

# Mineral Physics Lectures Overview:

1. Overview of Earth Materials (L)
2. Deep Earth Mineralogy (A)
3. Thermodynamics (L)
4. Elasticity (A)
5. Lattice Dynamics (L)
6. Transport Properties (A)
7. Ab Initio Methods (L)
8. Experimental Challenges (A)
9. “building a planet” (L&A)

# Earth Mineralogy:

1. ions and radii
2. X-ray diffraction review
3. Pauling's rules
4. Pressure trends
5. Earth mineralogy
6. Post-perovskite phase transformation?

The Periodic Table of the Elements is shown with several groups highlighted by green circles:

- Group 1 (IA):** Hydrogen (H) is circled in green.
- Group 2 (IIA):** Lithium (Li) and Beryllium (Be) are circled in green.
- Group 13 (IIIA):** Boron (B) is circled in green.
- Group 14 (IVA):** Carbon (C) and Silicon (Si) are circled in green.
- Group 15 (VA):** Nitrogen (N) and Phosphorus (P) are circled in green.
- Group 16 (VIA):** Oxygen (O) and Sulfur (S) are circled in green.
- Group 17 (VIIA):** Fluorine (F) and Chlorine (Cl) are circled in green.
- Group 18 (0):** Helium (He) is circled in green.
- Group 13 (IIIA):** Aluminum (Al) is circled in purple.
- Group 14 (IVA):** Tin (Sn) and Lead (Pb) are circled in green.
- Group 15 (VA):** Antimony (Sb) and Tellurium (Te) are circled in green.
- Group 16 (VIA):** Selenium (Se) and Tellurium (Te) are circled in green.
- Group 17 (VIIA):** Bromine (Br) and Iodine (I) are circled in green.
- Group 18 (0):** Xenon (Xe) is circled in green.

\* Lanthanide Series

58	59	60	61	62	63	64	65	66	67	68	69	70	71
Ce	Pr	Hd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
90	91	92	93	94	95	96	97	98	99	100	101	102	103
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

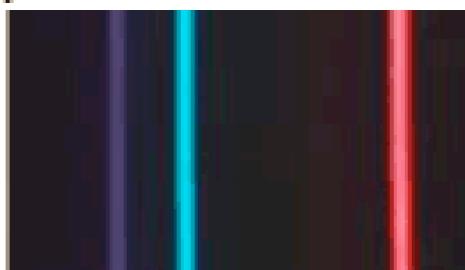
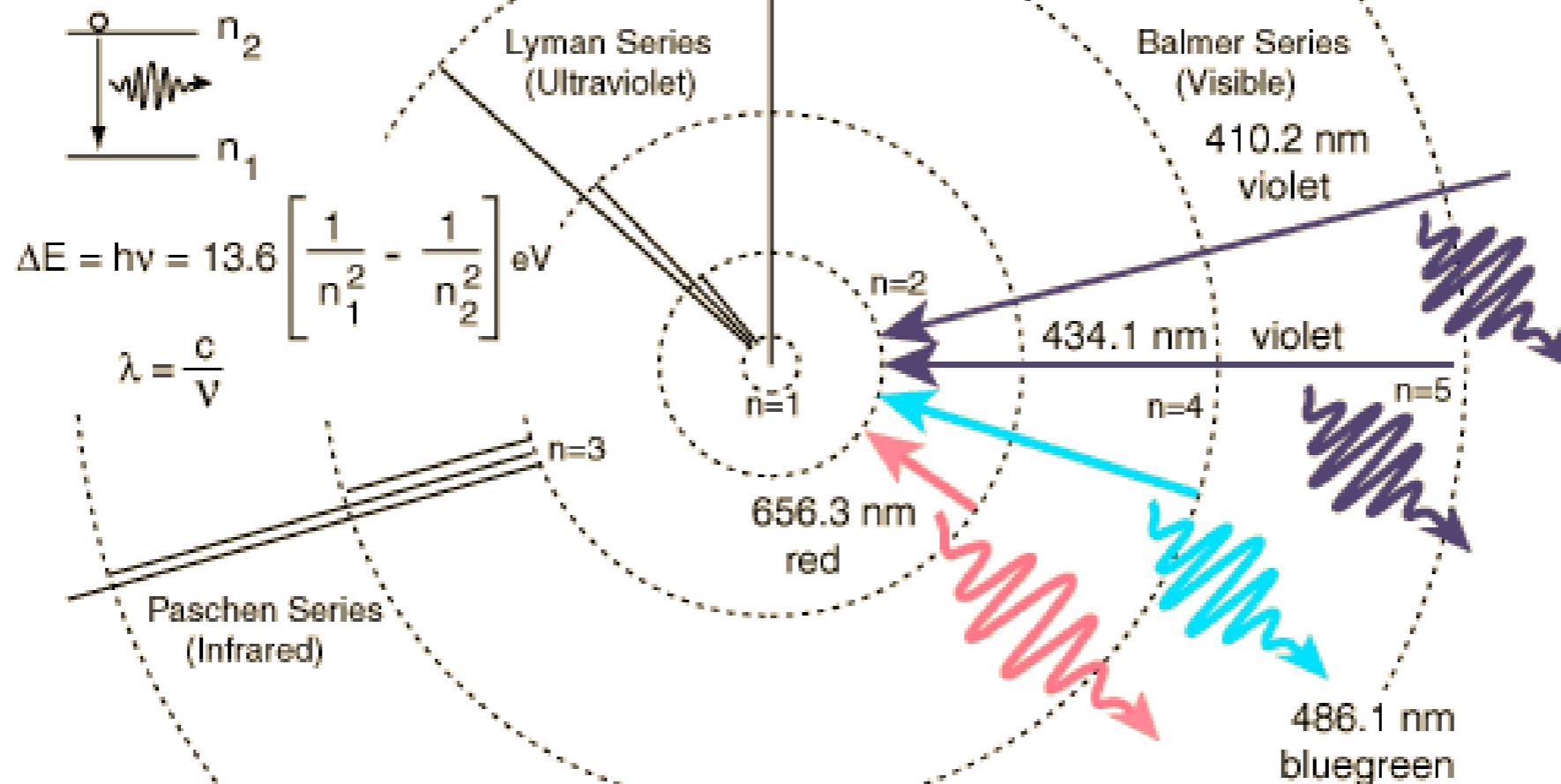
today: Fe in core/ O, Si, Mg in mantle

