AB_2 Structures

- Ionic compounds: CaF_2
- Covalent compounds: MoS_2, FeS_2
- In ionic compounds, size considerations determine structure.
- In covalent compounds, size considerations are also important, but there are more exceptions.

AB_2 Structure Types

- Most common:
  1. CaF_2: 3-D
  2. Rutile (TiO_2): 3-D
  3. TiS_2 or $CdCl_2$: 2-D
  4. MoS_2: 2-D
  5. Pyrite (FeS2): 3-D
  6. Maracasite (FeS2): 3-D

AB_2 Structure Types

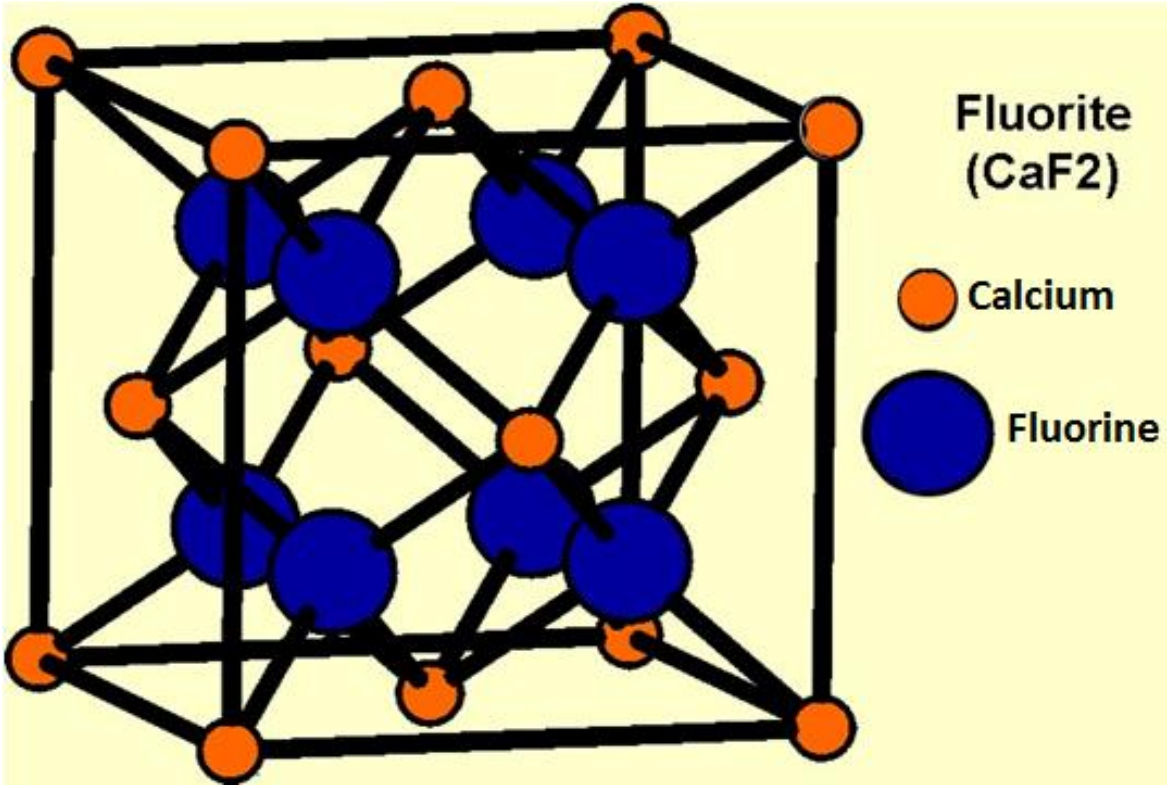
- Less common:
  1. SiO_2: 3-D
  2. Cu_2O: 3-D
  3. HgI_2: 2-D
  4. SiS_2: 1-D
  5. $PdCl_2$: 1-D
  6. PdS_2: 3-D

In AB_n materials:

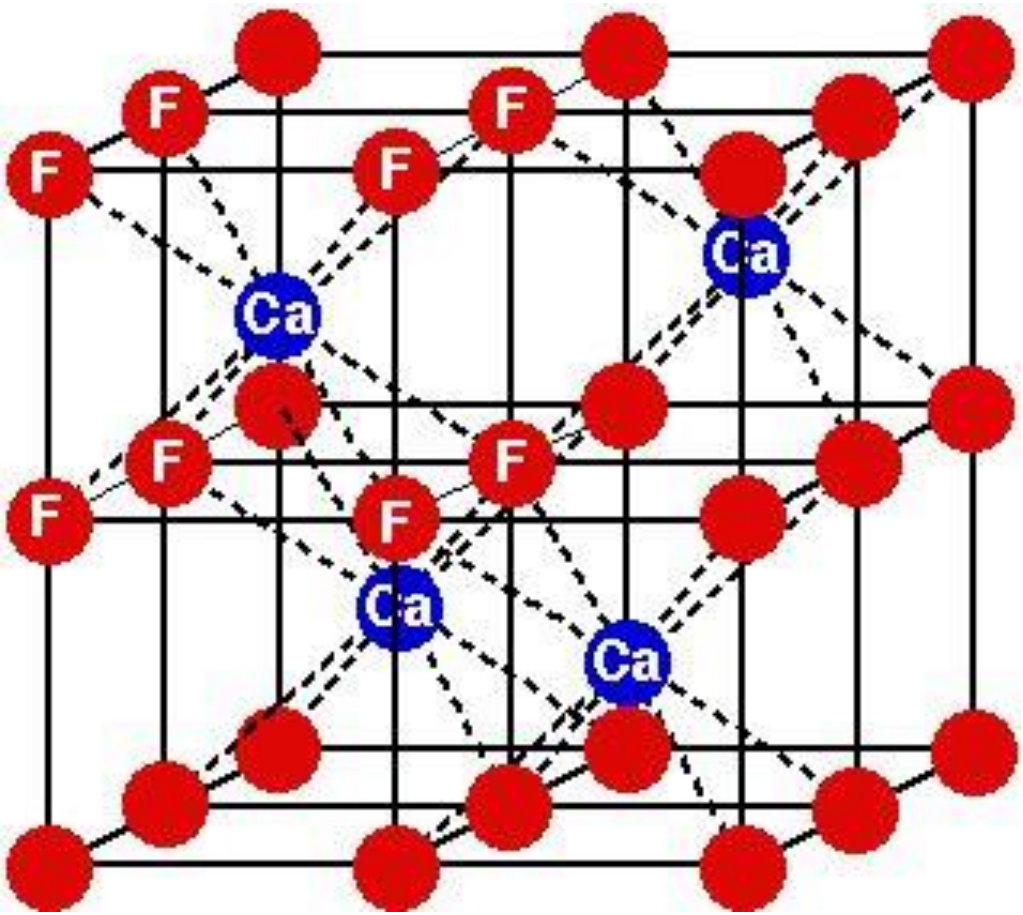
$$\frac{\text{coord. number of A}}{\text{coord. number of B}} = n$$

Fluorite: CaF_2

- $(Sr,Ba)F_2$, HgF_2
- CeO_2, PrO_2, ThO_2
- $CoSi_2$, LaH_2, CeH_2 ,$NiSi_2$
- Na_2S (anti-fluorite)

