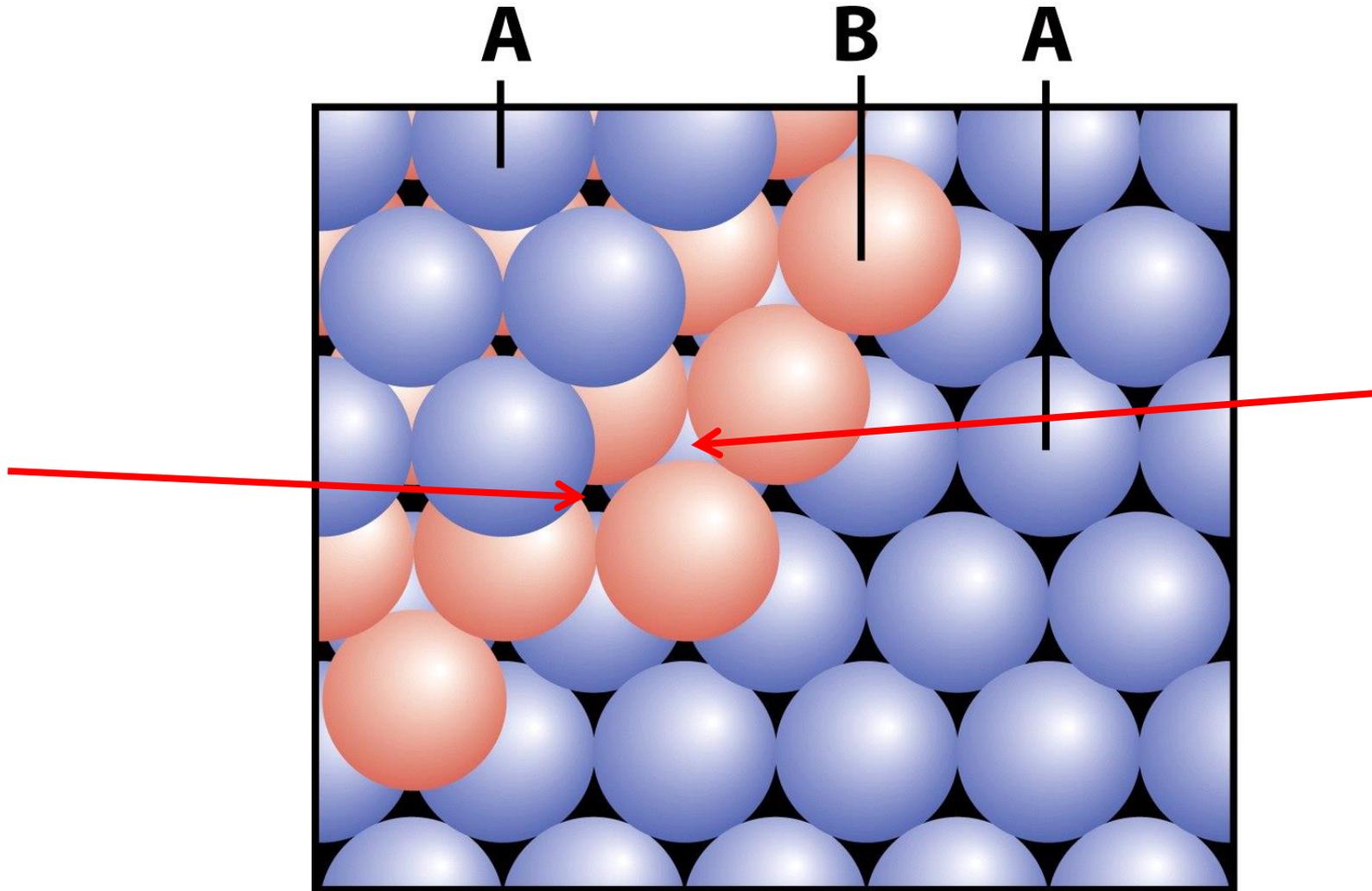


Strato di sfere a impaccamento compatto con evidenza  
la coordinazione esagonale



Politipi a impaccamento compatto: ABAB....

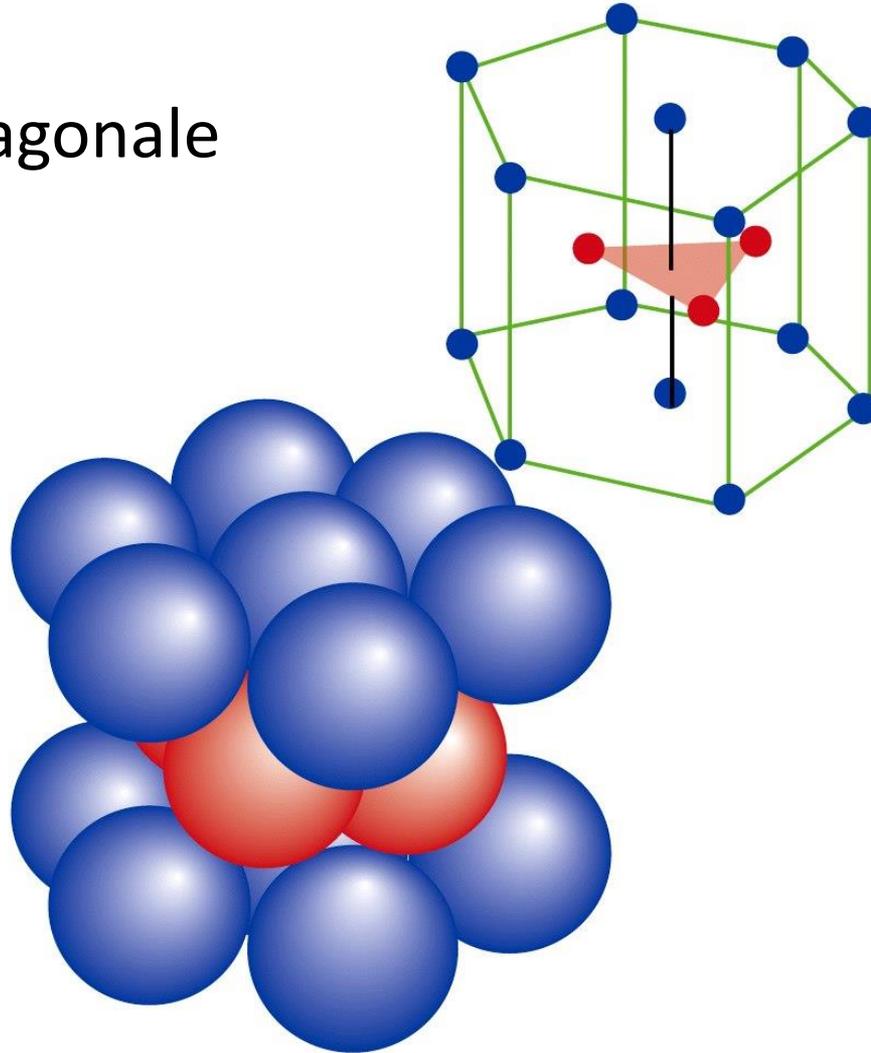
Esagonale compatto (*hcp*)