Al--elasticity lecture

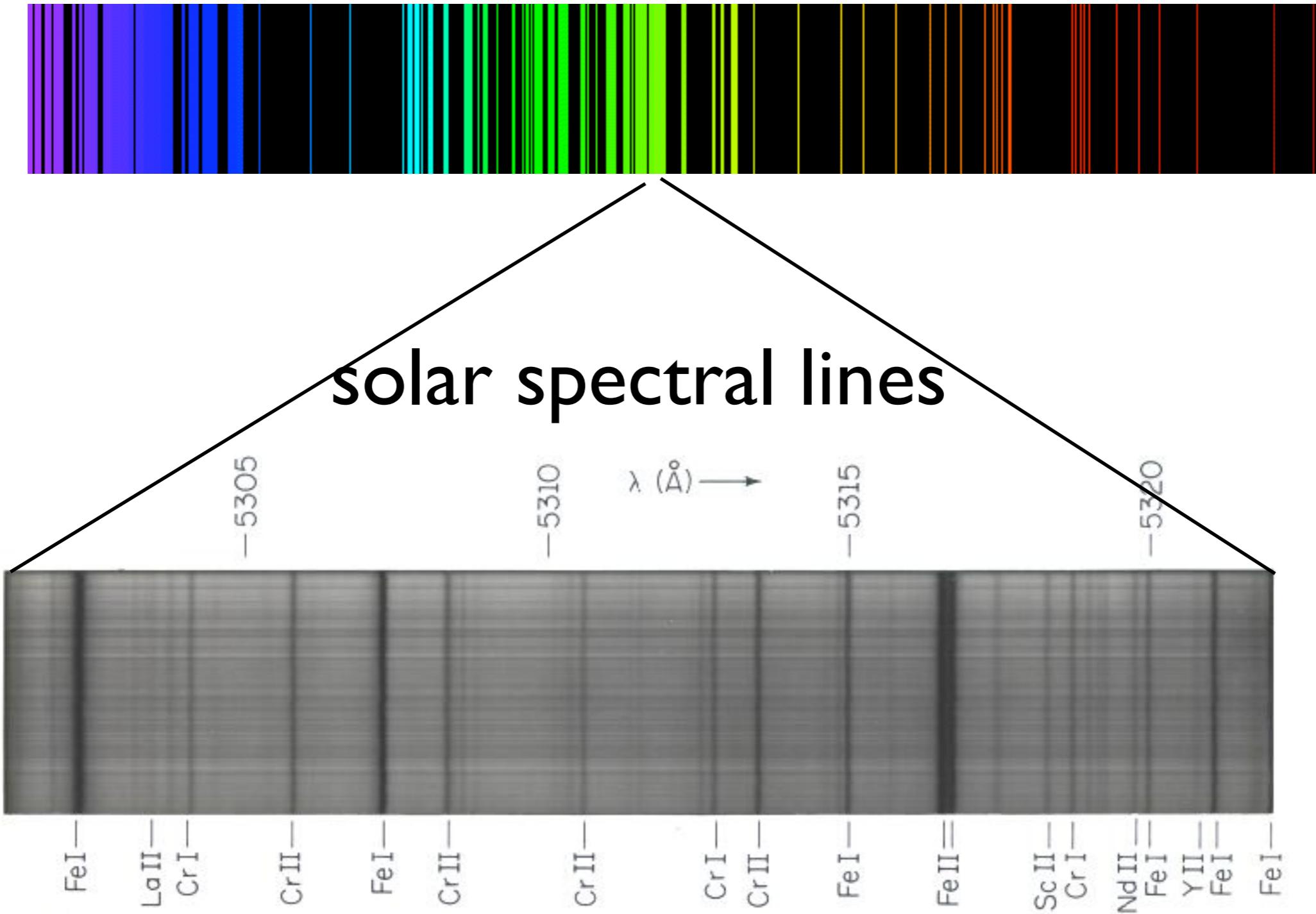
H--rheology (transport) lecture

# hydrogen spectrum

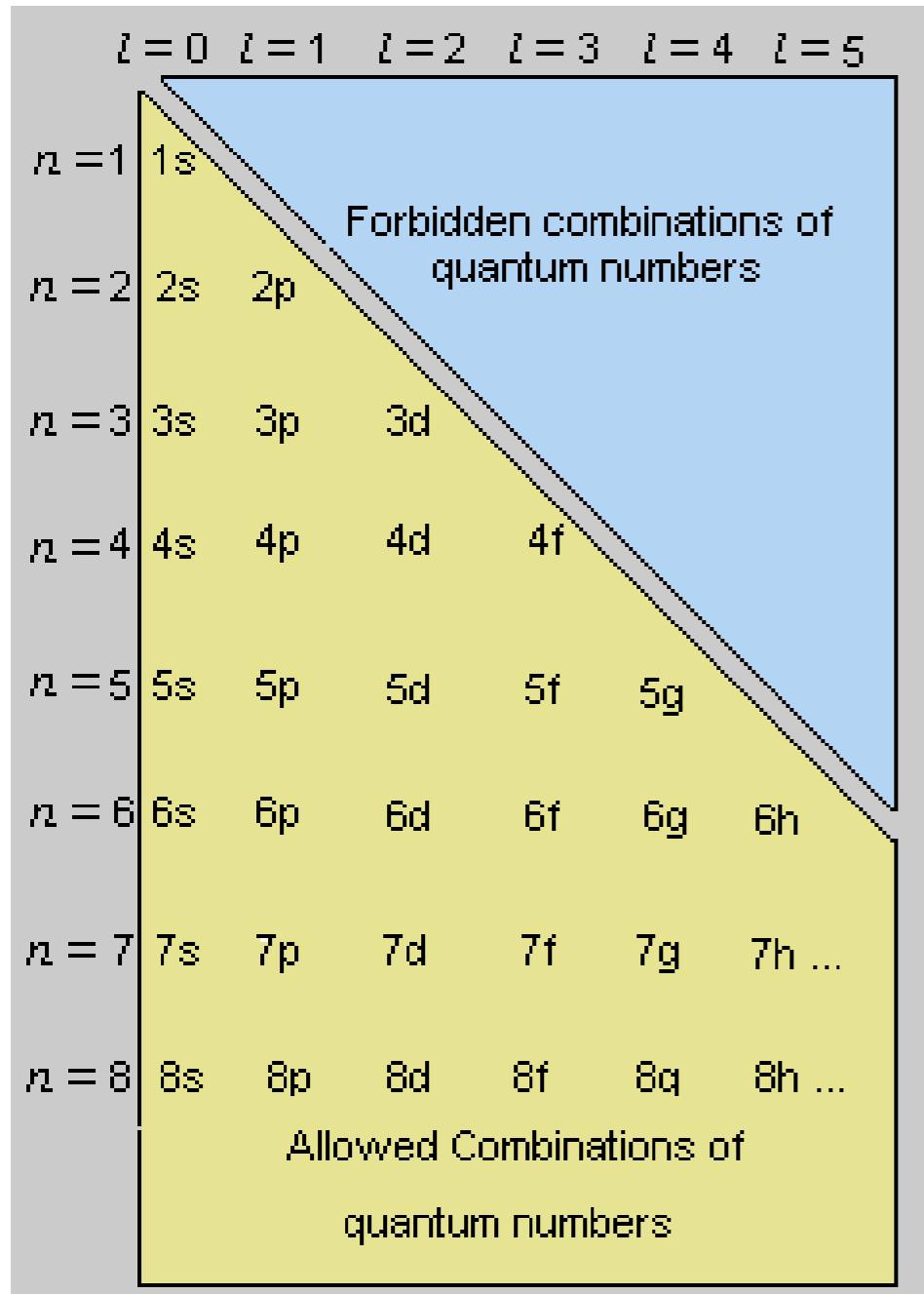
**From Bohr model:**



# emission spectra of Fe

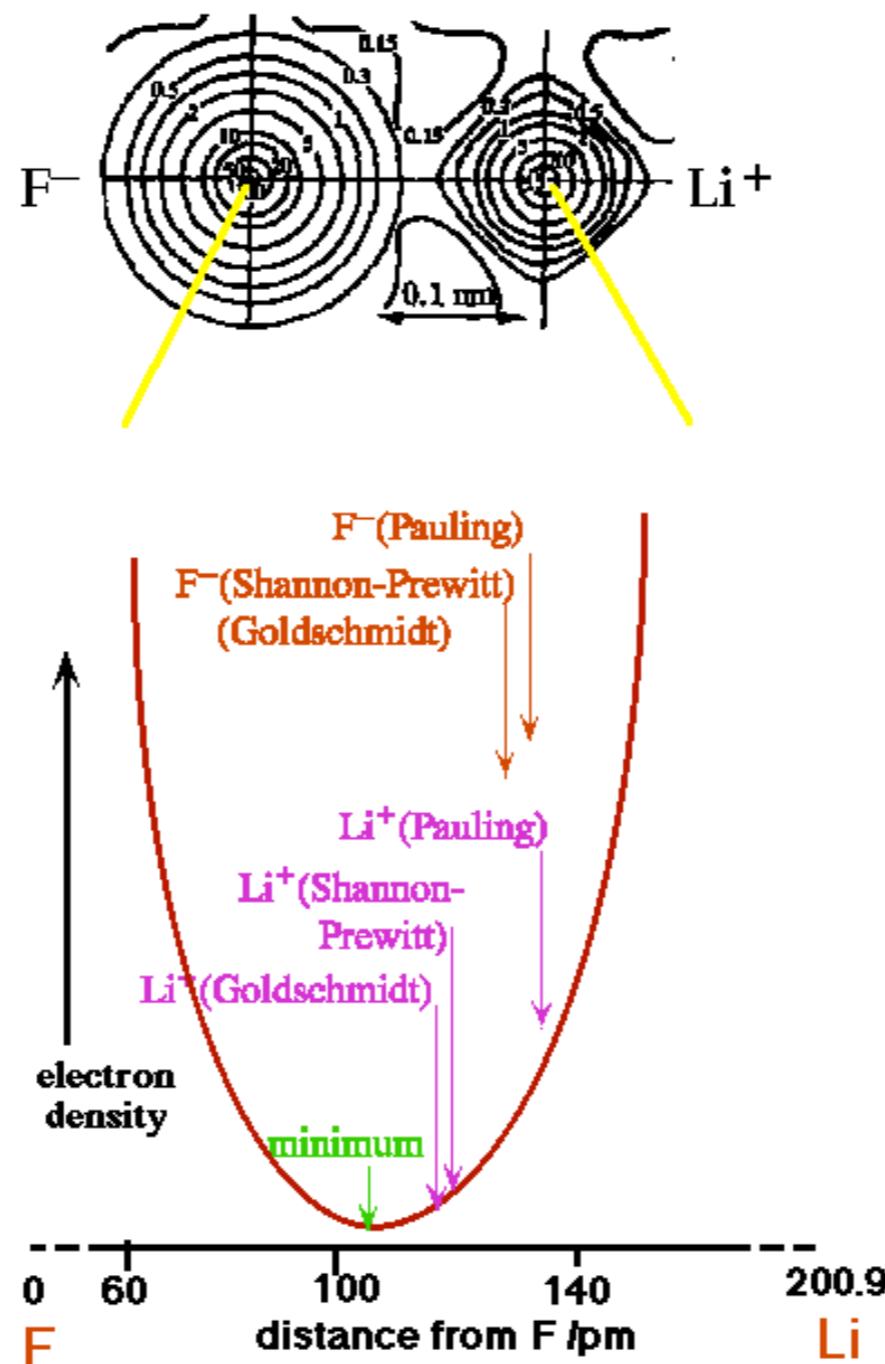


# electronic structure: hund's rules



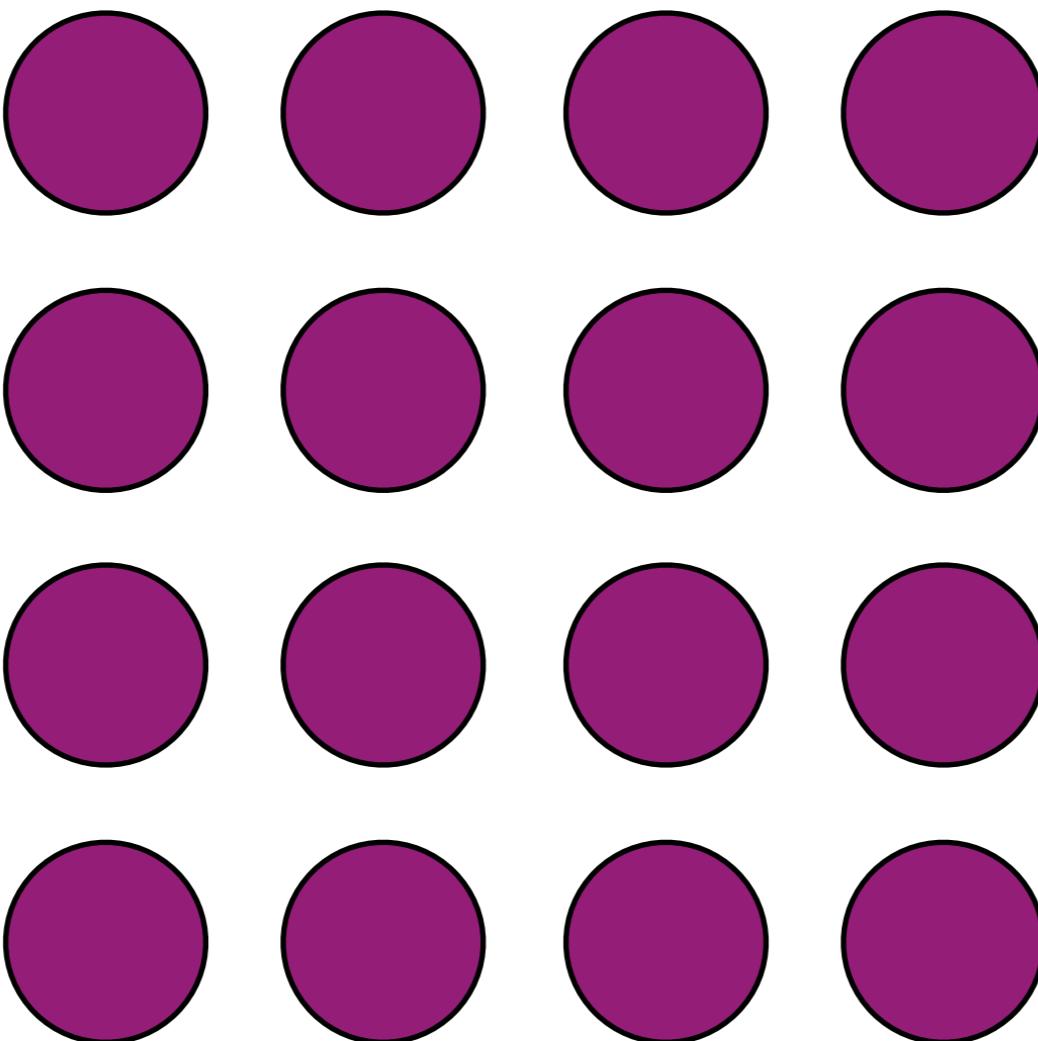
element	electron configuration	ionic radius
O	$1s^2 2s^2 2p^4$	
Si	$1s^2 2s^2 2p^6 3s^2 3p^2$	
Mg	$1s^2 2s^2 2p^6 3s^2$	
Fe*	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$	

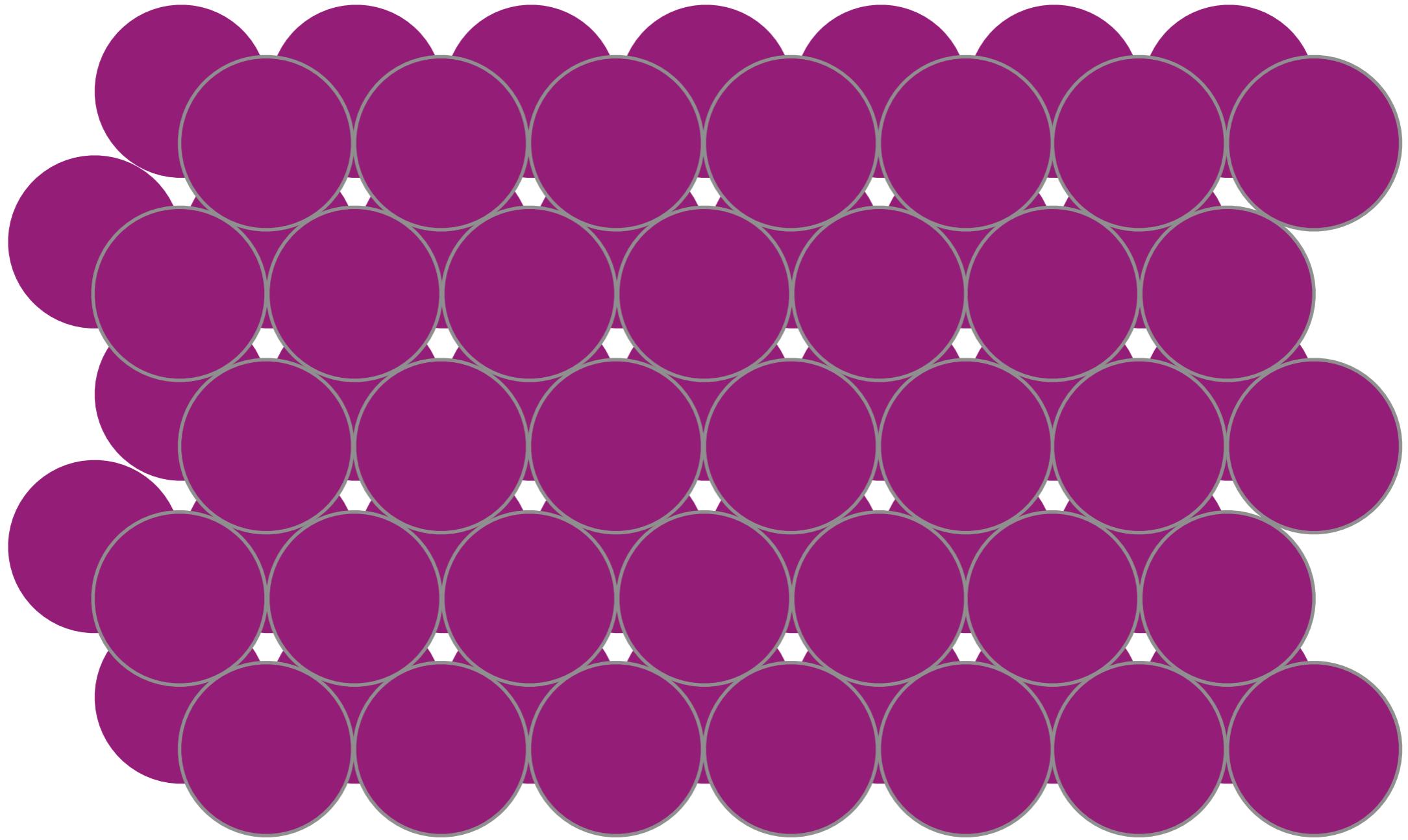
# how are ionic radii determined?