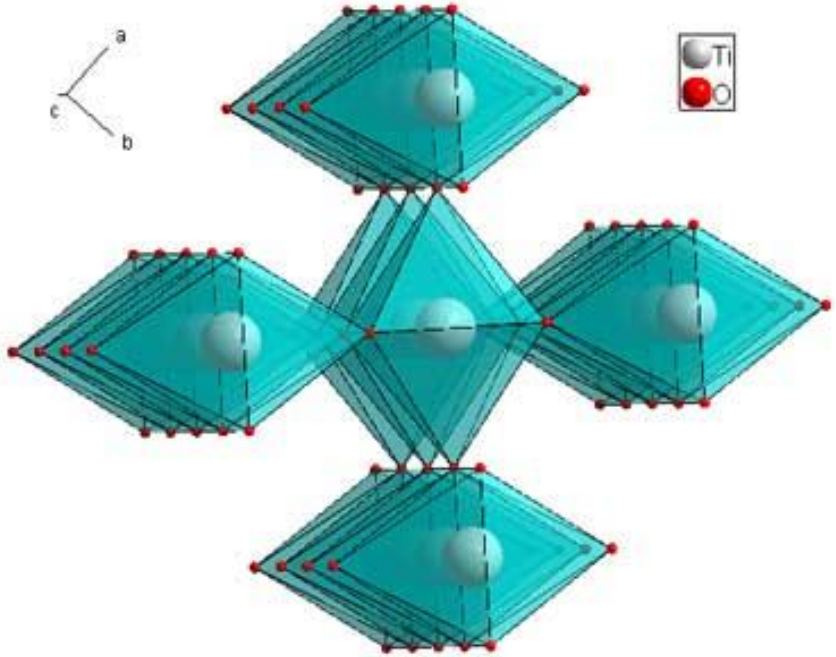


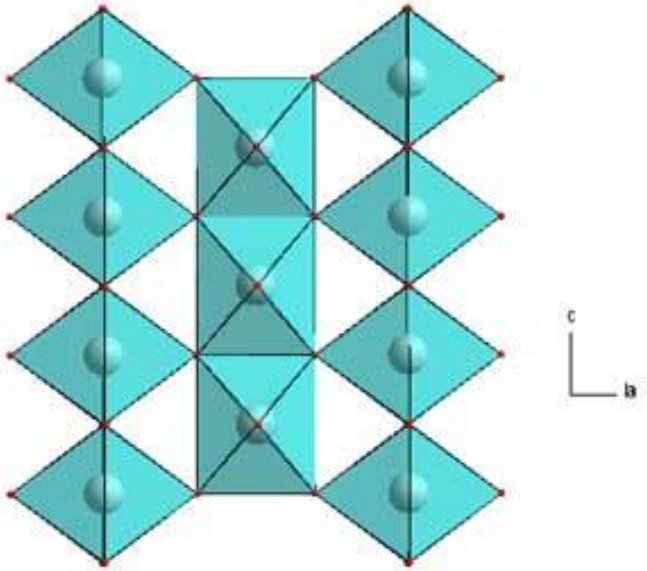
8-coordinate Ca^{2+}



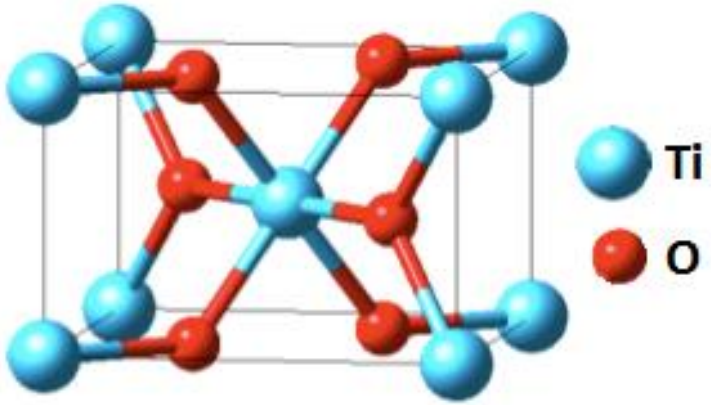
tetragonal

Rutile: TiO_2



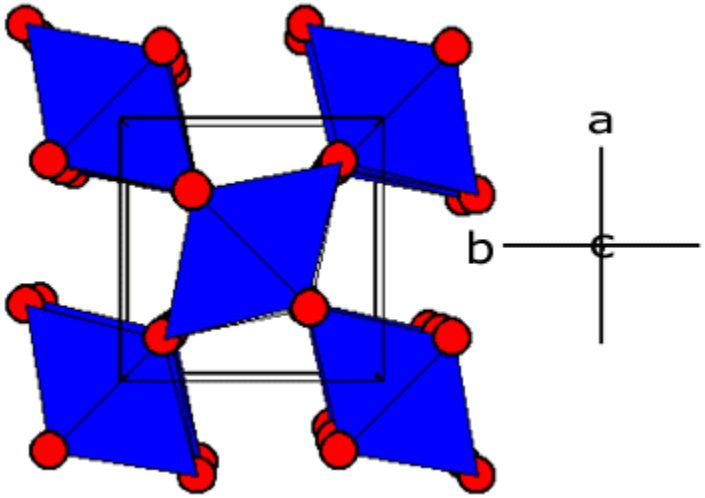


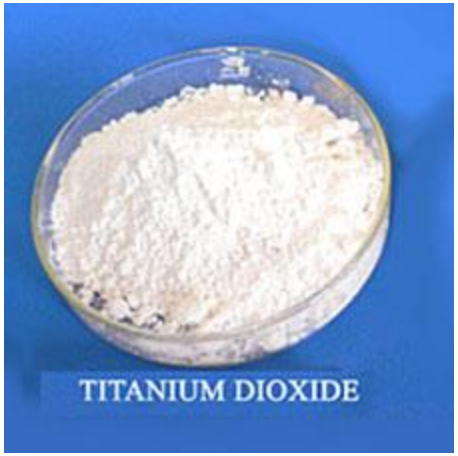
- MgF_2, MgF_2, FeF_2, NiF_2, ZnF_2
- VO_2, OsO_2, RuO_2, IrO_2, SnO_2,