# Impaccamento esagonale compatto (*hcp*)

*hexagonally close packed*

Cella unitaria esagonale

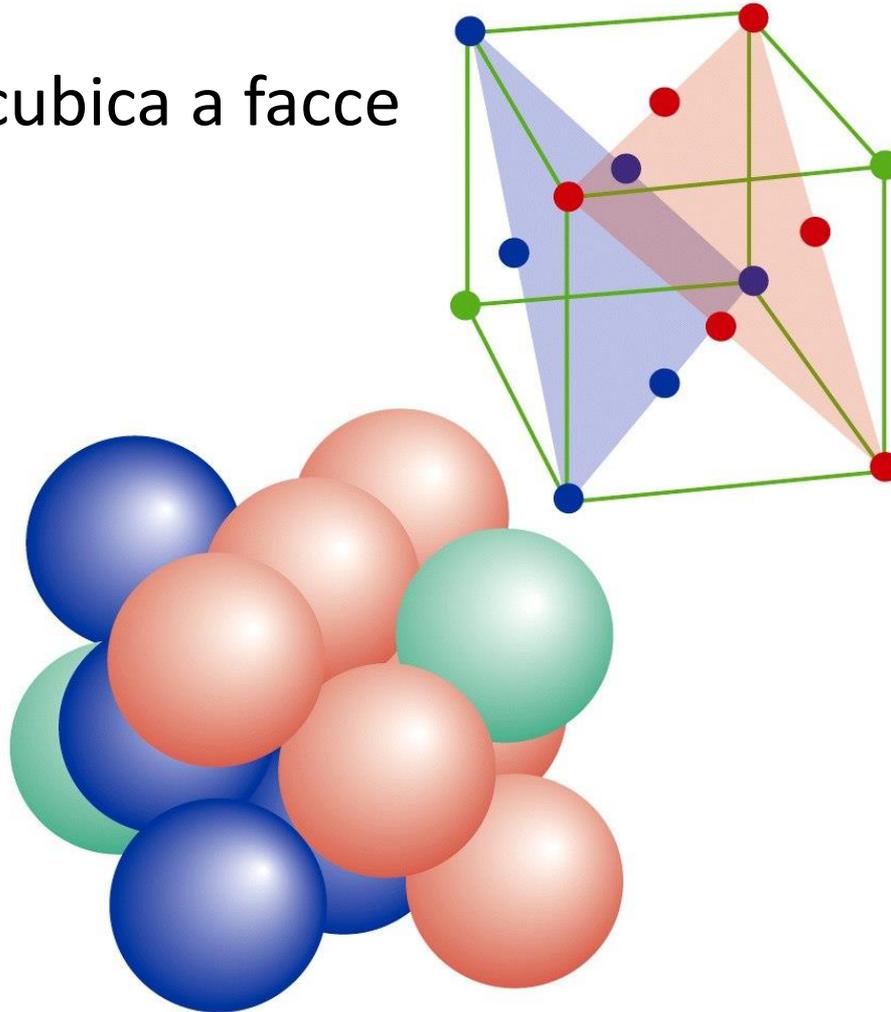




# Impaccamento cubico compatto (*ccp*)

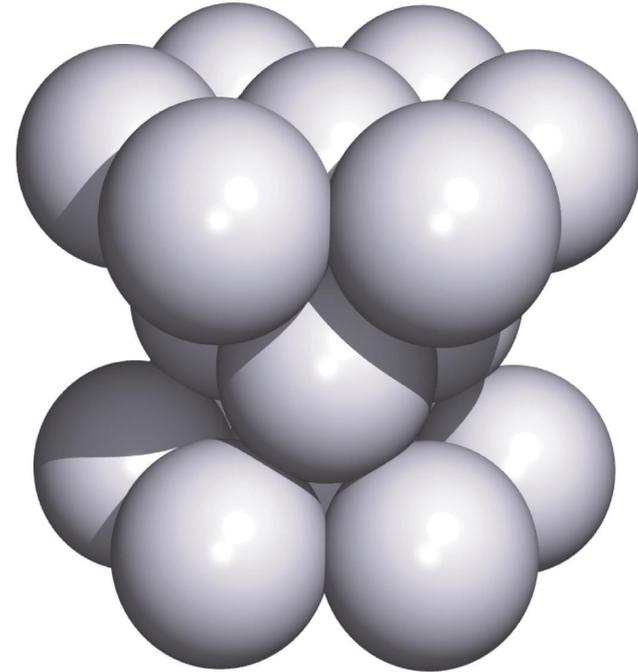
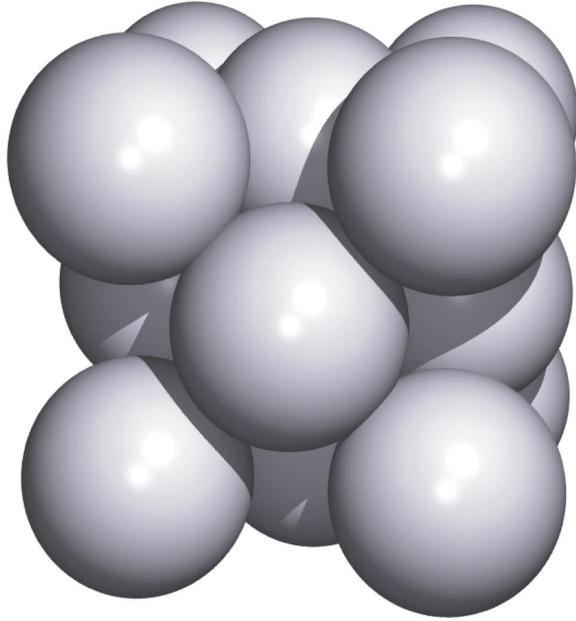
*cubic close packed*

Cella unitaria cubica a facce centrate (fcc)