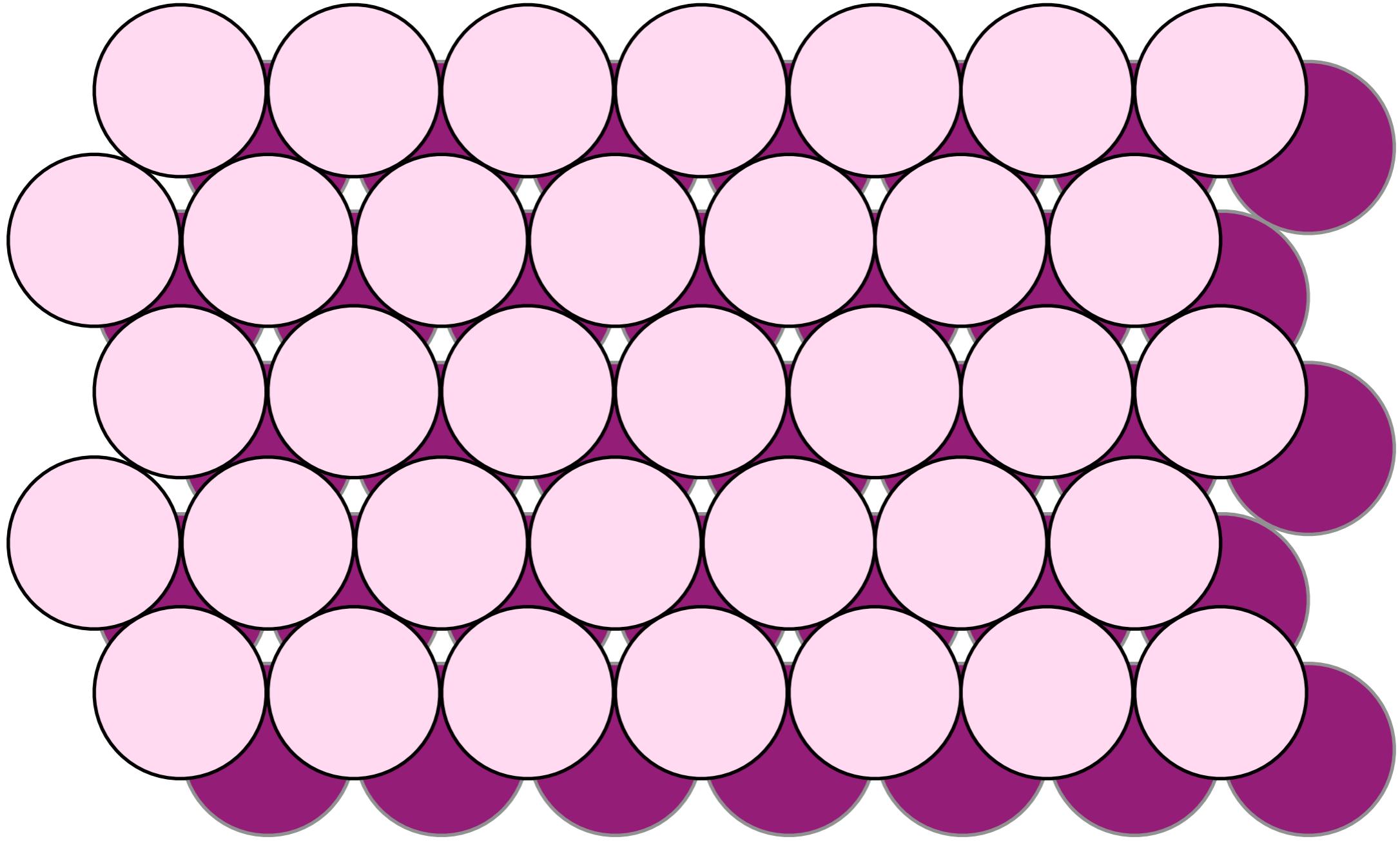
# Goldschmidt & Pauling rules for creating structures:

- I. geometric considerations
2. charge neutrality
3. Other effects



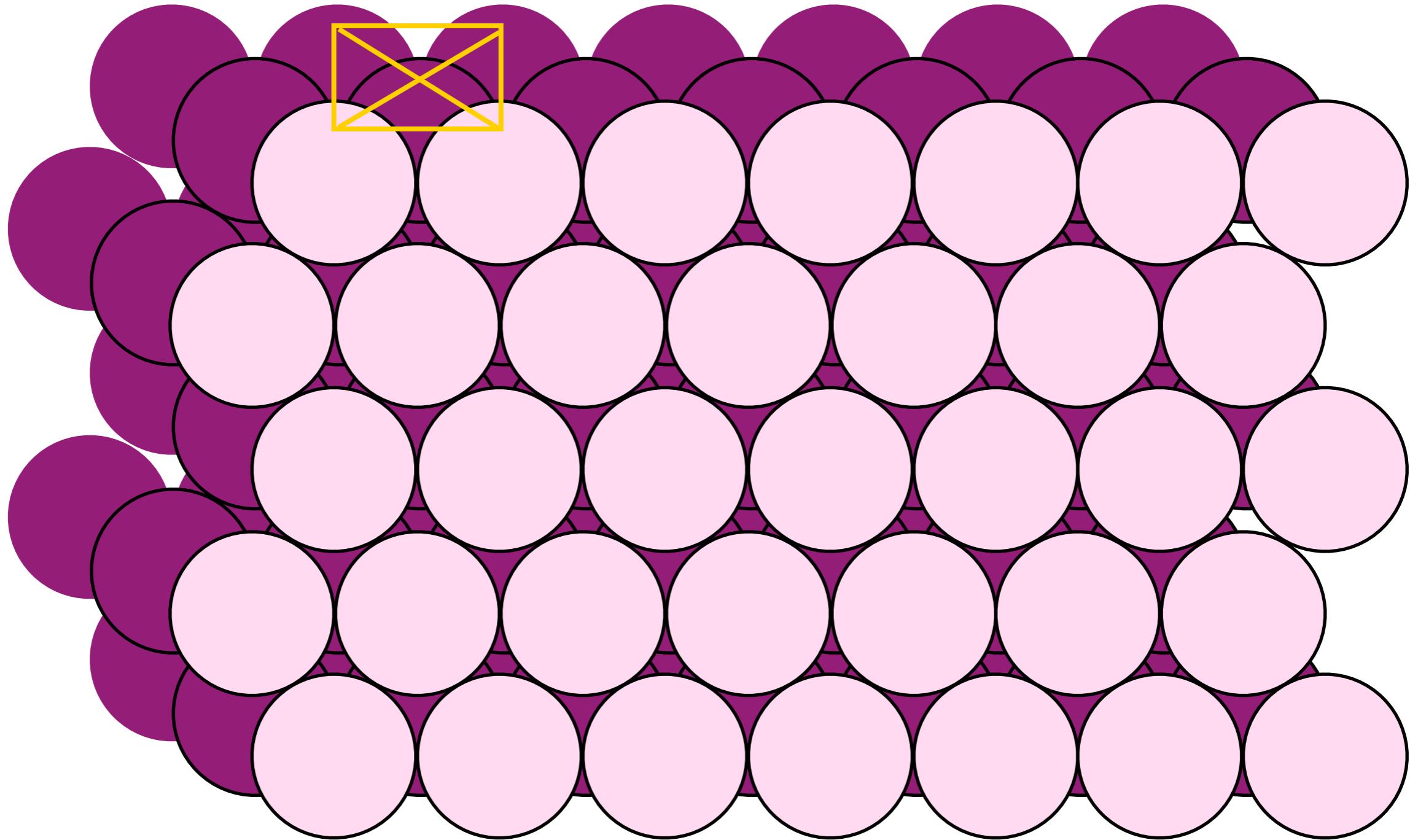


A B



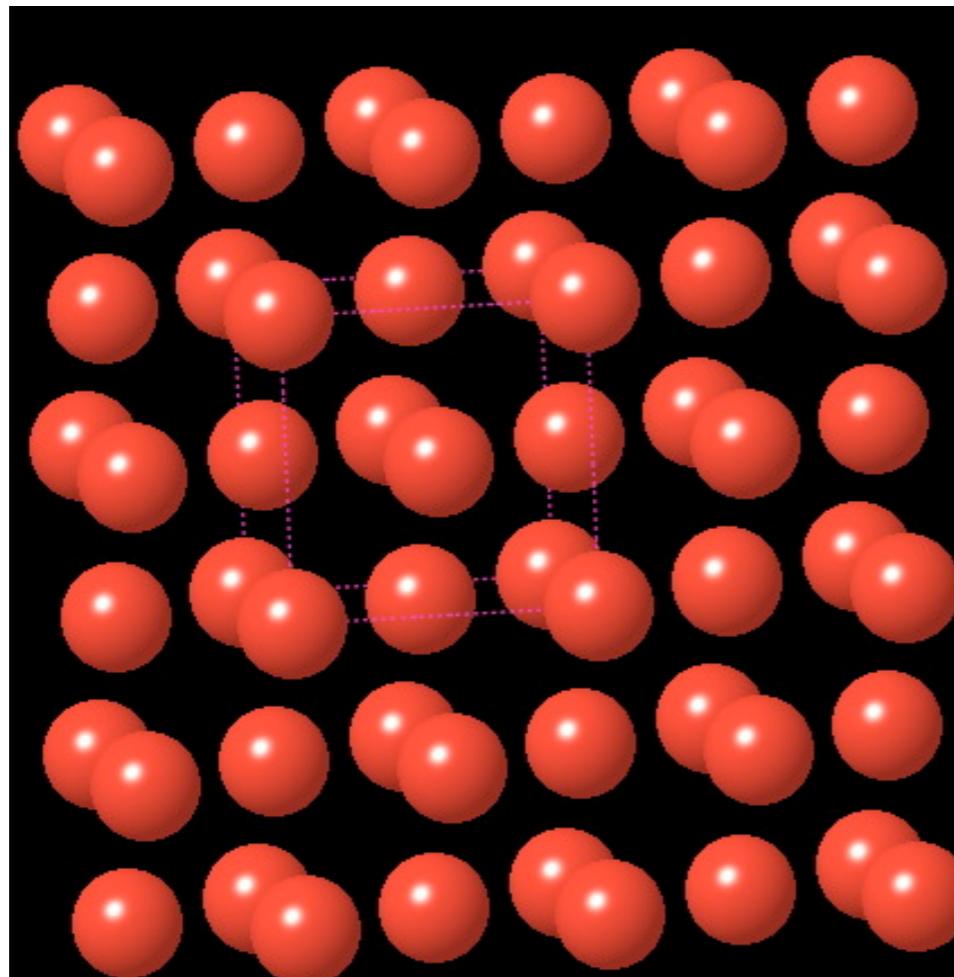
A B A B...