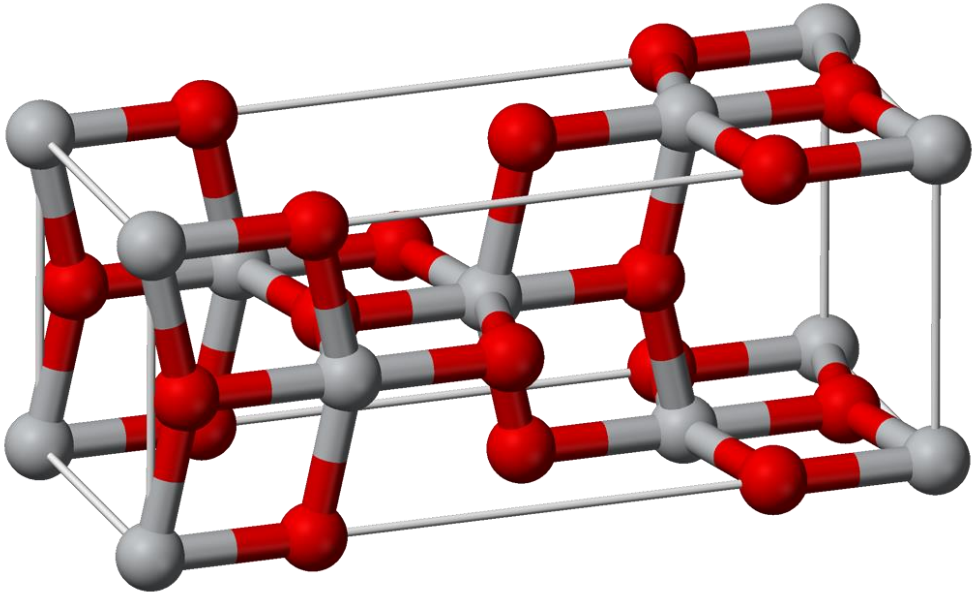
Rutile: TiO_2

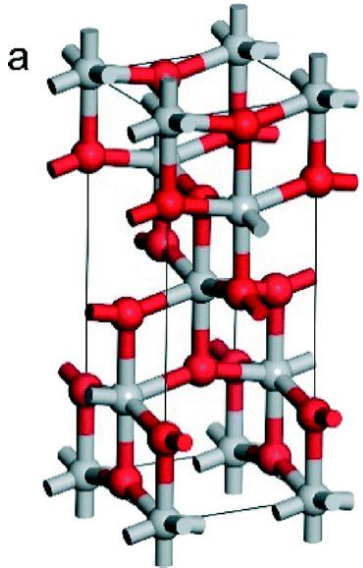

FUNDAMENTAL PHOTOGRAPHS
http://www.fphoto.com

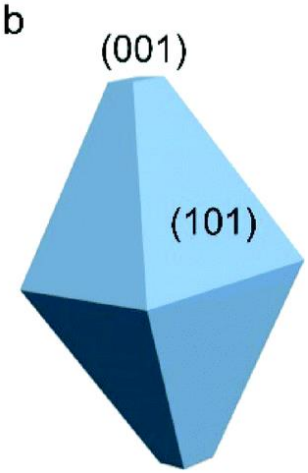

a
b
c

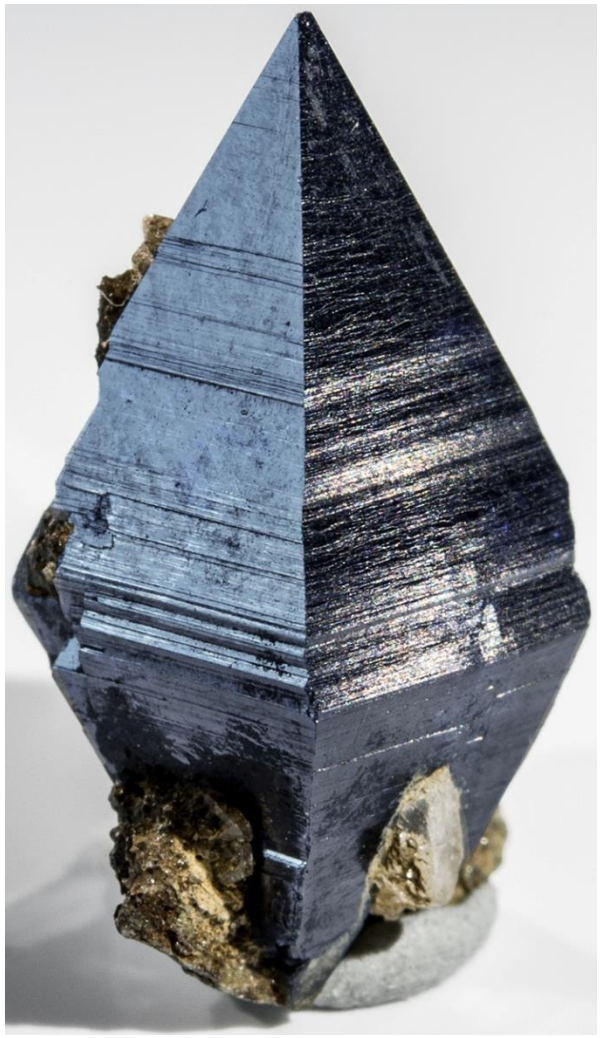

TITANIUM DIOXIDE

Anatase: TiO_2

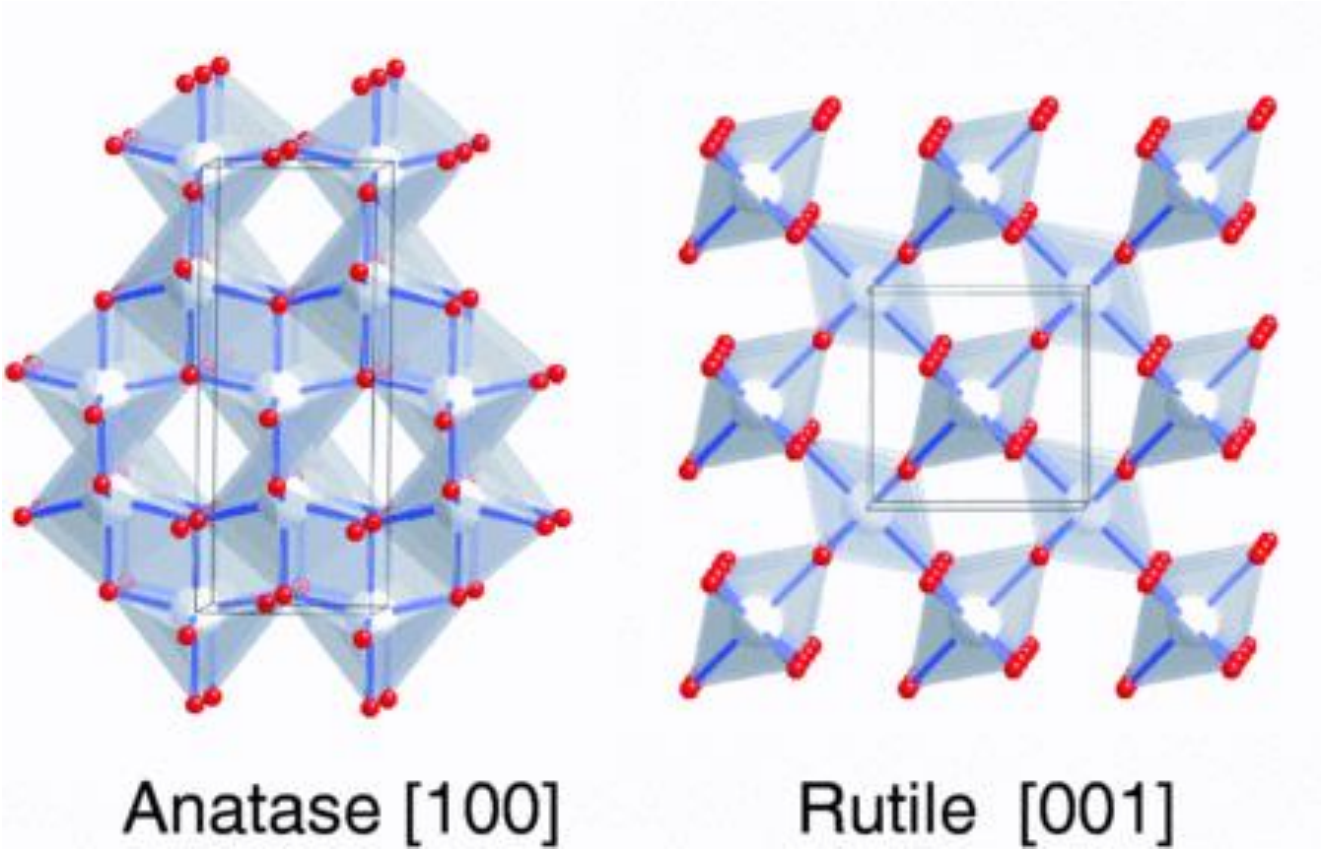