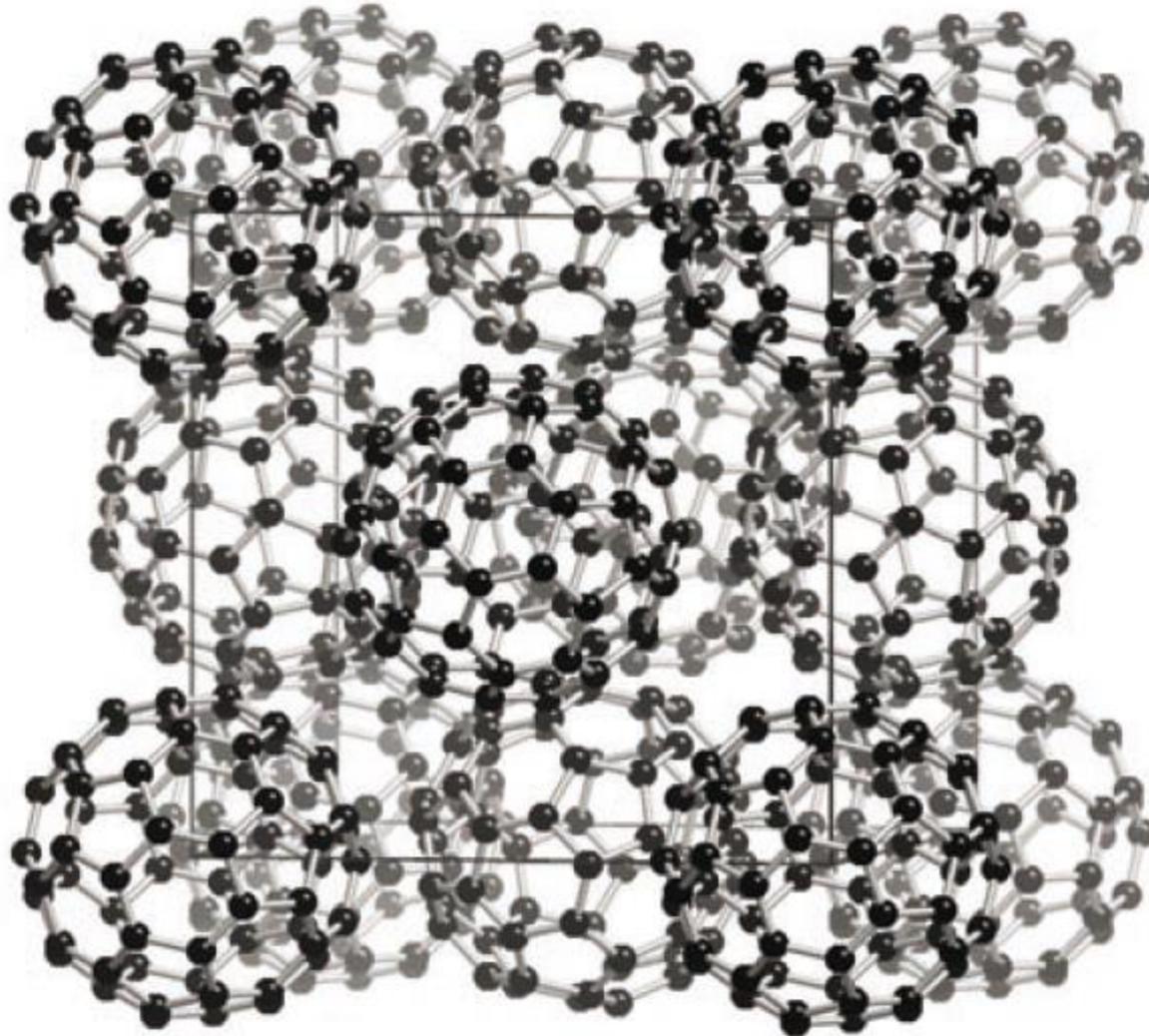
# Celle unitarie fcc e hcp a confronto

Numero di coordinazione 12

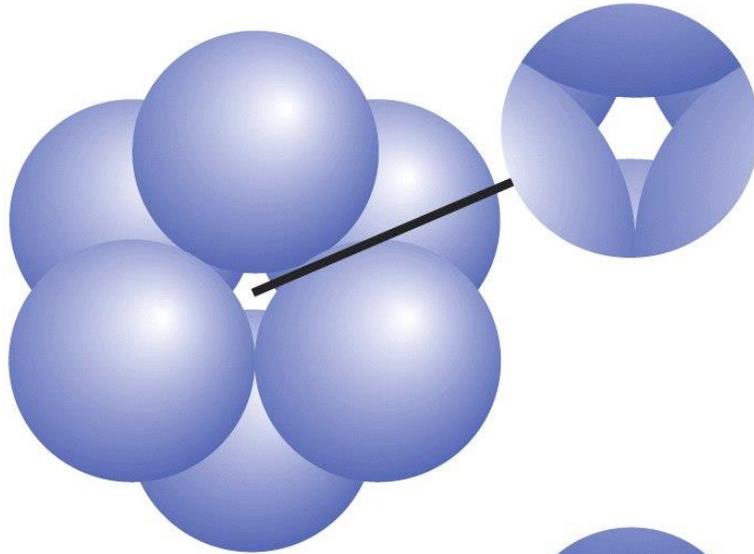


Spazio vuoto = 26%

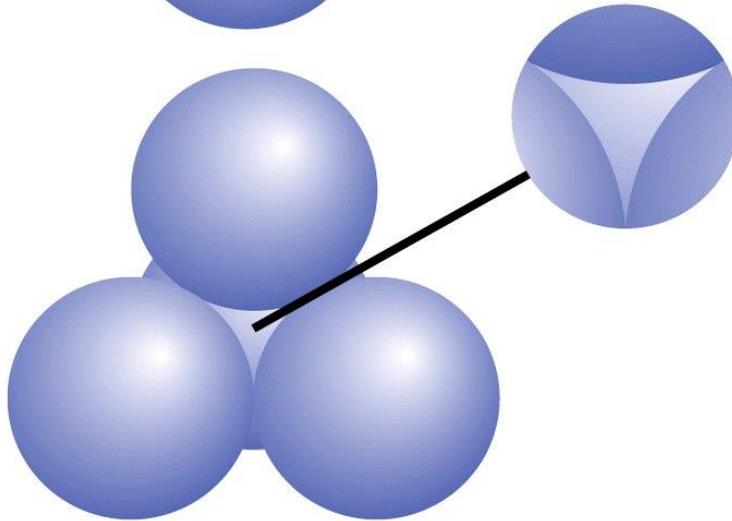
# Arrangiamento ccp di $C_{60}$



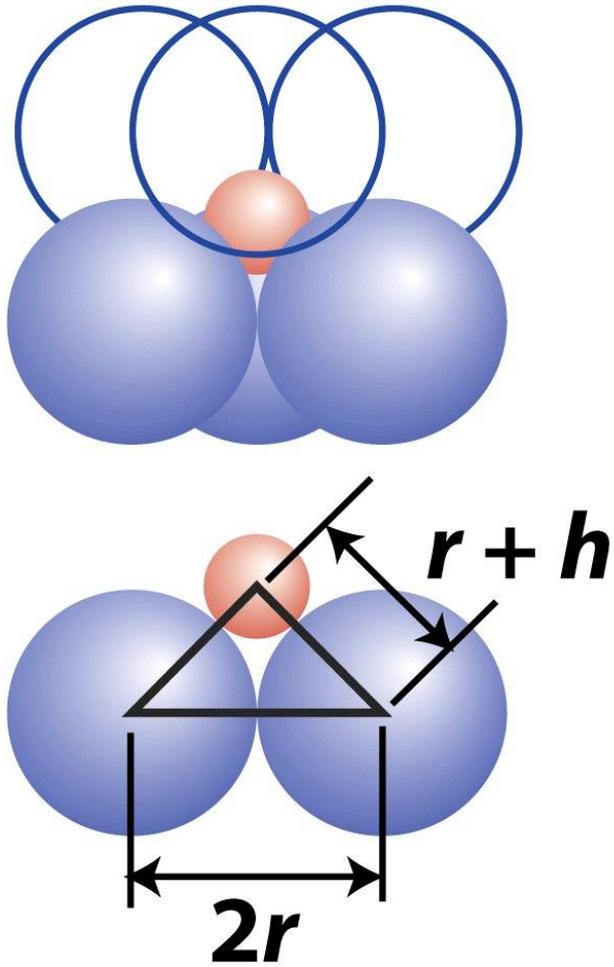
# Interstizi negli impaccamenti compatti



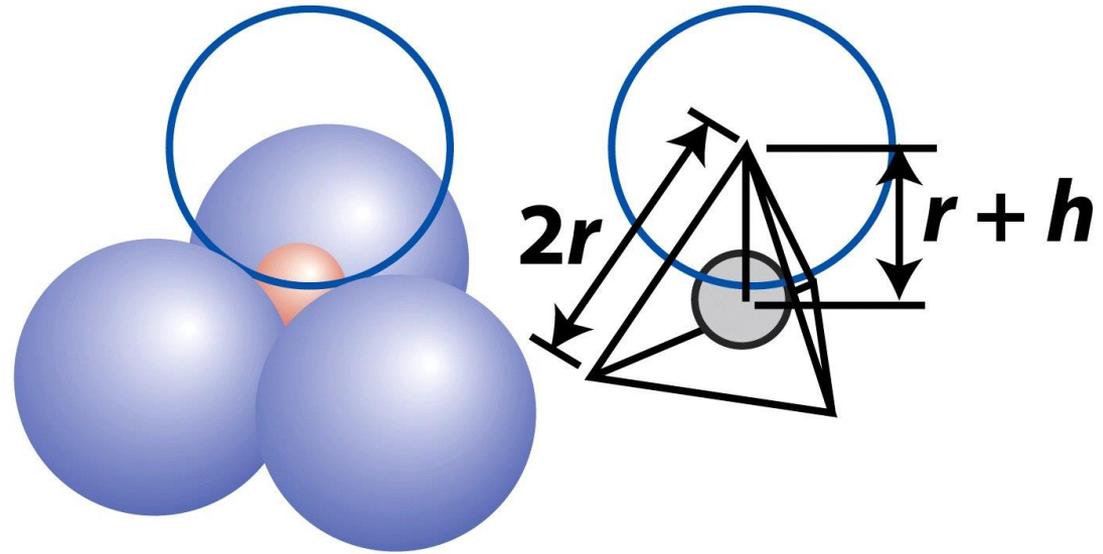
Interstizio ottaedrico  
 $r_h = 0.414r$