hexagonal close packed

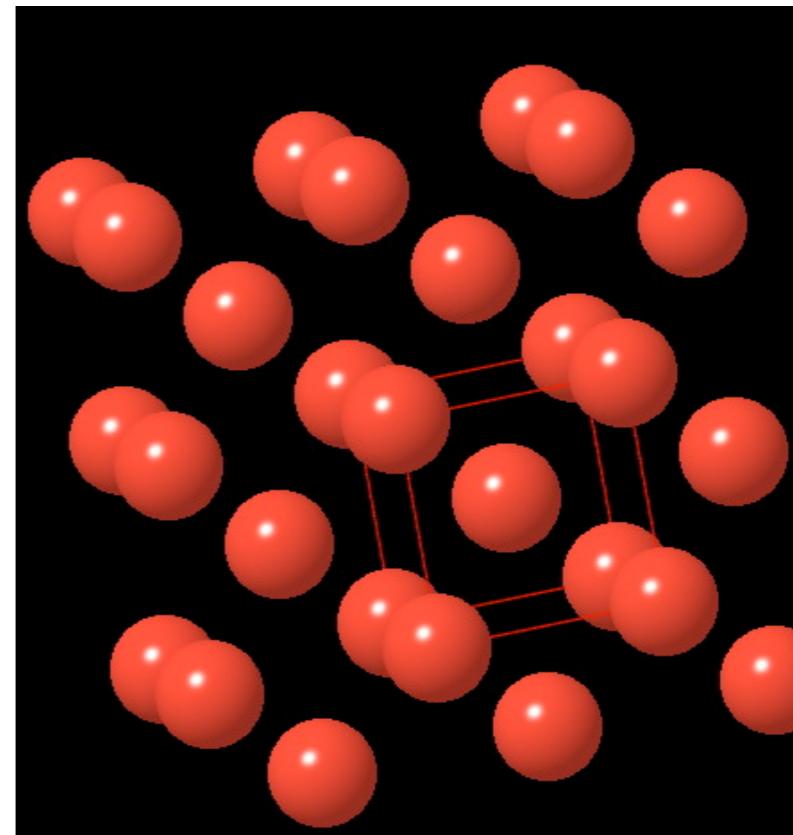


cubic close packed  
A B C A B C...  
or  
face centered cubic

# Fe in the core?

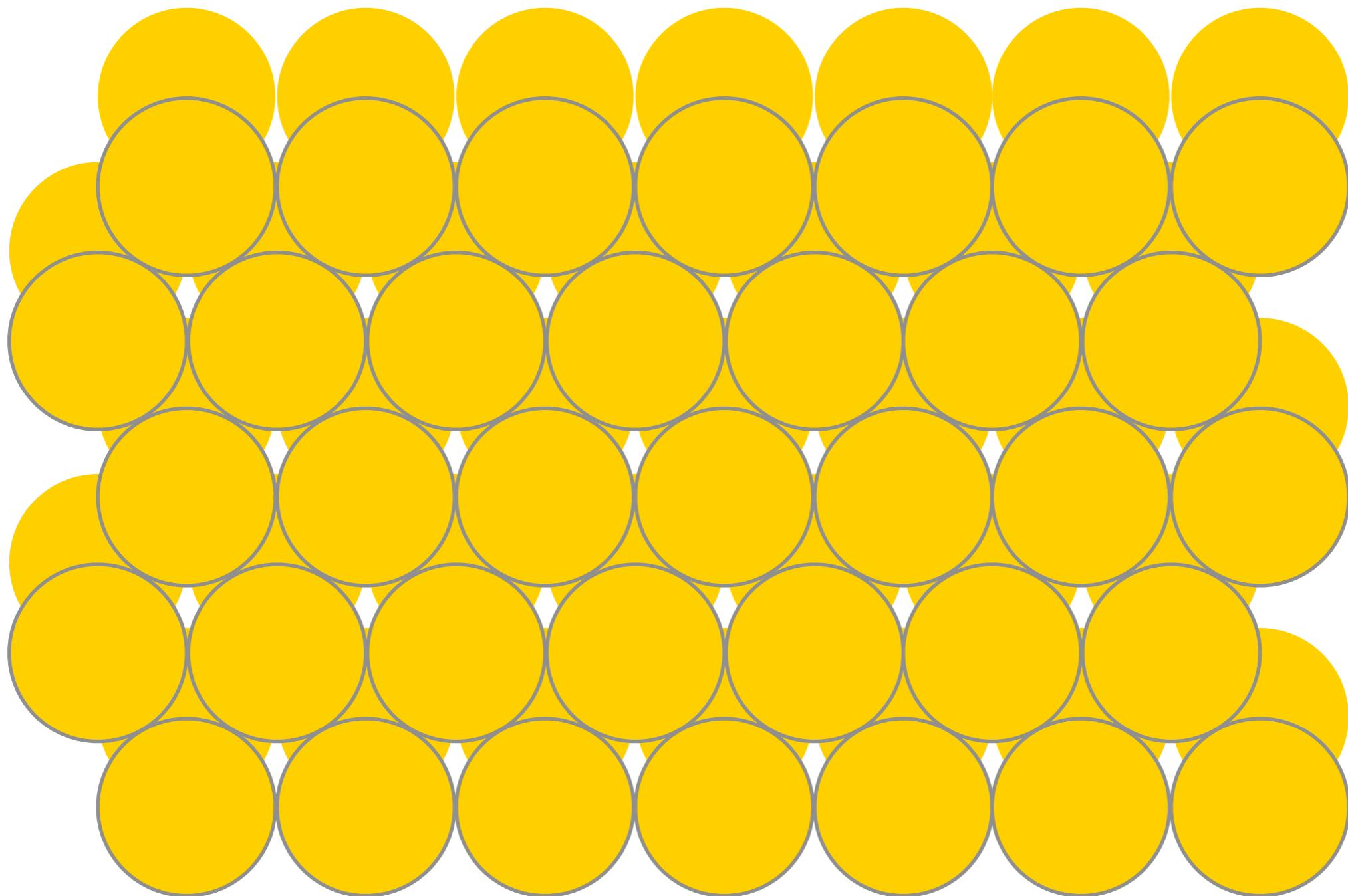


fcc

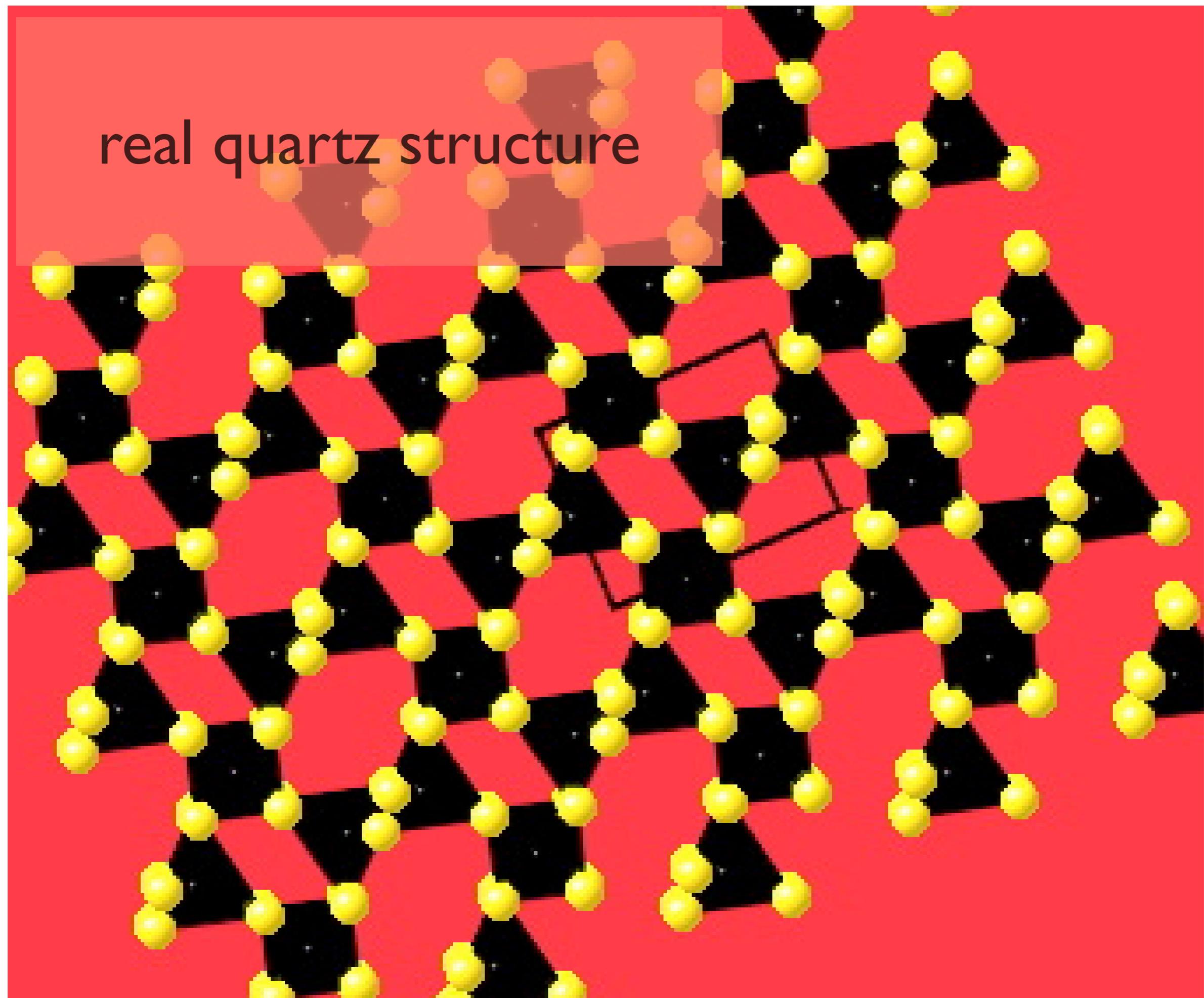


bcc

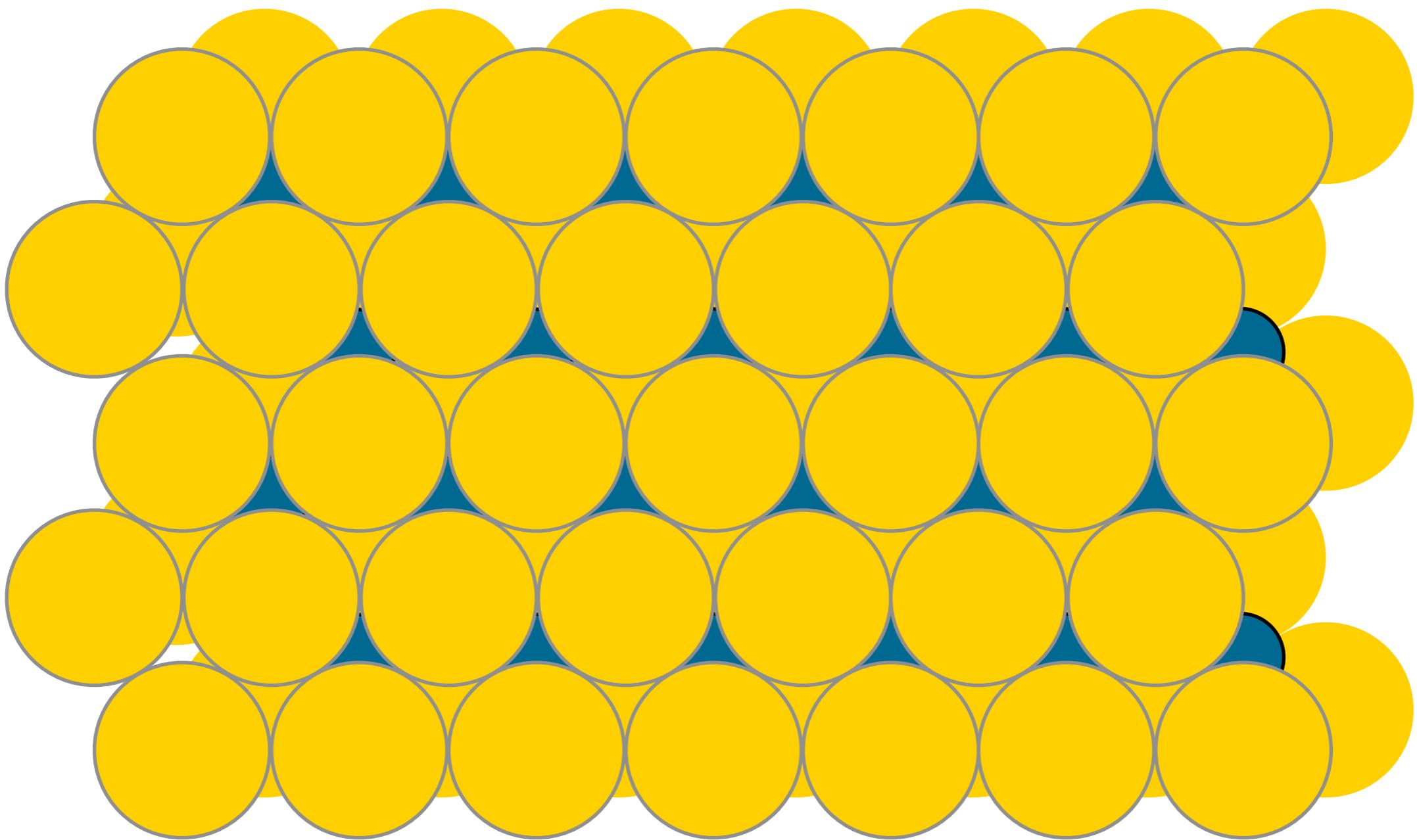
**two different sized spheres:  
O and Si**