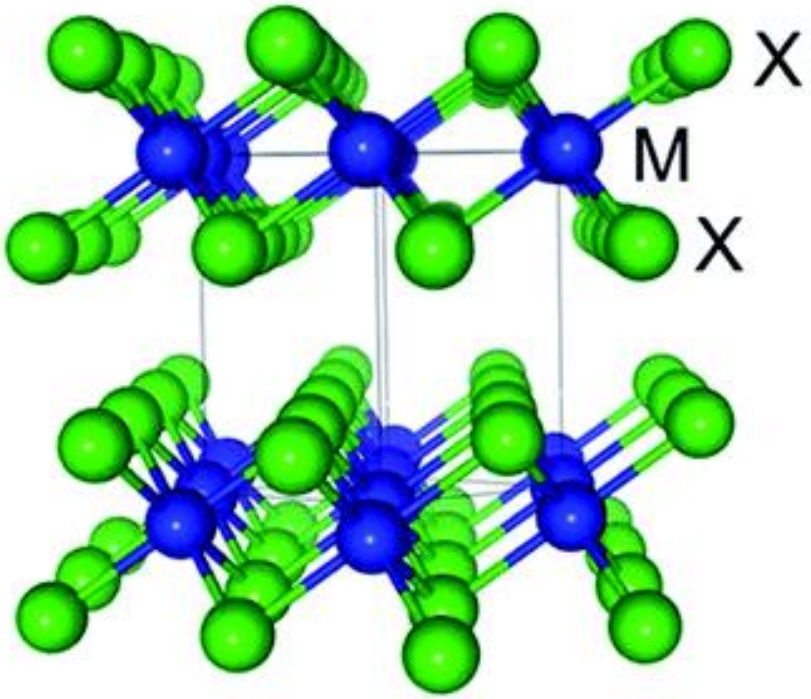
Rutile-Anatase comparison: TiO_2



TiS_2 or $CdCl_2$ type

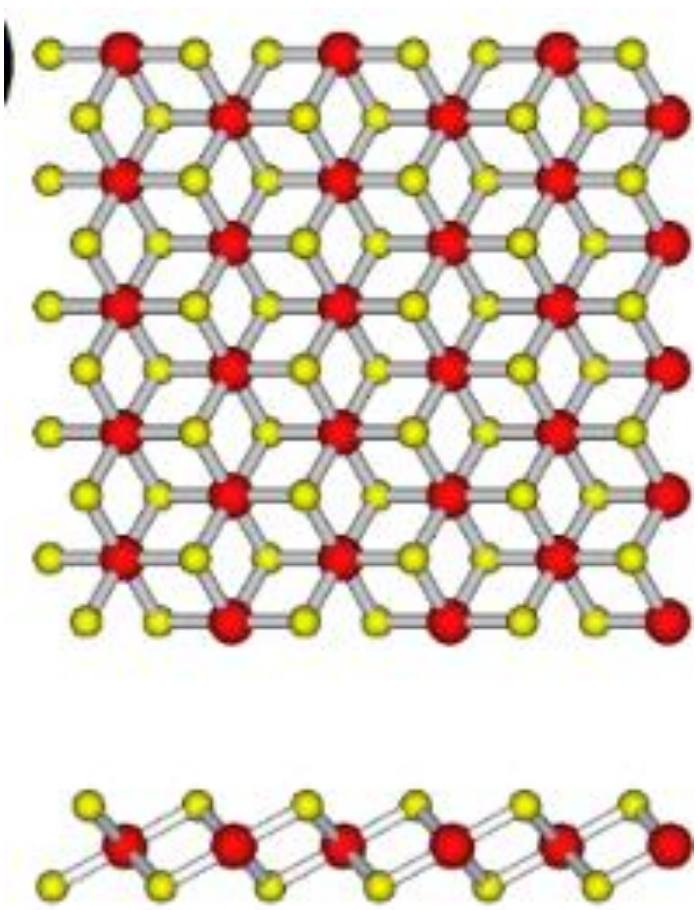
- Defect NiAs structure

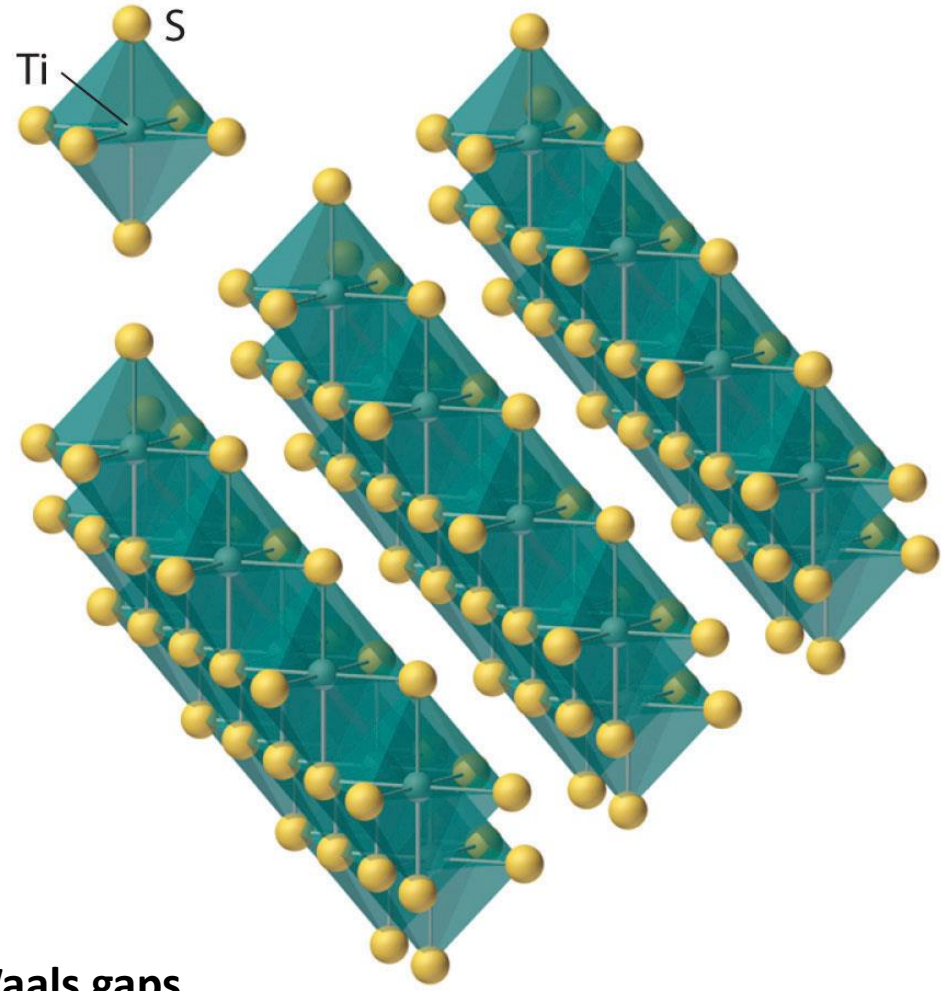
- ZrS_2, $TiSe_2$, VS_2
- $MgCl_2$, $FeCl_2$
- $NiCl_2$, $MnCl_2$