Interstizio tetraedrico  
 $r_h = 0.225r$

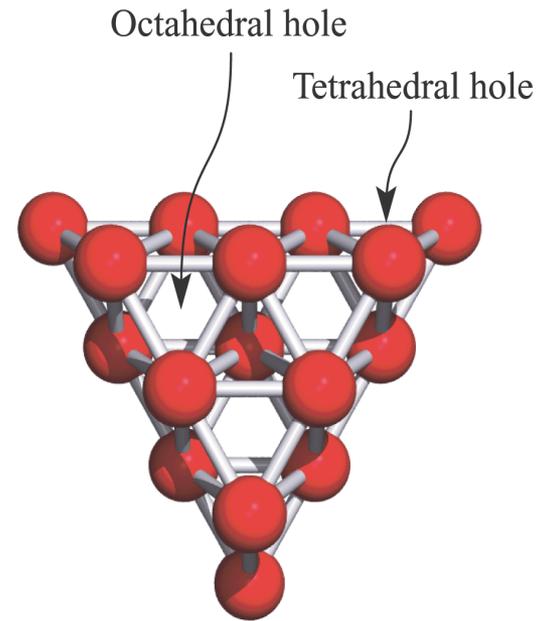
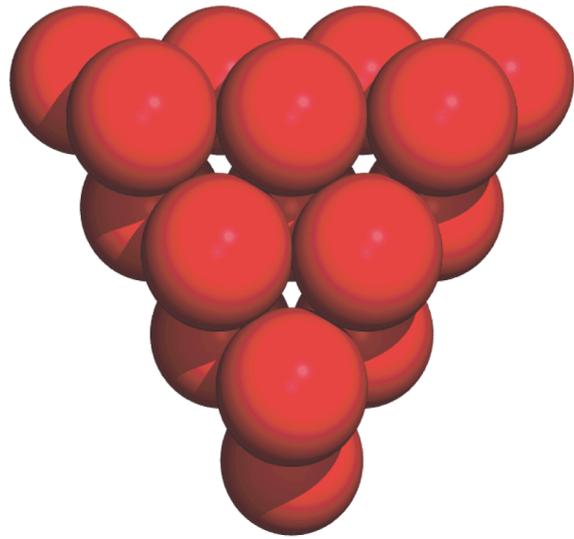


Interstizio ottaedrico  
 $r_h = 0.414r$

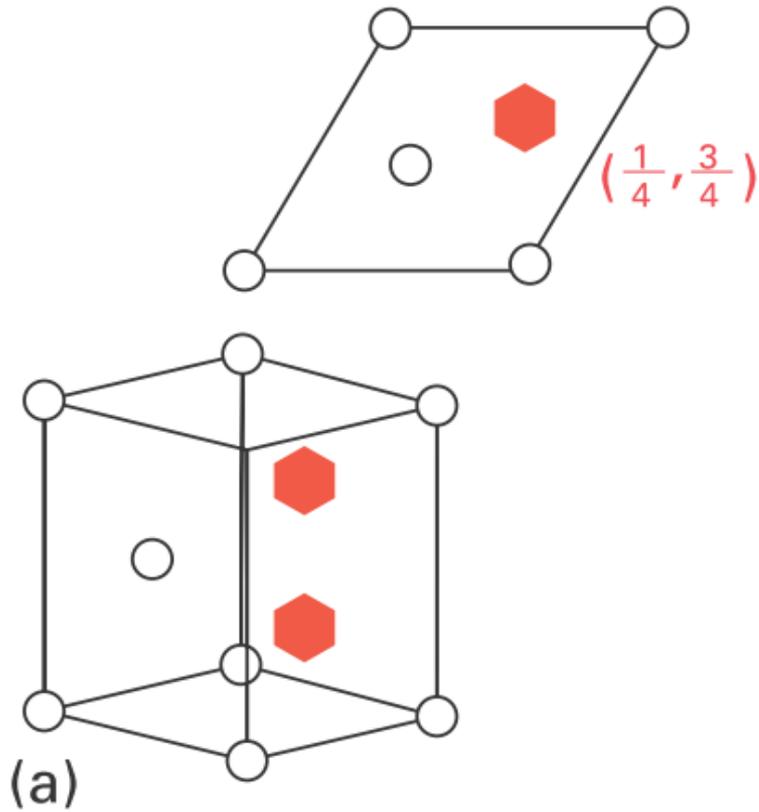


Interstizio tetraedrico  
 $r_h = 0.225r$

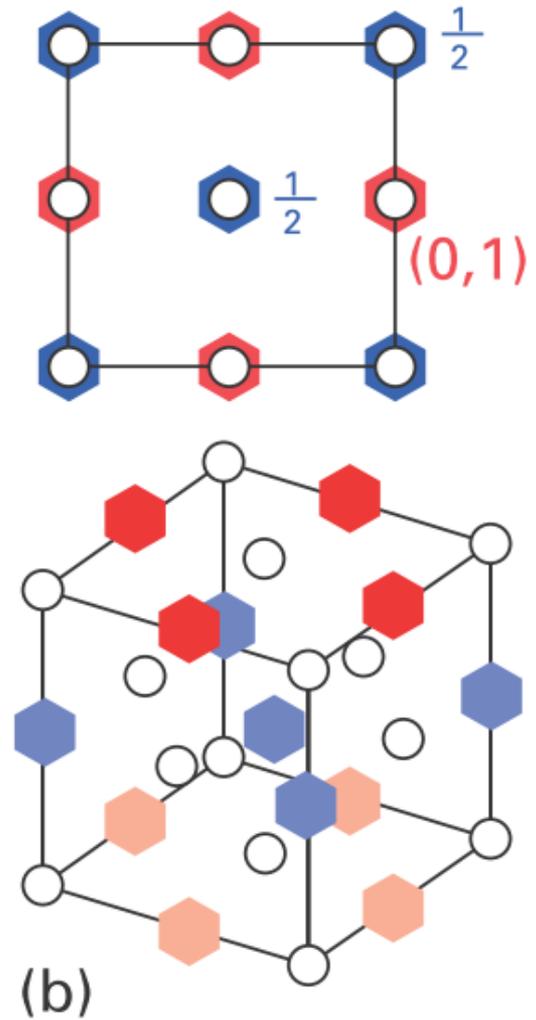
# Interstizi ottaedrici e tetraedrici



# Interstizi ottaedrici nelle strutture compatte

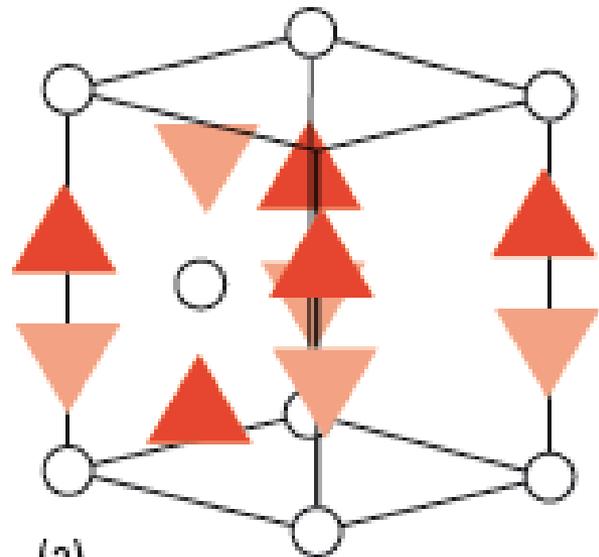
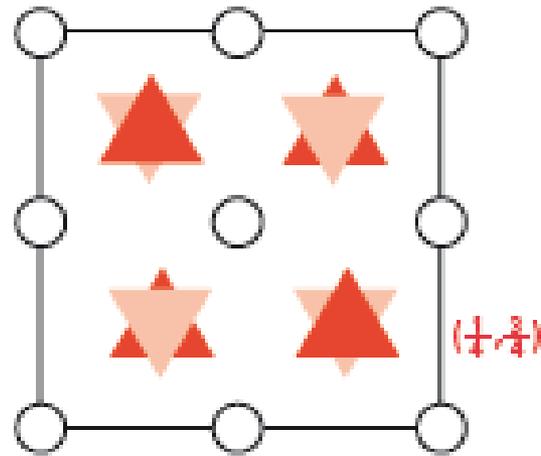
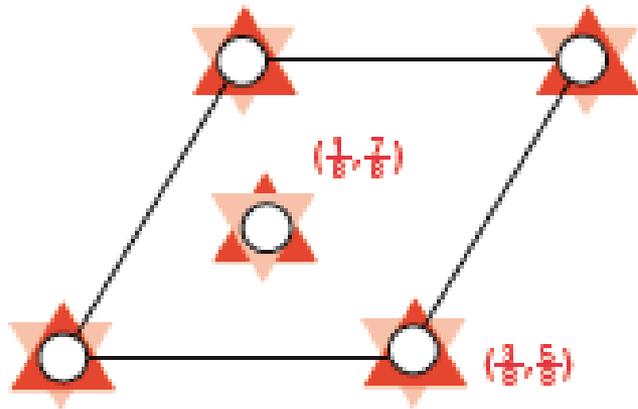