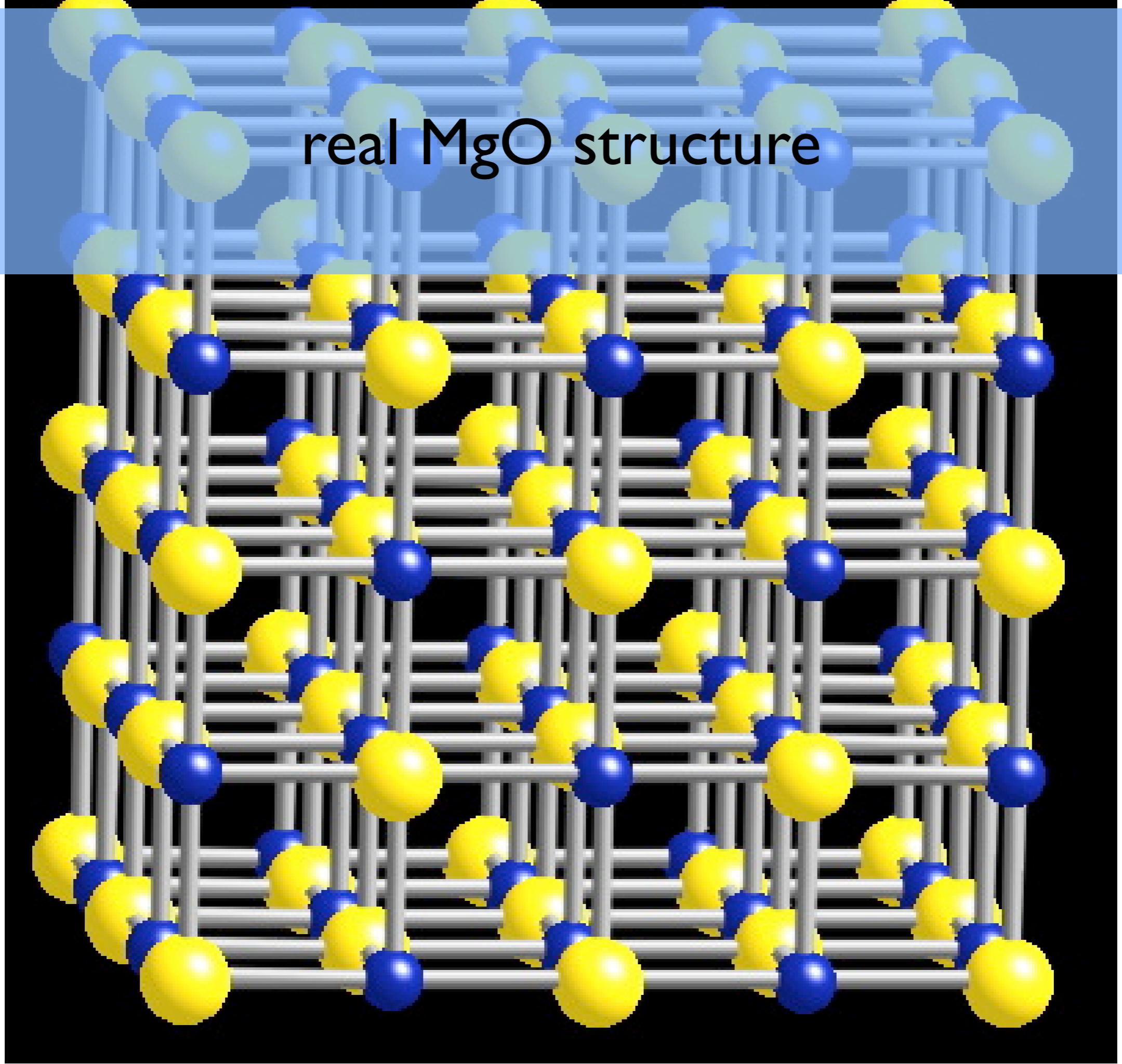
real quartz structure



two different sized spheres:  
O and Mg

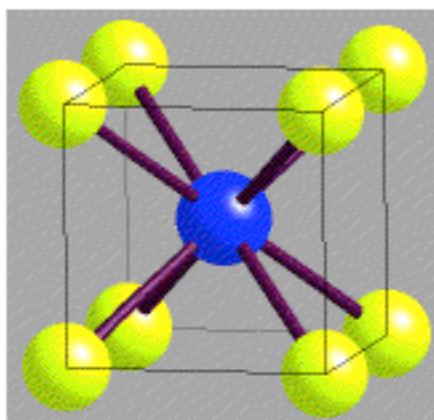


real MgO structure



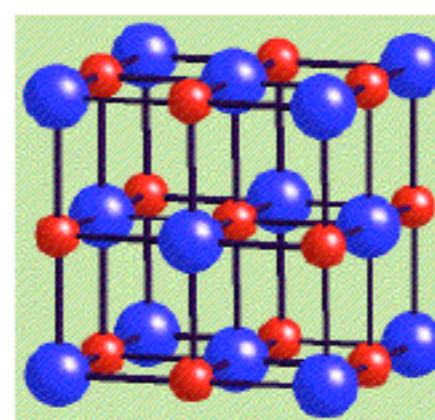
# Limiting Radius Ratios

**CsCl 8:8**



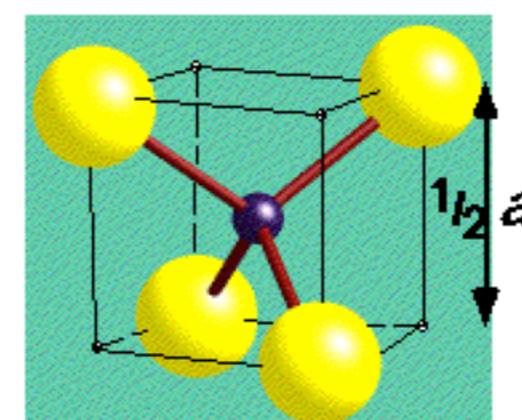
*unit cell*

**NaCl 6:6**



*unit cell*

**ZnS 4:4**

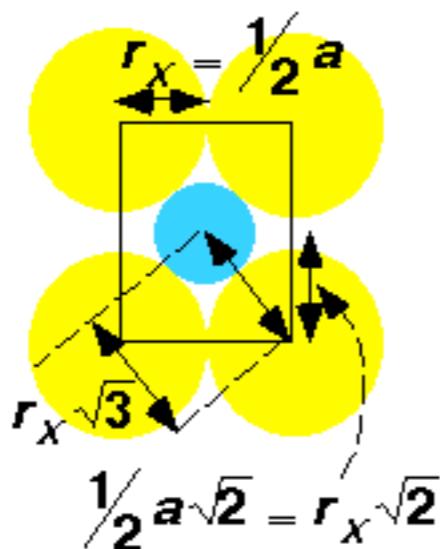


*1/8<sup>th</sup> unit cell*

cell side  $a$

face diagonal  $a\sqrt{2}$

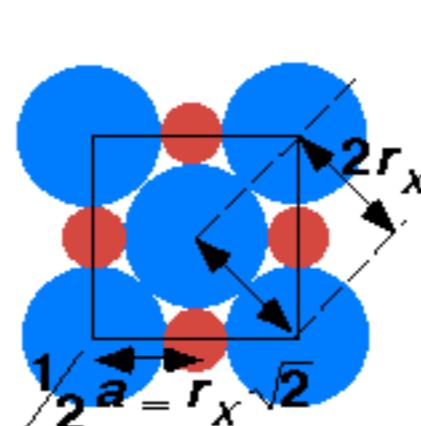
body diagonal  $a\sqrt{3}$



$$r_M + r_X = r_X \sqrt{3}$$

$$r_M / r_X = \sqrt{3} - 1$$

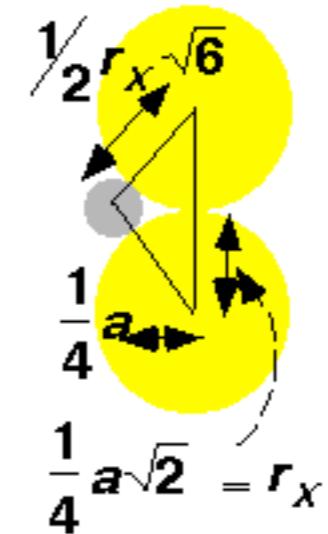
$$= 0.732$$



$$r_M + r_X = r_X \sqrt{2}$$

$$r_M / r_X = \sqrt{2} - 1$$

$$= 0.414$$



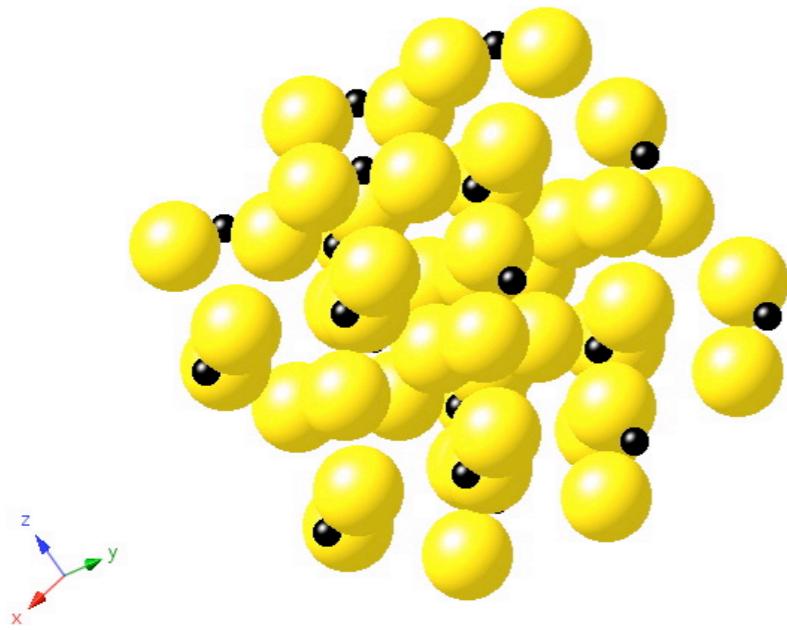
$$r_M + r_X = \frac{1}{2} r_X \sqrt{6}$$

$$r_M / r_X = \frac{1}{2} \sqrt{6} - 1$$

$$= 0.225$$

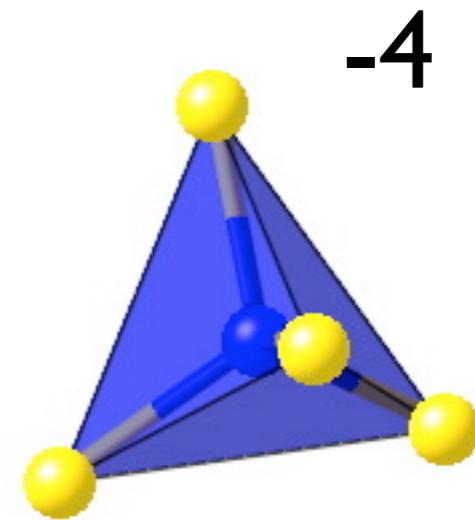
# rules for creating structures:

1. geometric considerations
2. charge neutrality
3. Other effects



fully networked  
silicate tetrahedra  
(quartz)

everything  
in between  
=crustal  
mineralogy



isolated  
silicate tetrahedra  
(olivine)

rules for creating structures:

I. geometric considerations

2. charge neutrality

3. Other effects

i. Energetics:

(polyhedra face sharing>edge sharing>vertex)

ii. Principal of Parsimony:

fewer rather than more structures

# pressure rules:

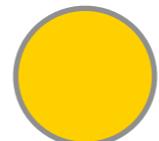
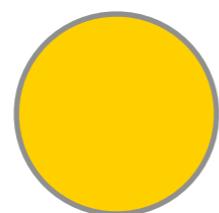
pressure