$TiS_2, TiSe_2$
$ZrS_2, ZrSe_2$

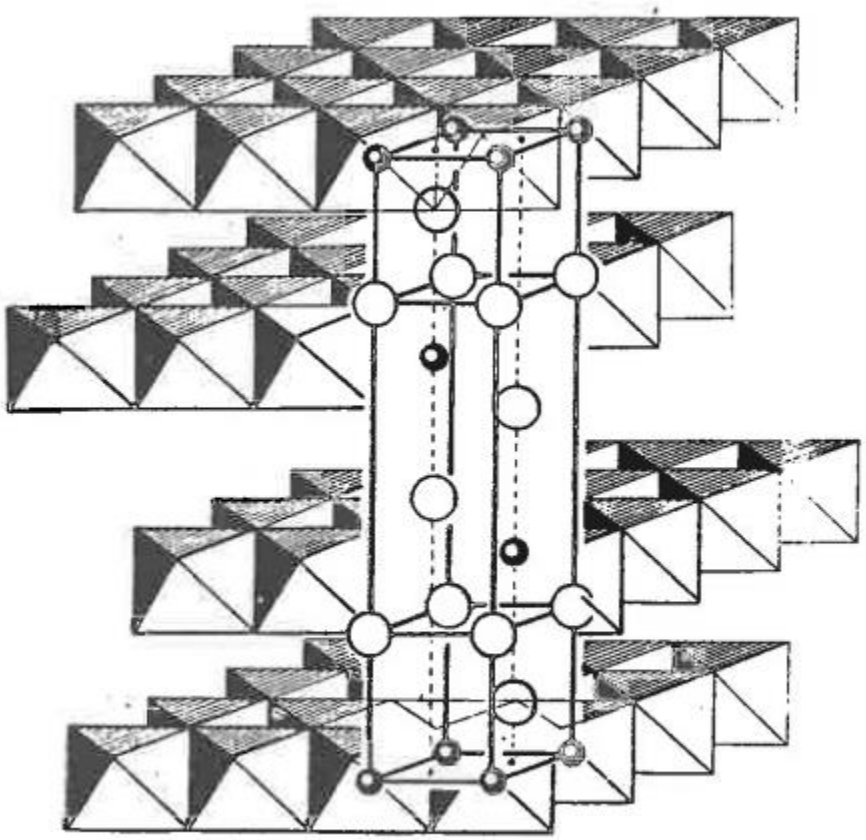
TiS_2 or $CdCl_2$ type



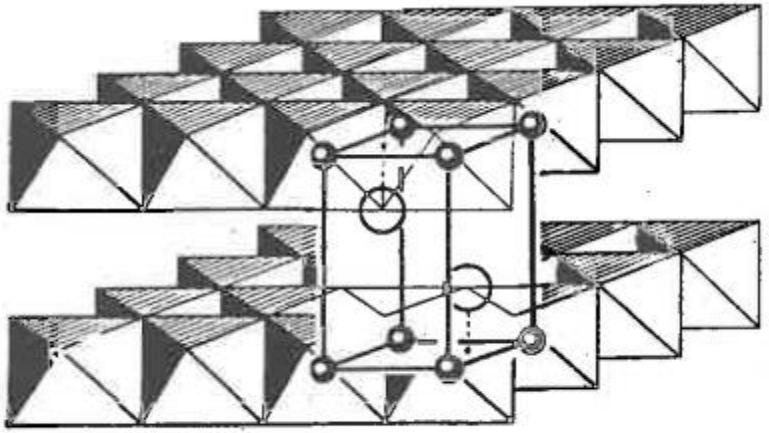


Van der Waals gaps

TiS_2: Polyhedral Representations

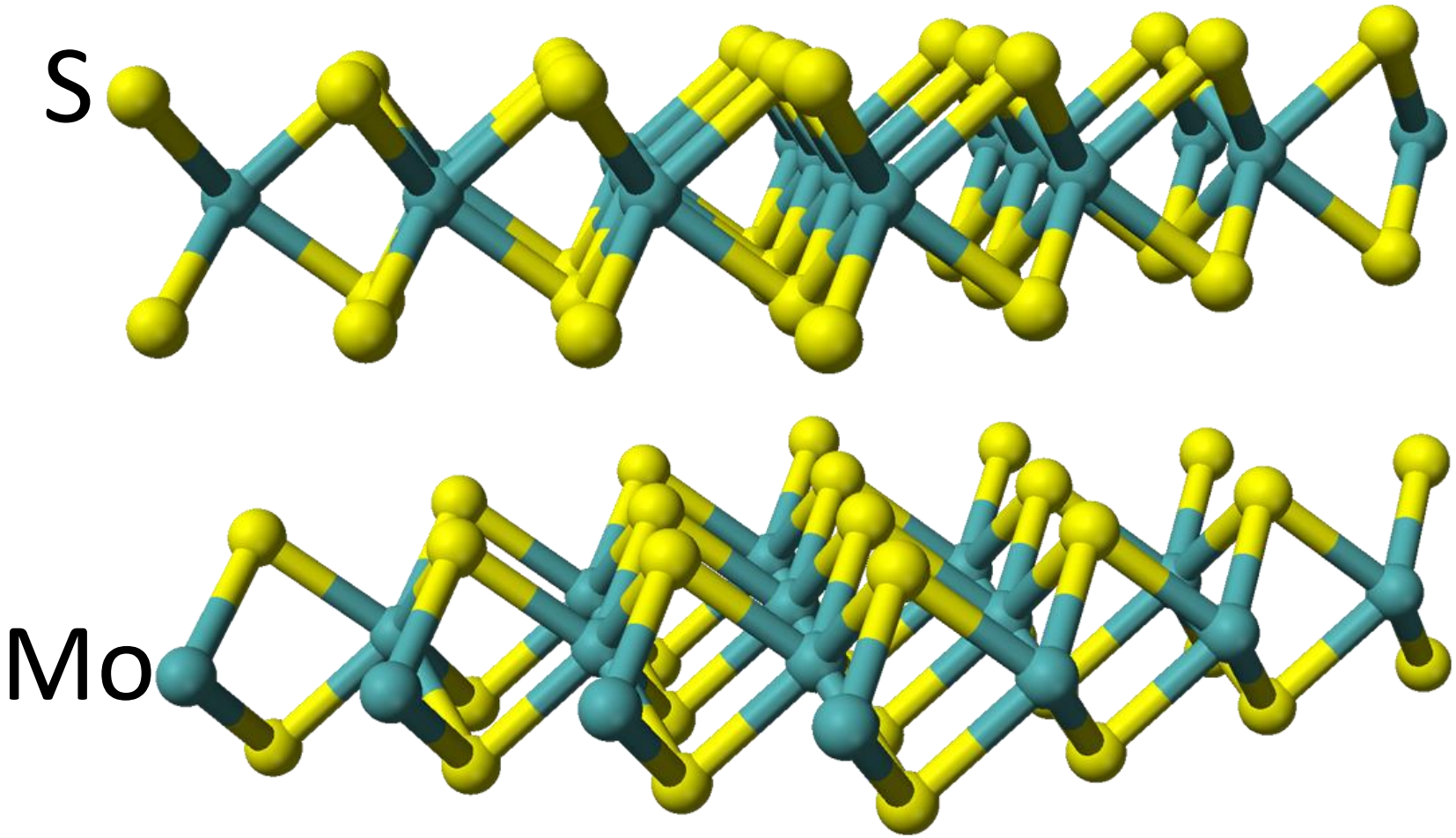


The $CdCl_2$ structure.