hcp



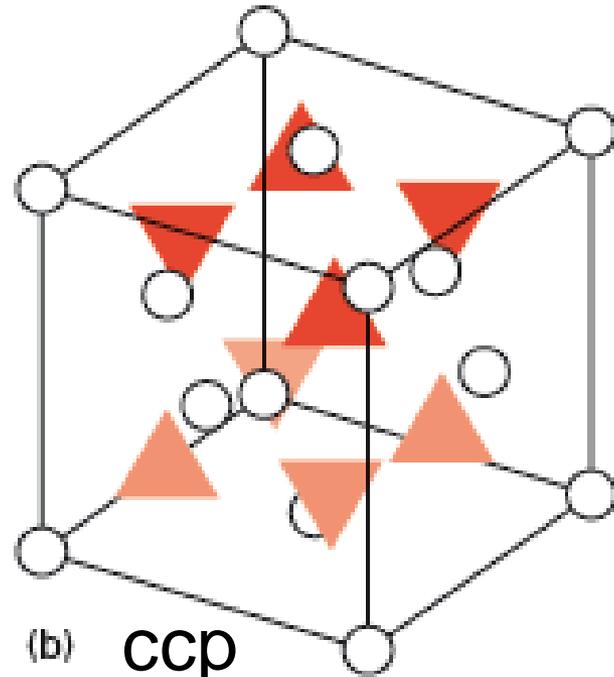
ccp

# Interstizi tetraedrici nelle strutture compatte



(a)

hcp



(b)

ccp

# Le strutture dei metalli

$$\rho_{\text{Os}} = 22,61 \text{ g cm}^{-3}$$

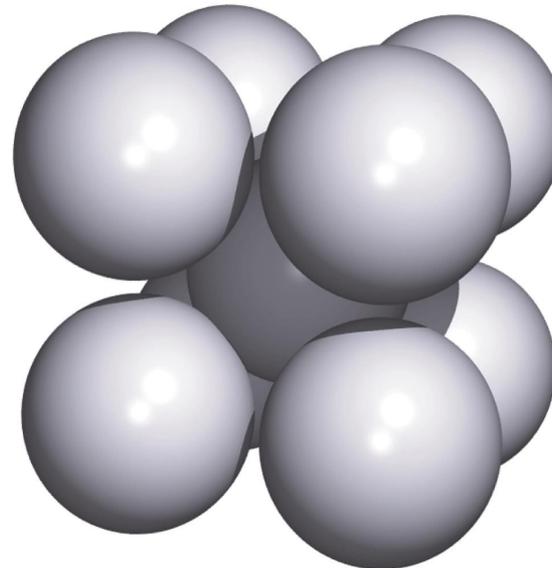
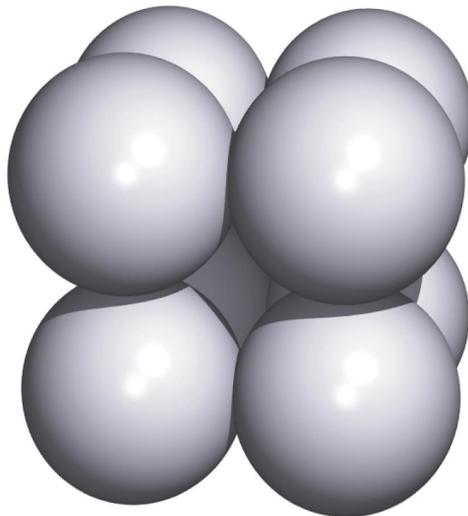
$$\rho_{\text{Pb}} = 11,3 \text{ g cm}^{-3}$$

Struttura cristallina	Elemento
Esagonale compatta (hcp)	Be, Ca, Co, Mg, Ti, Zn
Cubica compatta (ccp)	Ag, Al, Au, Cd, Cu, Ni, Pb, Pt
Cubica a corpo-centrato (bcc)	Ba, Cr, Fe, W, metalli alcalini
Cubica primitiva (cubica-P)	Po