0

15 GPa

25 GPa

O



Si



depth

crust

410 km

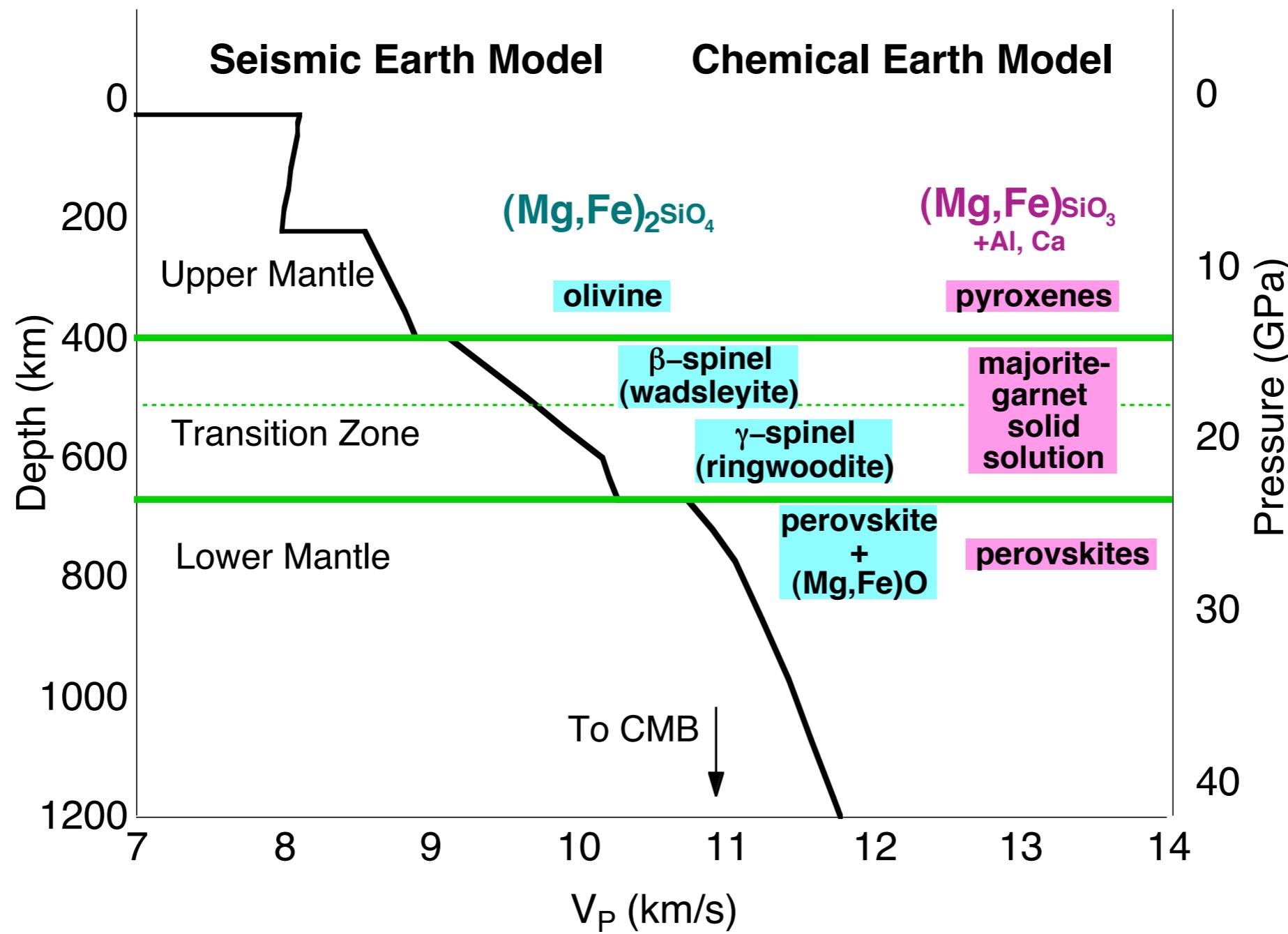
660 km

coordination

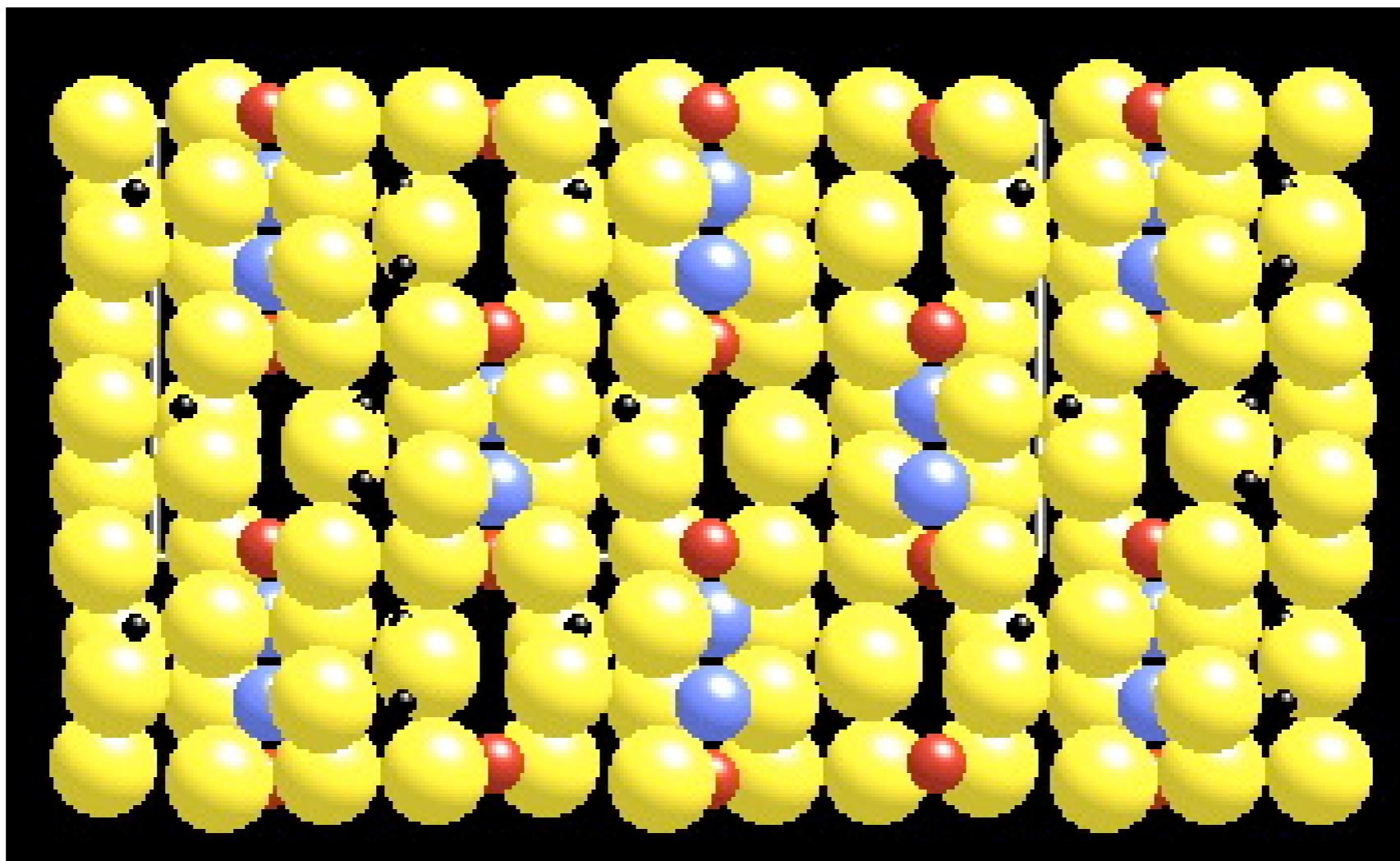
tetrahedral  
(4)

octahedral  
(6)

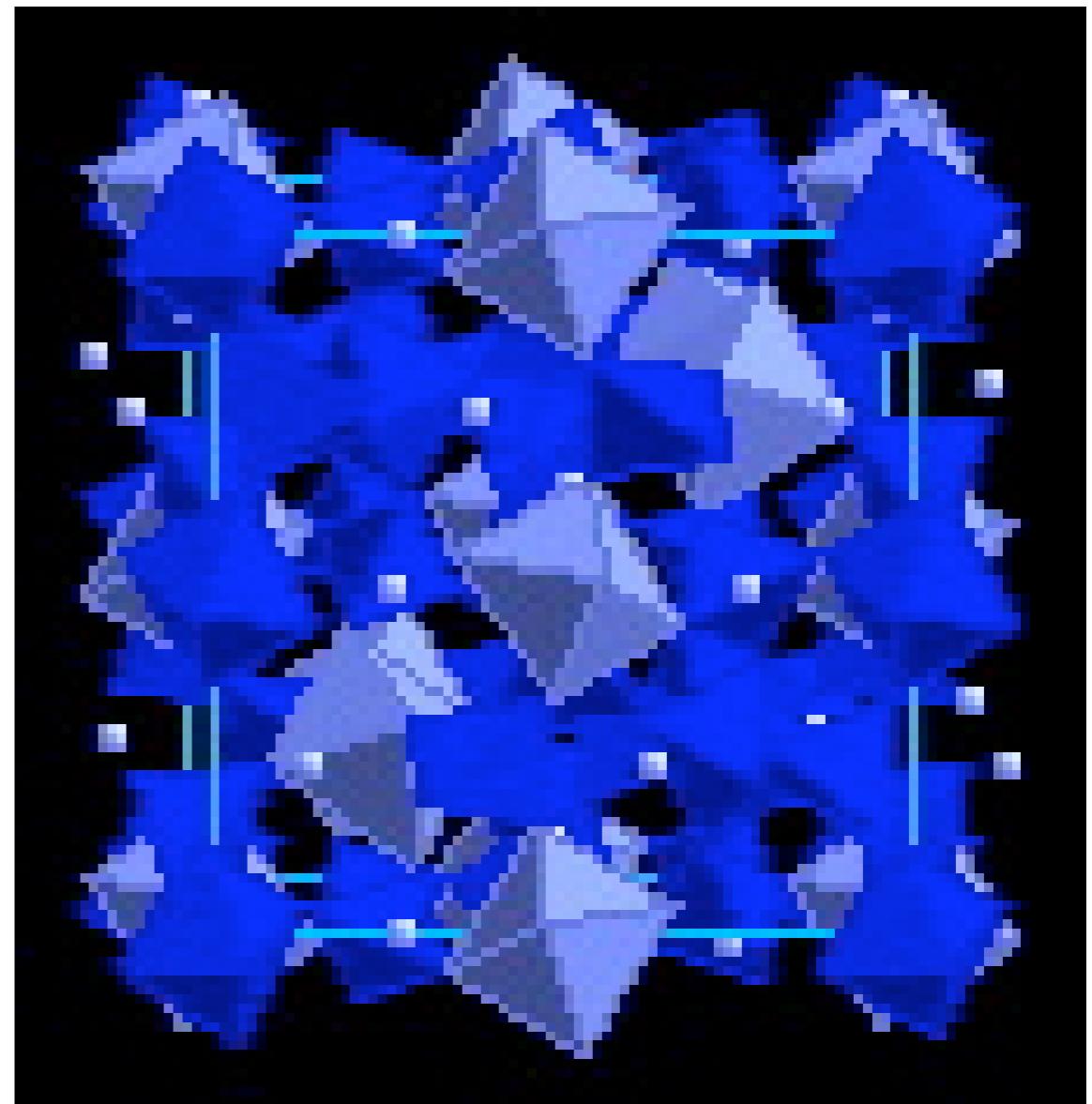
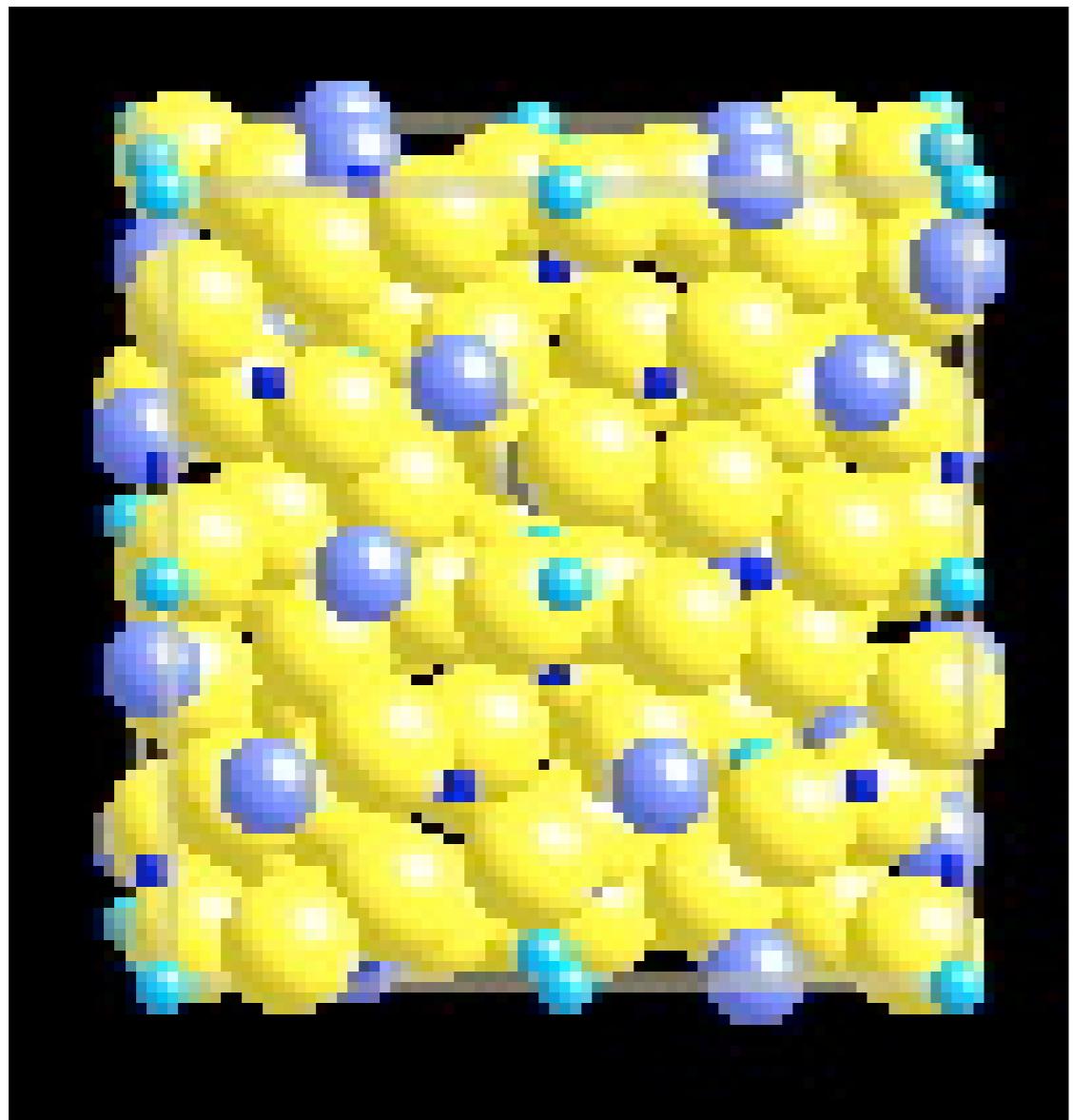
cubic  
(8)