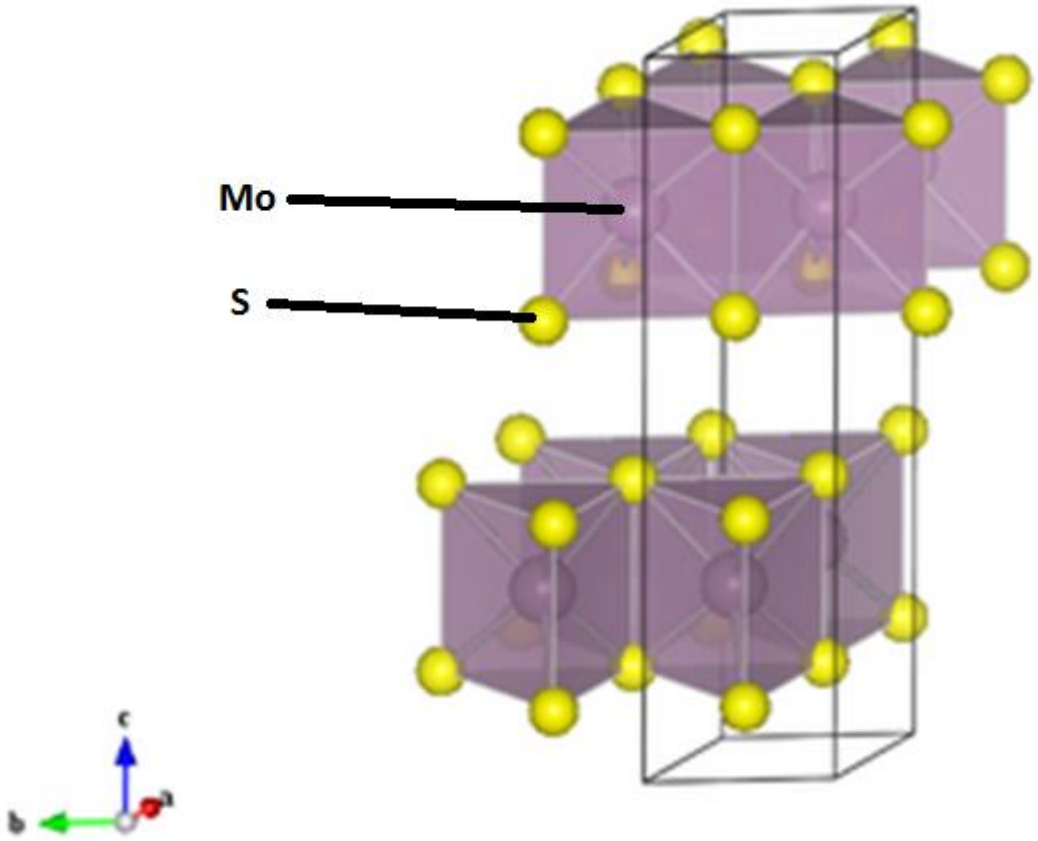


The CdI_2 structure.