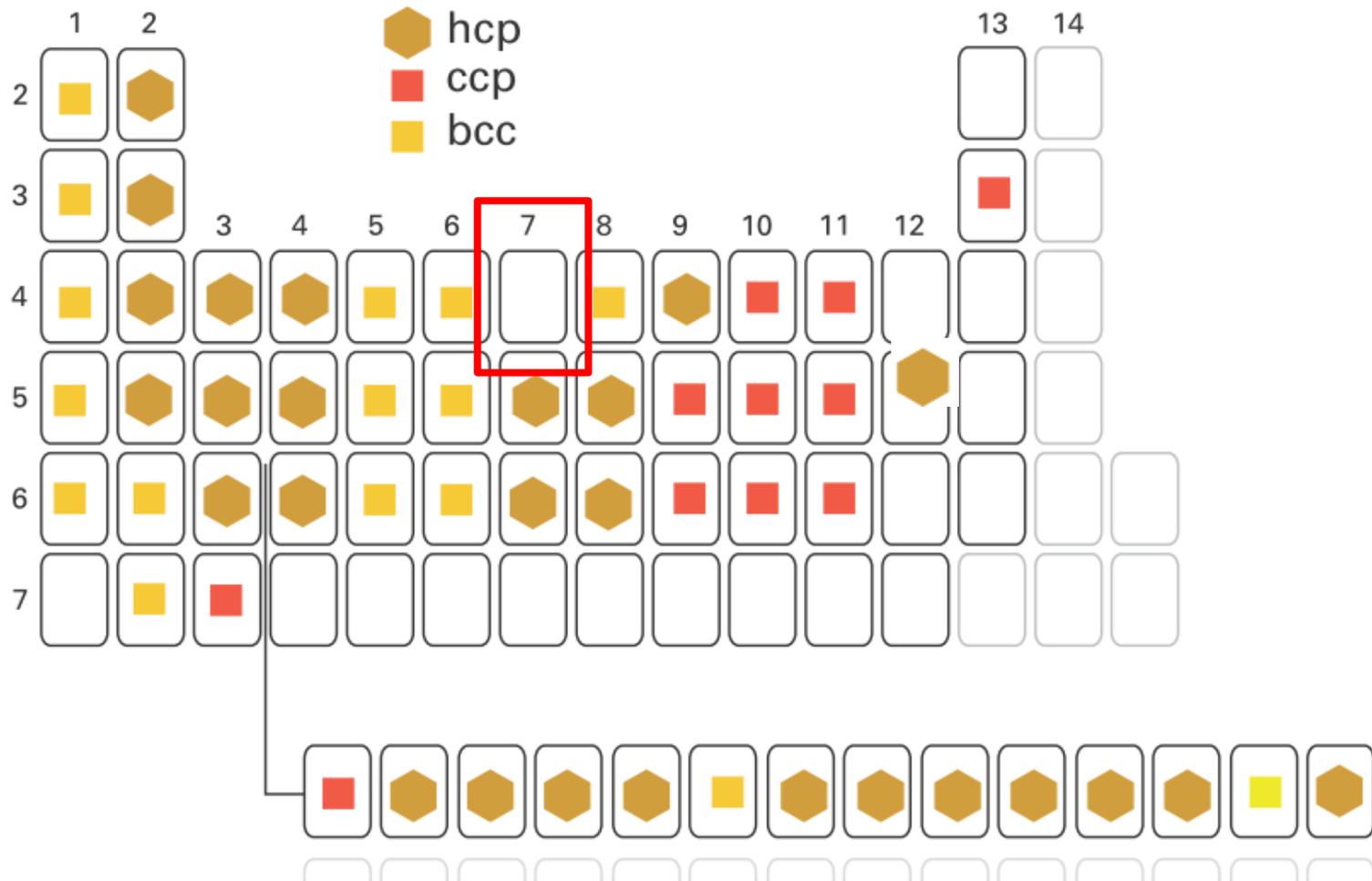
} 26% vuoto

32% vuoto

Cubica  
primitiva

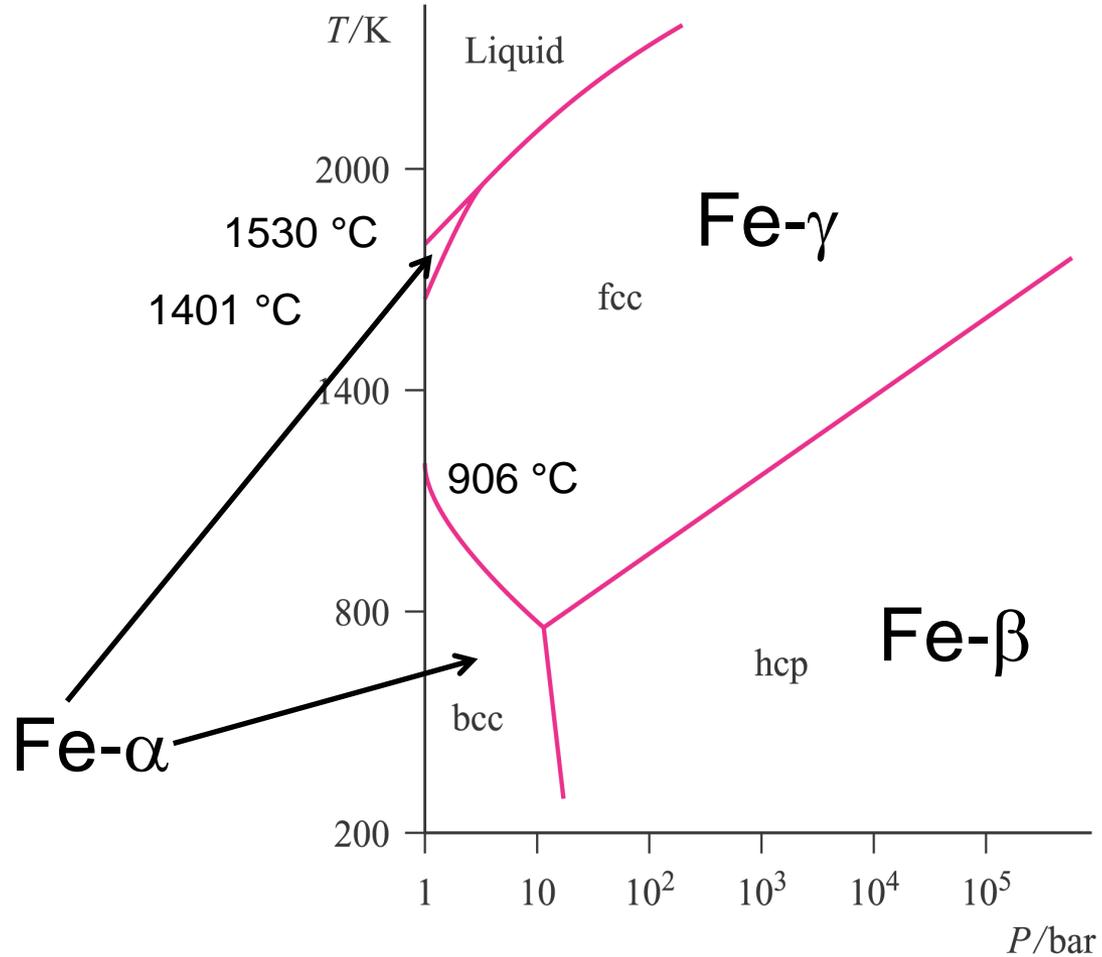


bcc



*Nel Mn gli atomi descrivono un complesso reticolo cubico nel quale ci sono quattro interni coordinativi, con numeri di coordinazione 12, 13 o 16*

# Allotropia (polimorfismo) del ferro



*Polimorfismo = la capacità di adottare forme cristalline diverse in condizioni di pressione e temperatura differenti*

# Allotropia dello stagno

*A 298 K e 1 bar di pressione, l'allotropo termodinamicamente stabile è lo stagno bianco ( $\beta$ -Sn), ma abbassando la temperatura a 286 K si ha la lenta transizione all'allotropo stagno grigio ( $\alpha$ -Sn). Alla transizione tra i due allotropi,  $\beta \rightarrow \alpha$ , corrisponde una variazione del numero di coordinazione da 6 a 4, e lo stagno grigio adotta un reticolo come quello del diamante. Di conseguenza nella transizione  $\beta \rightarrow \alpha$  la densità dello stagno diminuisce da 7.31 a 5.75 g·cm<sup>-3</sup> (mentre solitamente i polimorfi stabili a più basse temperature hanno una densità maggiore)*

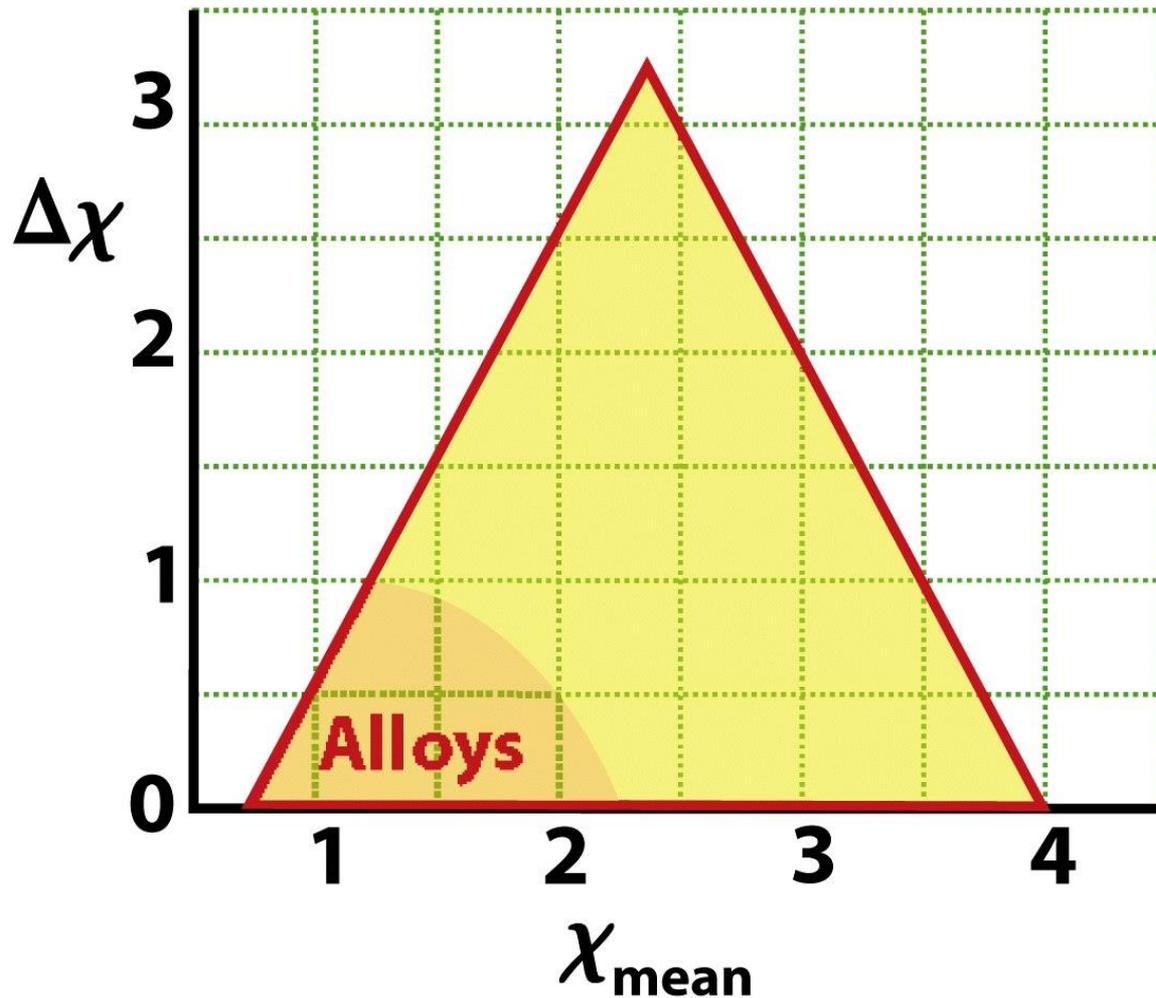
# Correzione di Goldschmidt dei raggi atomici

Numero di coordinazione	Raggio relativo
12	1
8	0,97
6	0,96
4	0,88

Correzione di Goldschmidt = raggio metallico (ipotetico) in una struttura a impaccamento compatto con coordinazione 12.