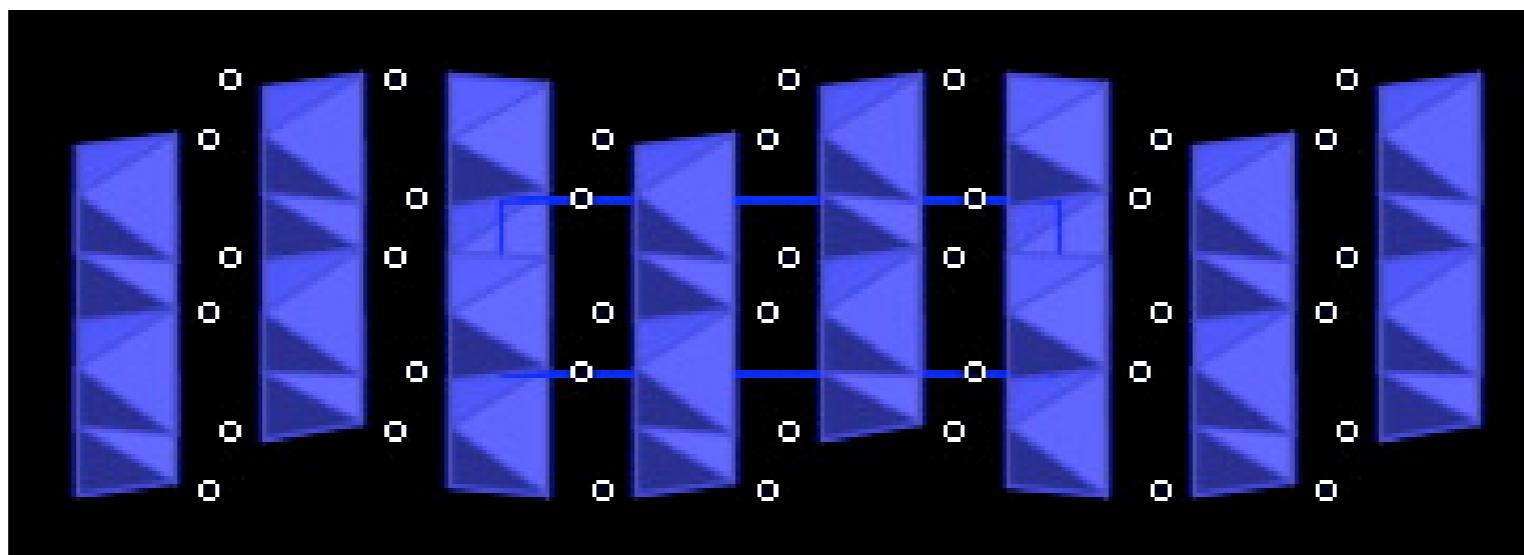
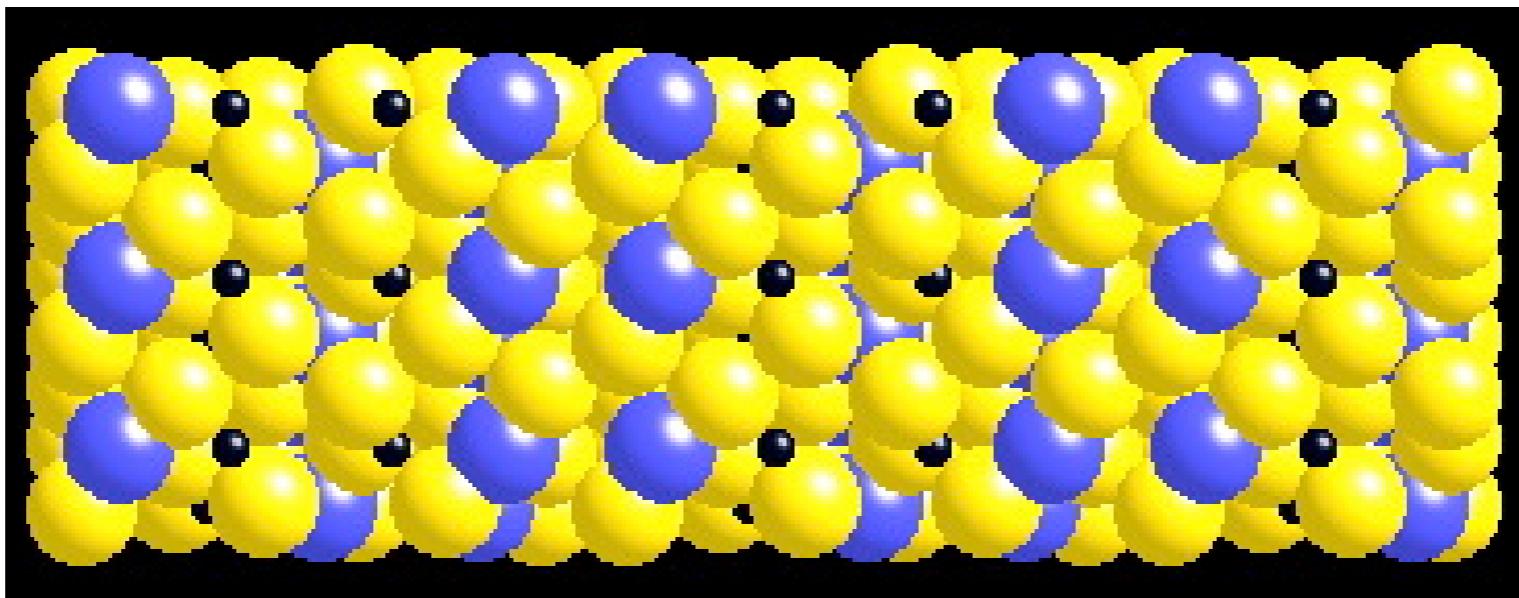
# Si:3O mantle mineralogy



orthopyroxene

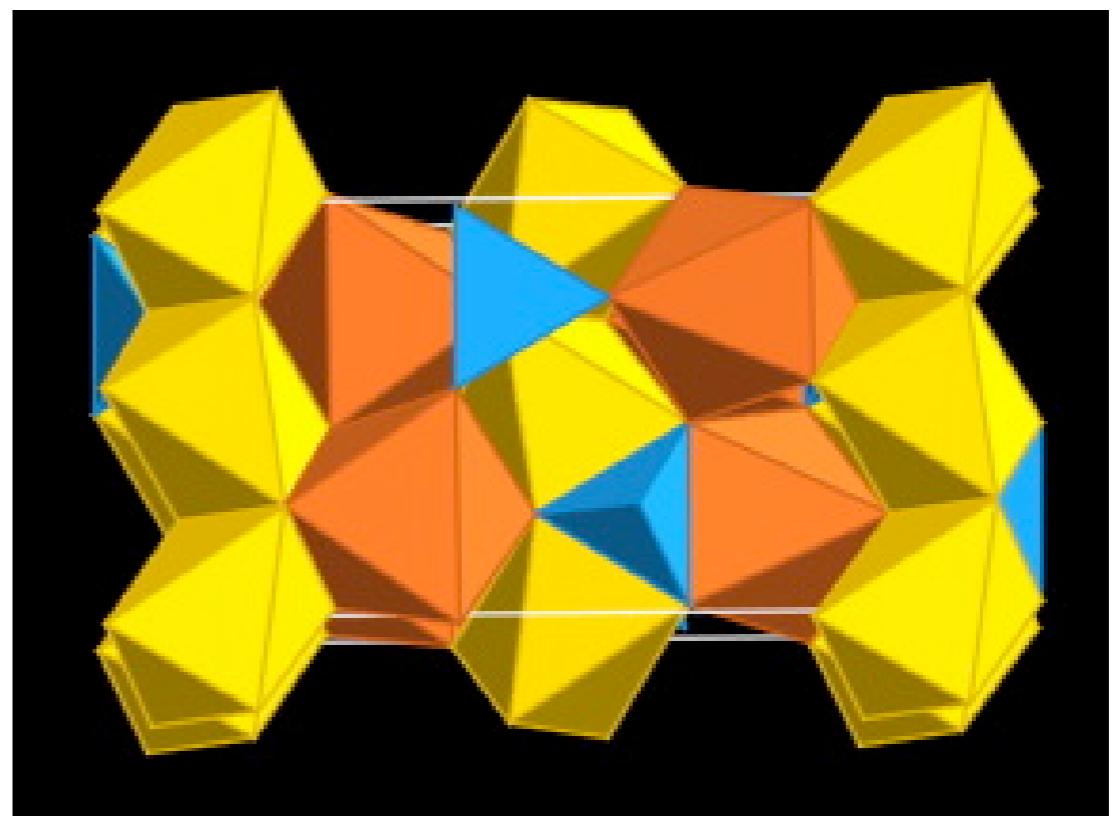
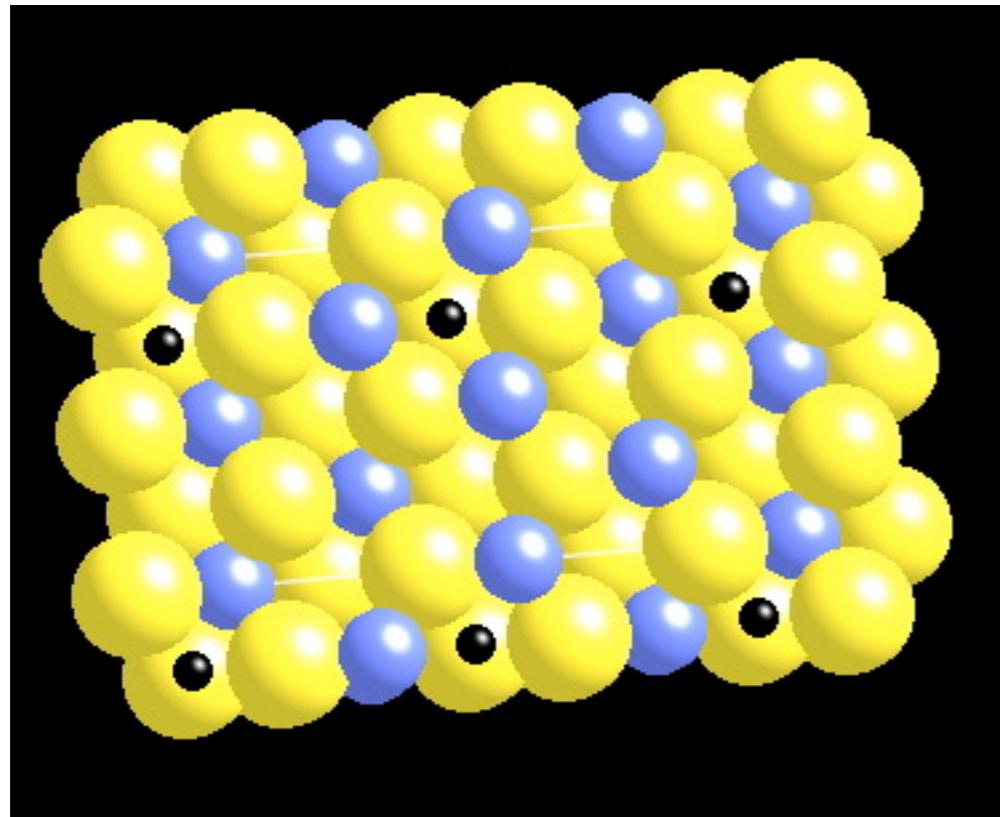