MoS_2

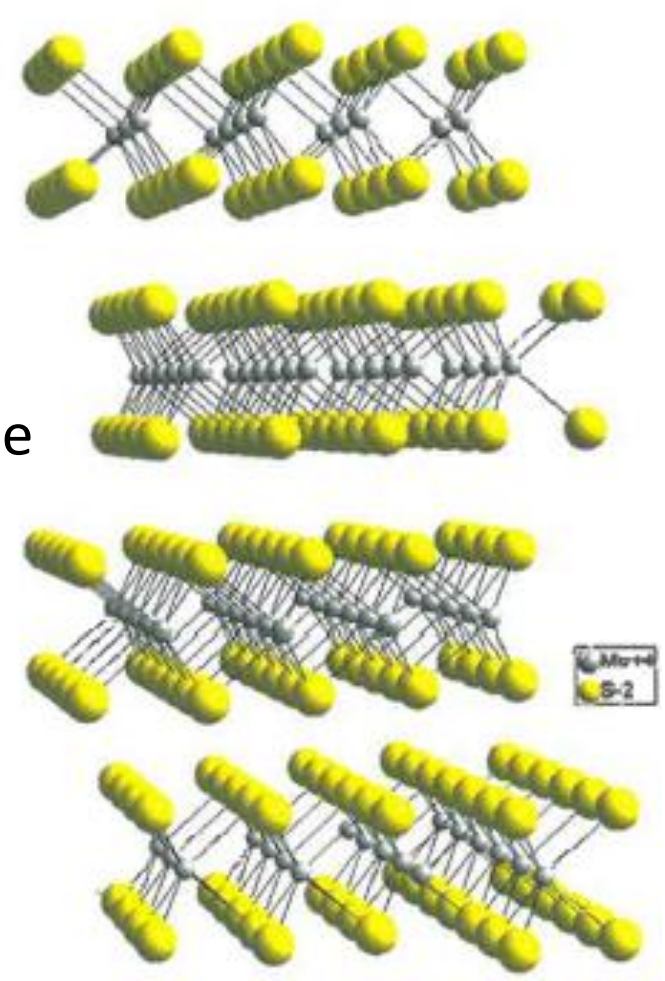


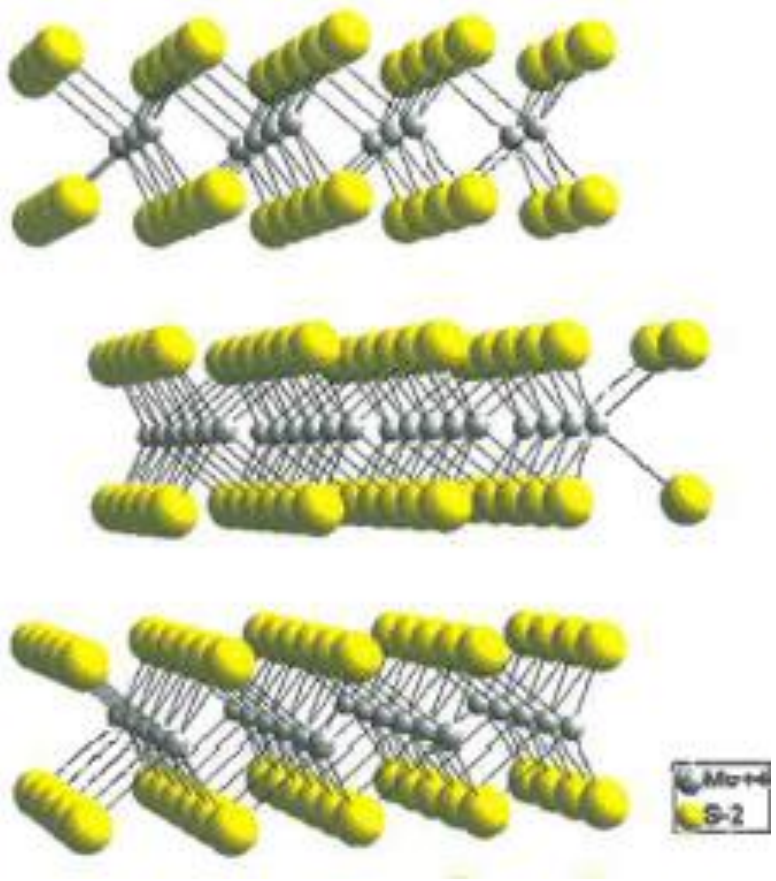
MoS_2



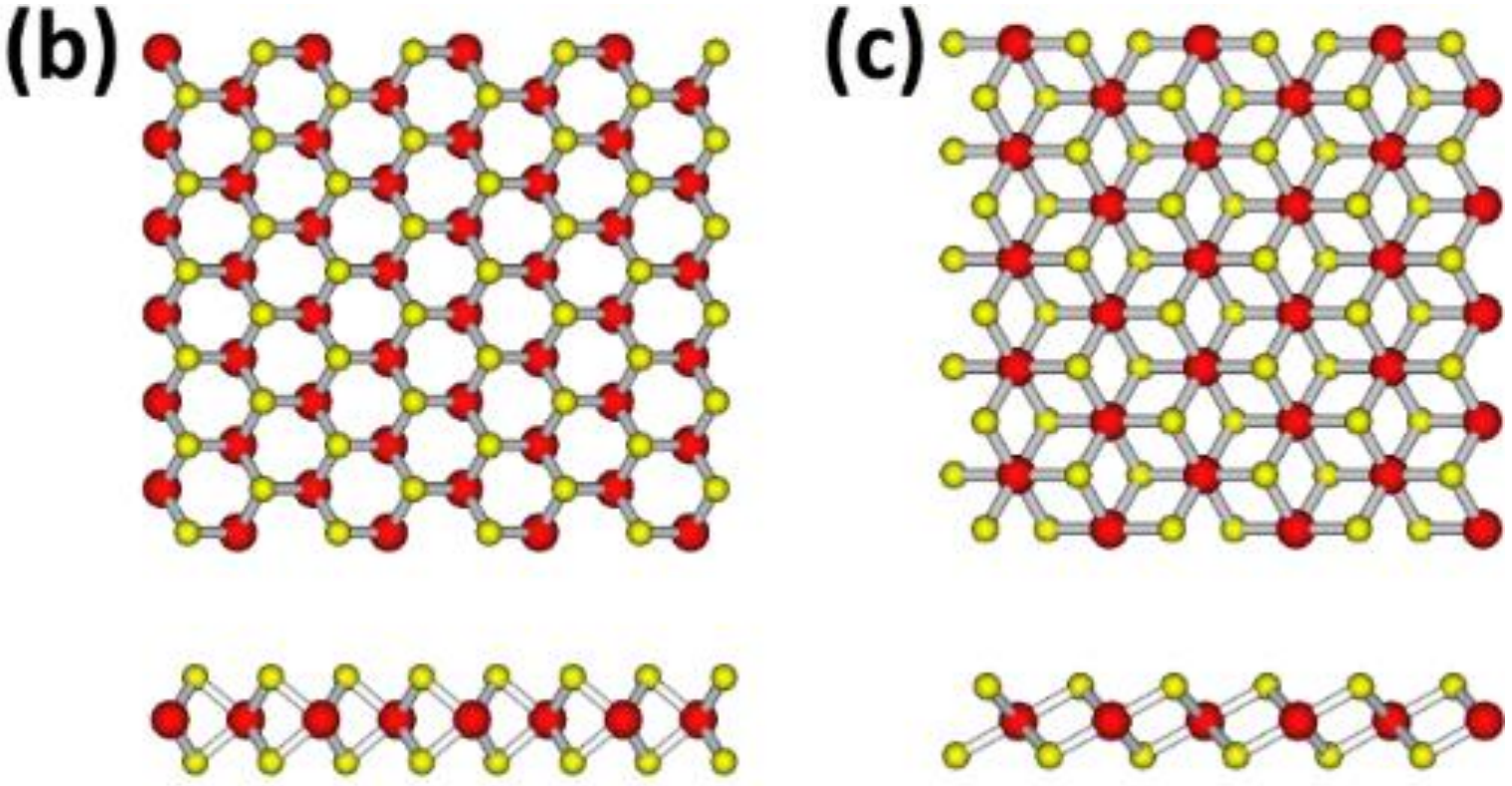
One dimensional structure

- TaS2
- WS2
- WSe2
- WTe2
- SiS2-type



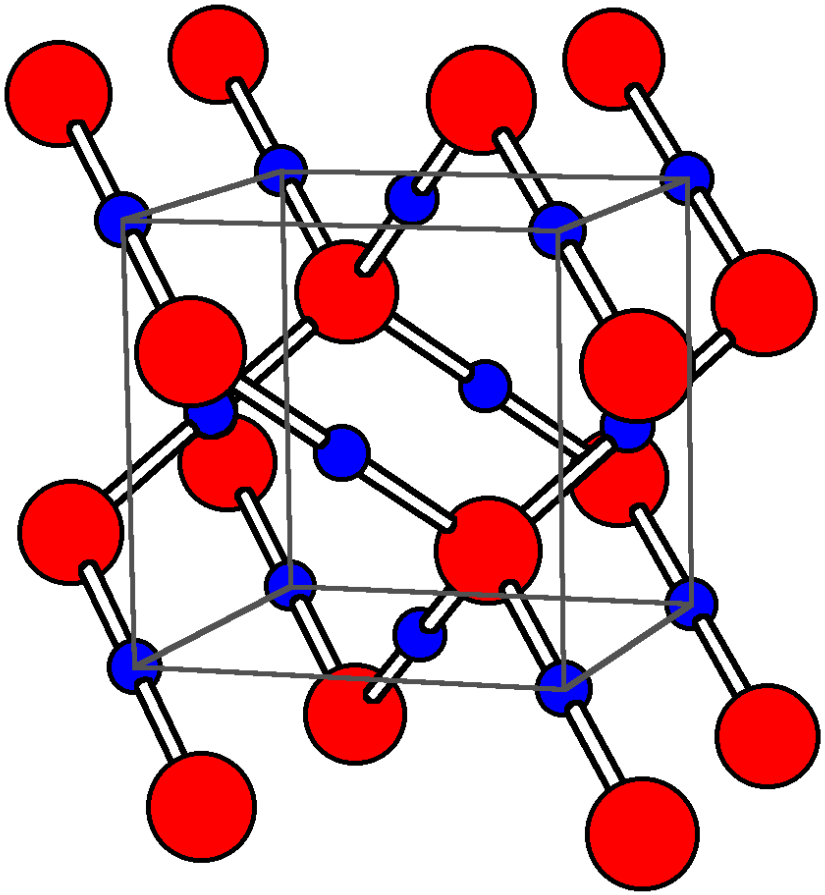


Comparison between TiS_2 and MoS_2 structures