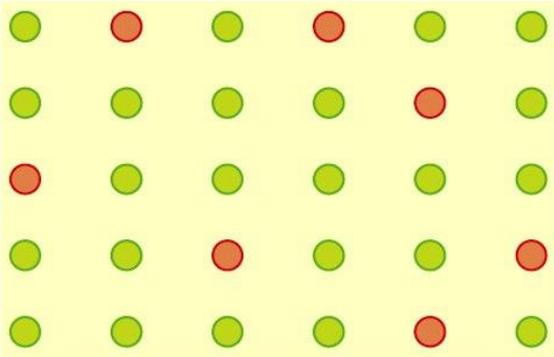
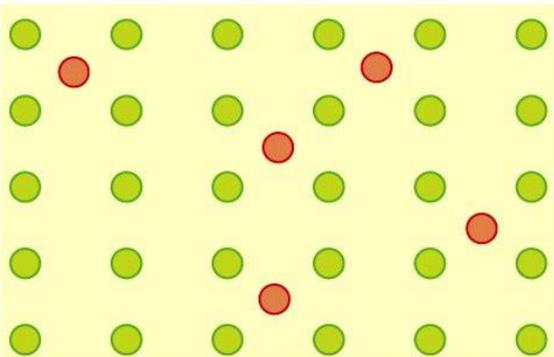
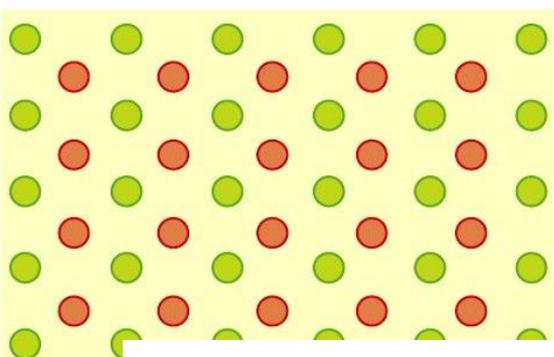
*Il raggio atomico empirico di Na è 185 pm per la struttura bcc, con numero di coordinazione 8. Per riportarlo alla coordinazione 12 si moltiplica questo raggio per  $1/0,97 = 1,03$  e si ottiene 191 pm.*

# Leghe metalliche



*La maggior parte delle leghe semplici può essere classificata come “sostituzionale” oppure come “interstiziale”*

# Leghe metalliche

- (a)  Soluzioni solide **sostituzionali**  
 $\Delta r < 15\%$   
(e.g. Cu/Ni, Cu/Sn/Pb (85/10/5, bronzo),  
 $\text{Cu}_{1-x}/\text{Zn}_x$ ,  $0 < x < 0.38$  (ottoni  $\alpha$ ), acciai inox)
- (b)  Soluzioni solide **interstiziali** (con nonmetalli) o composti non-stechiometrici  
 $r < 0.414R$   
e.g. Fe/C (acciai al carbonio,  $0.2 < \text{C}\% < 1.6$ )
- (c)  Composti interstiziali  
 $r < 0.414R$   
e.g. WC