majorite garnet

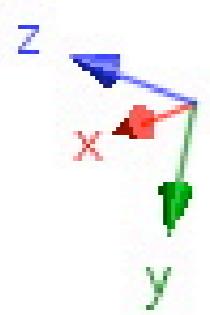
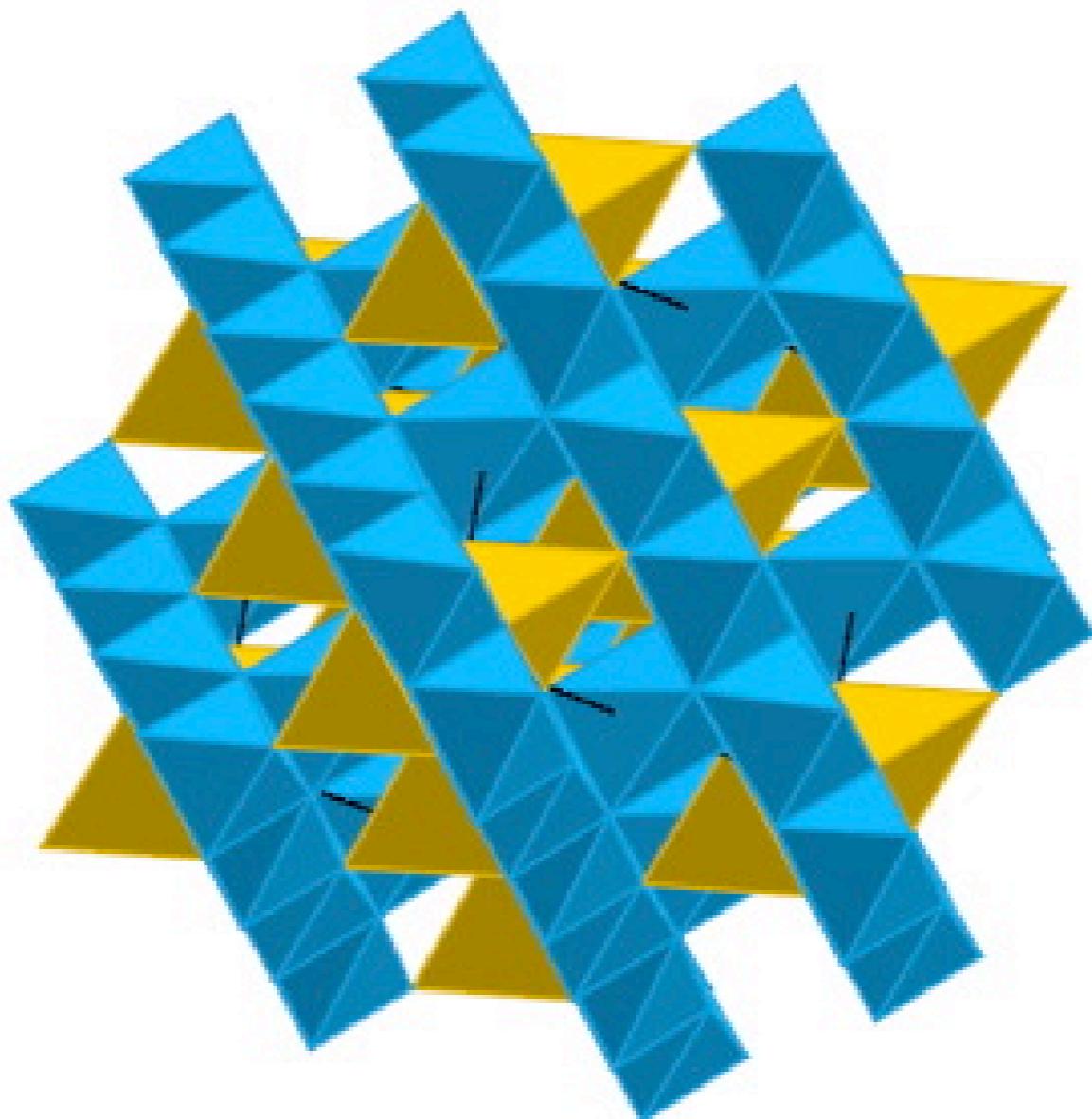


akimotoite

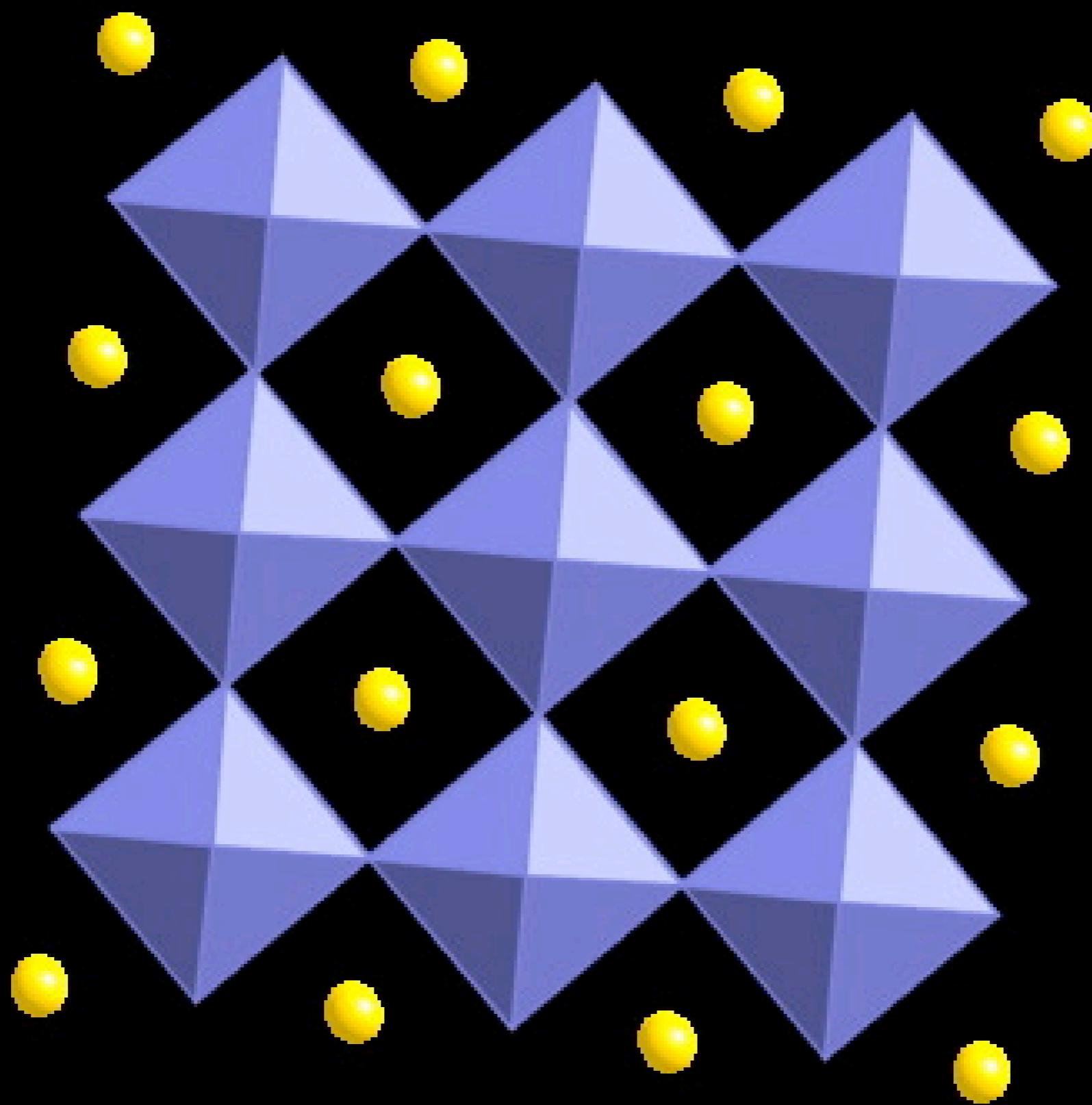
# Si:2O mantle mineralogy



olivine



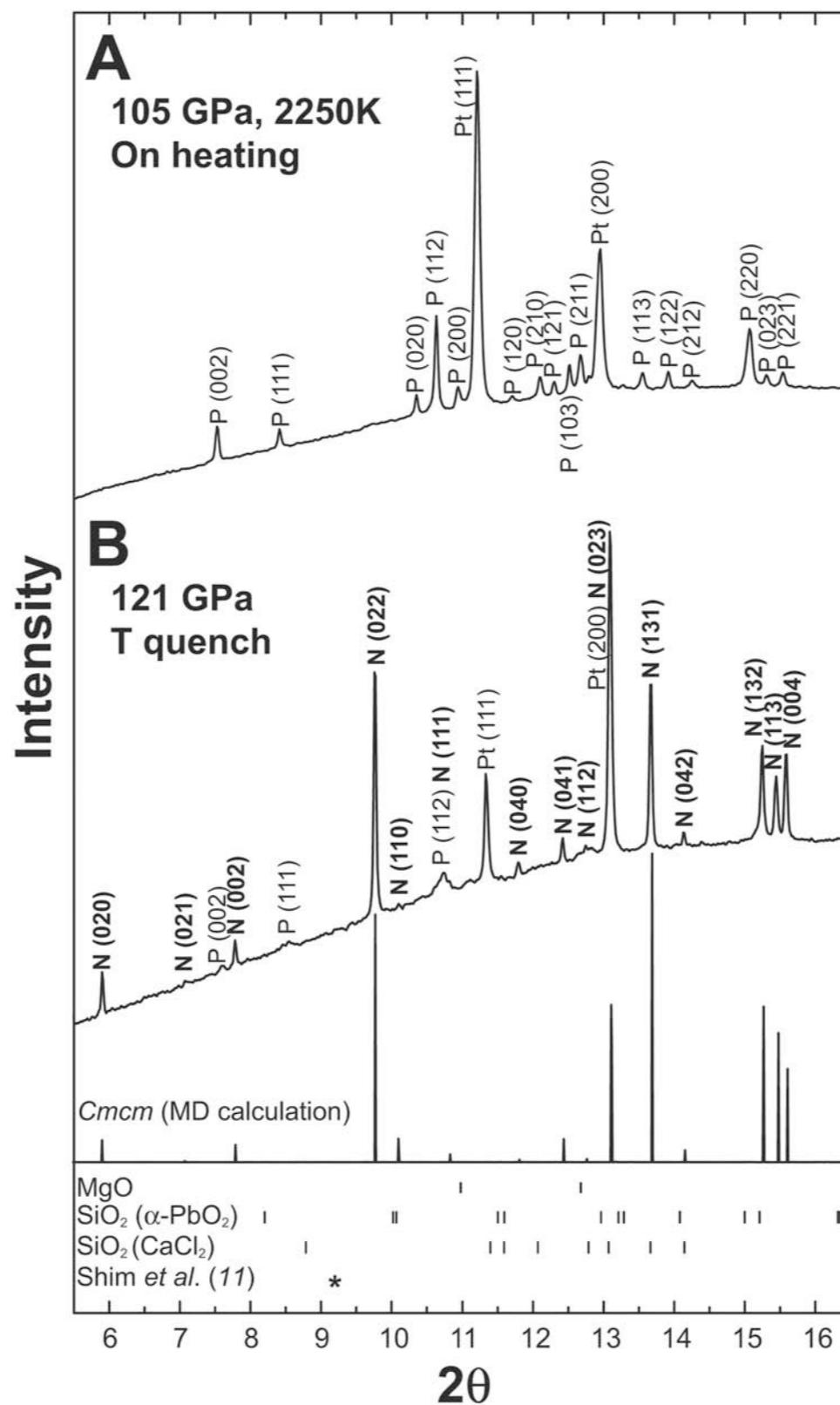
ringwoodite



perovskite



# Murakami et al, 2004



# post-perovskite phase transformation?