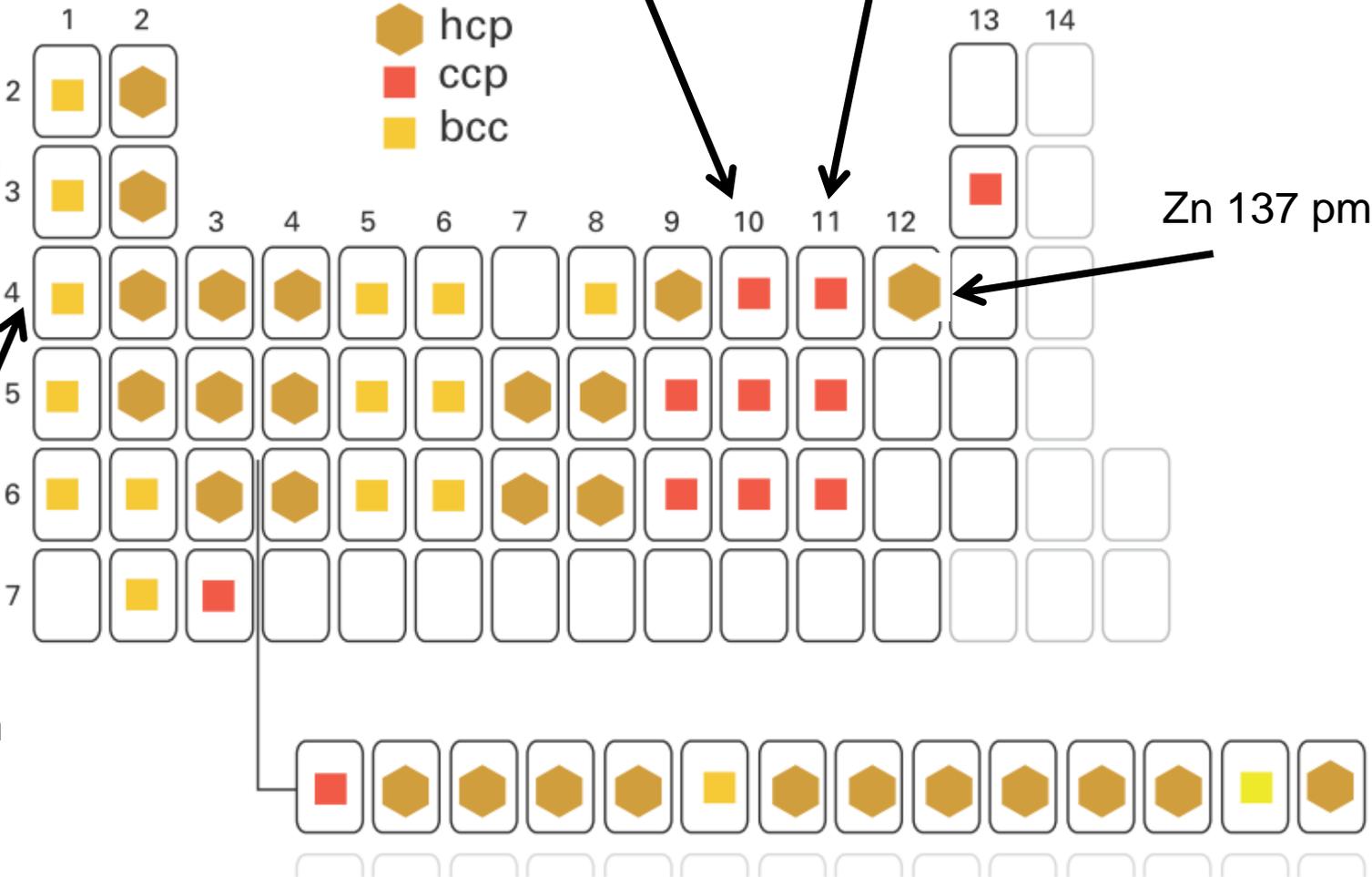
Na 191 pm

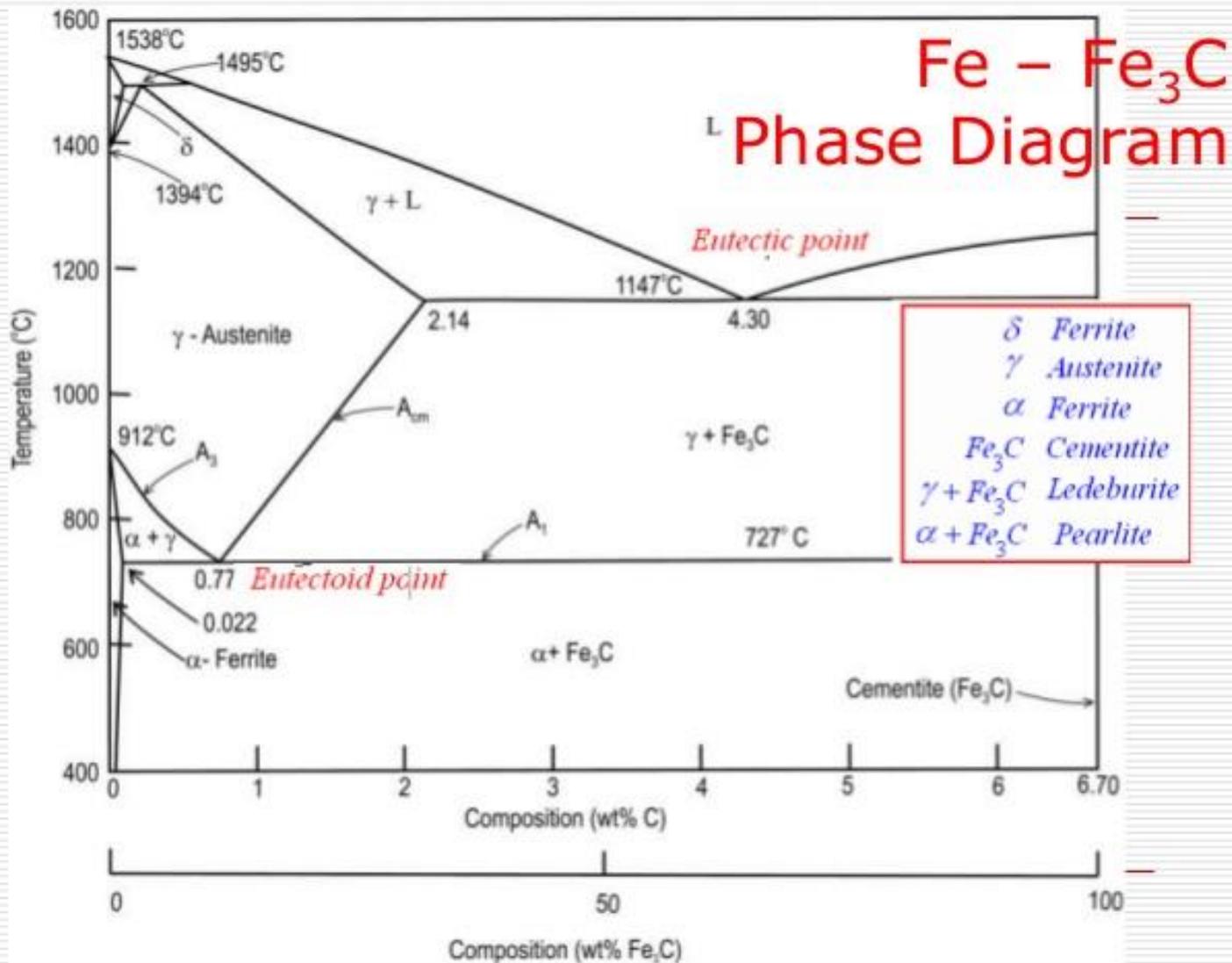
Ni 125 pm, Cu 128 pm

Zn 137 pm

K 235 pm

 hcp  
 ccp  
 bcc



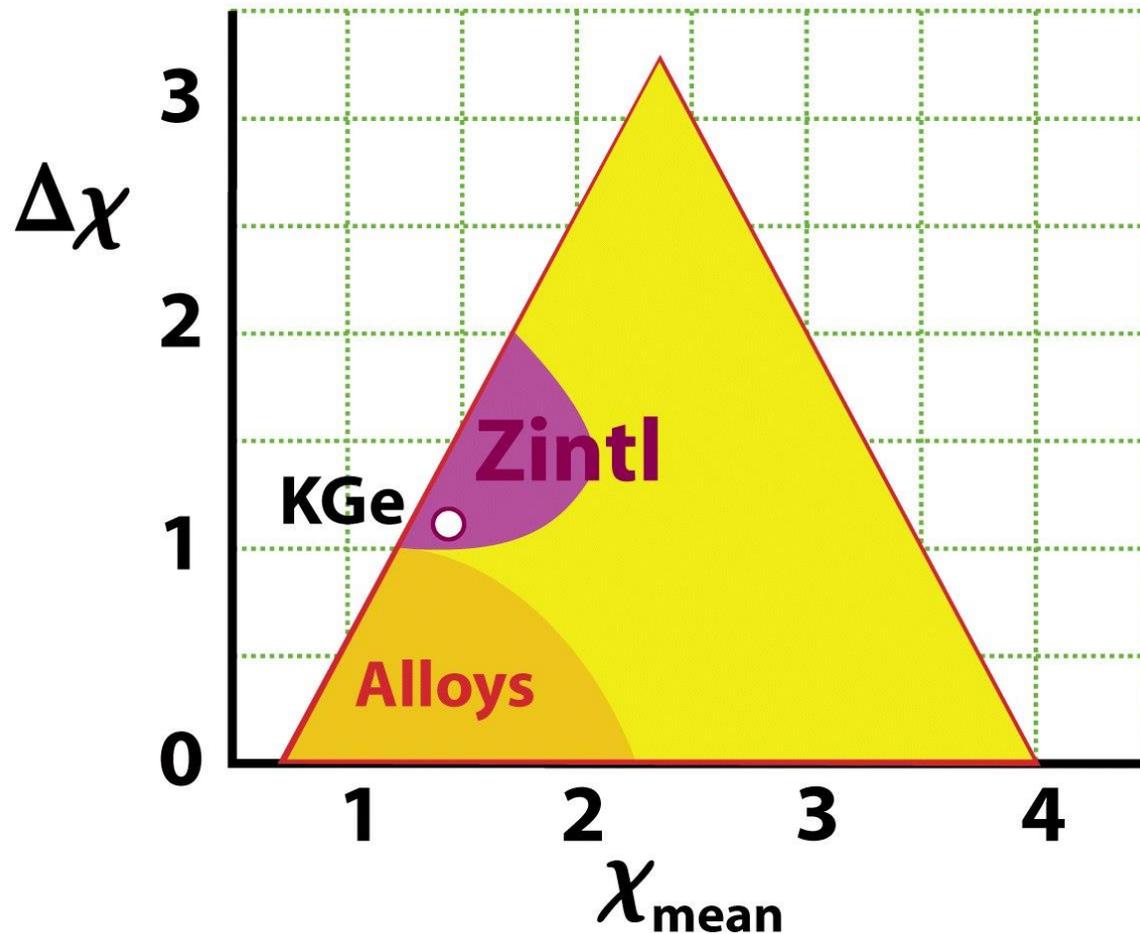


*Nelle soluzioni solide interstiziali la struttura cristallina originale del metallo viene mantenuta*

# Composti intermetallici e *fasi di Zintl*

*ottone- $\beta$  (CuZn), alnico, LaNi<sub>5</sub>, Nitinol, MgZn<sub>2</sub>, Cu<sub>3</sub>Au, NaTl, Na<sub>5</sub>Zn<sub>21</sub>*

*La struttura è diversa da quella di entrambi i componenti metallici*



# Struttura della *fase di Zintl* $K_4Ge_4$