Cu_2O Structure

- Cuprite

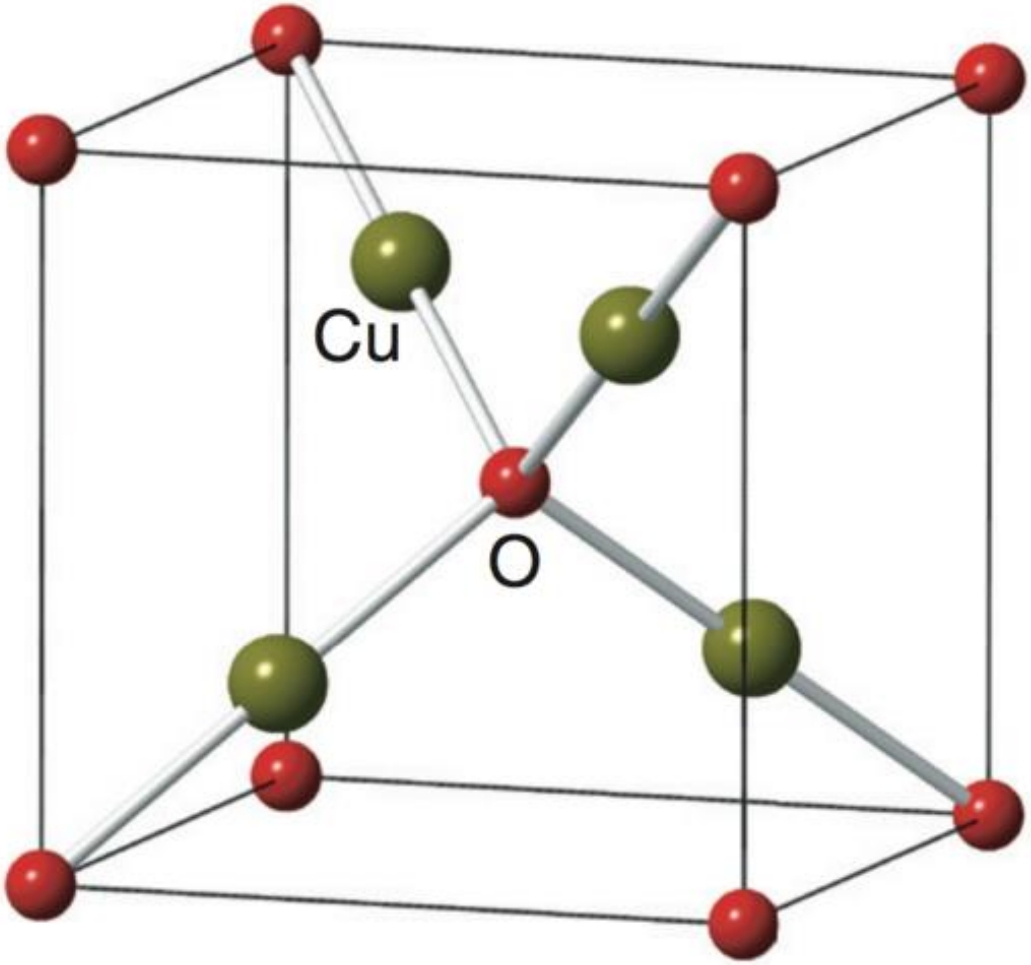


Oxygen

Cu

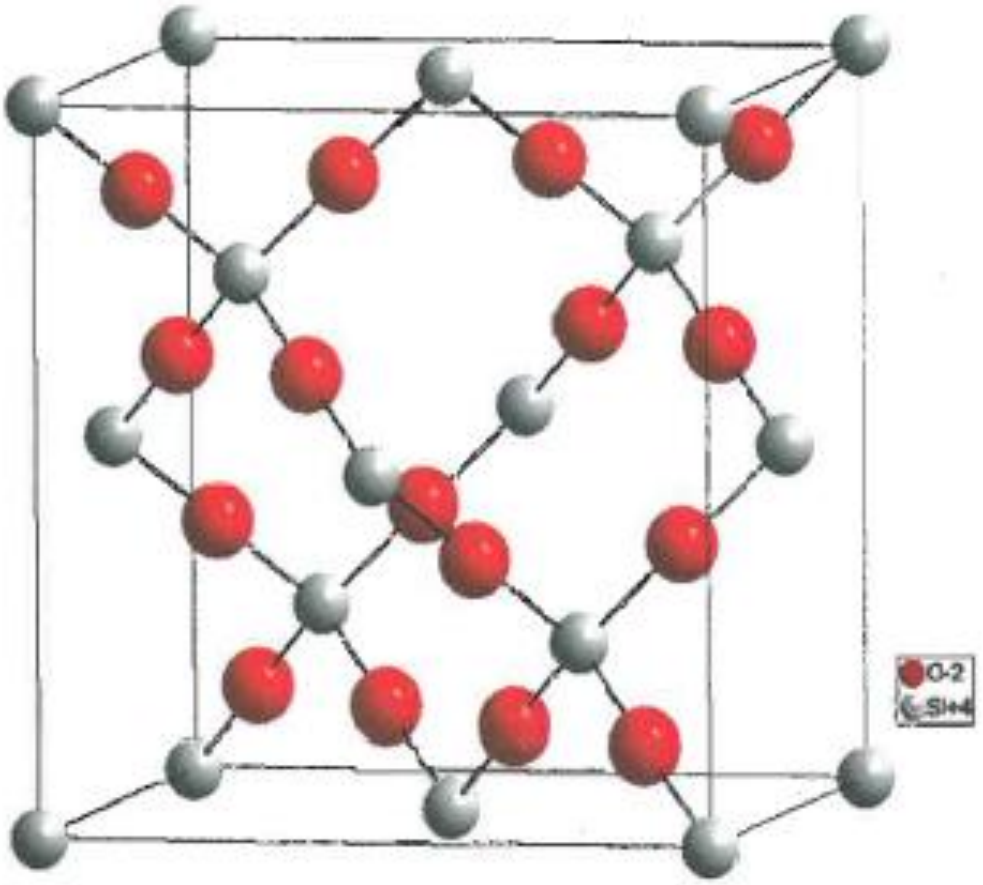
Ag2O

Cu_2O



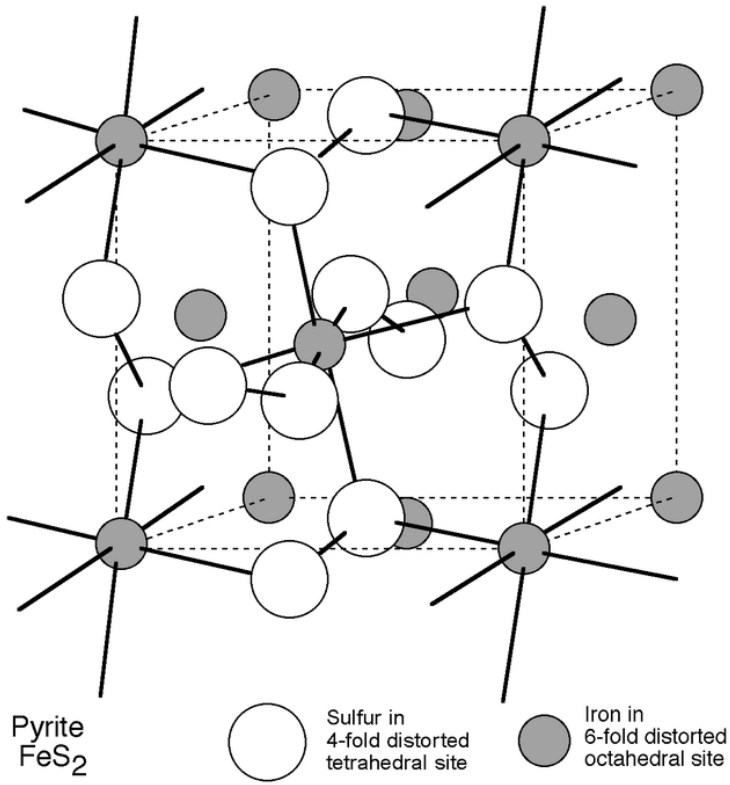
SiO_2

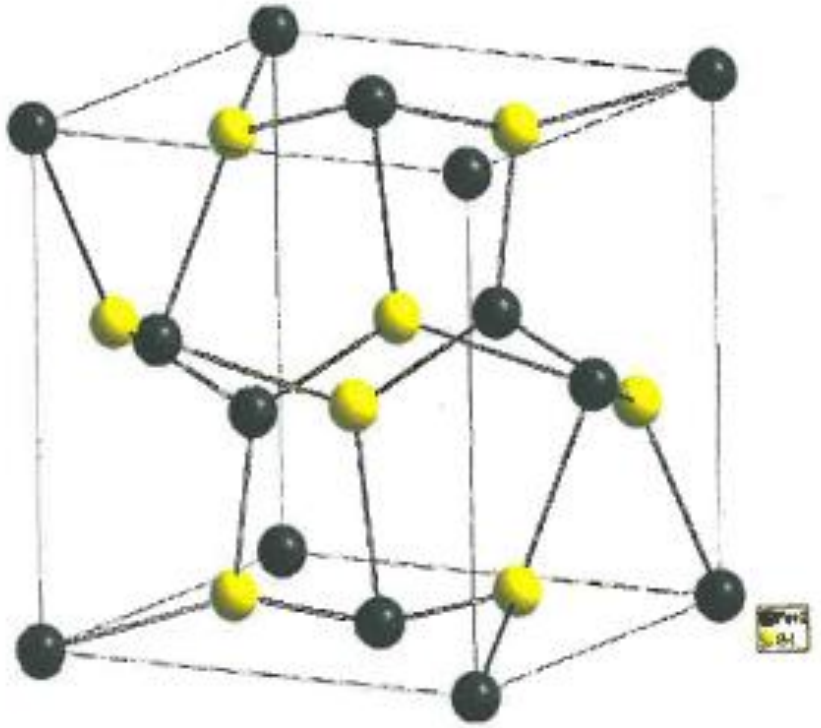
- Crystobalite is related to sphalerite…



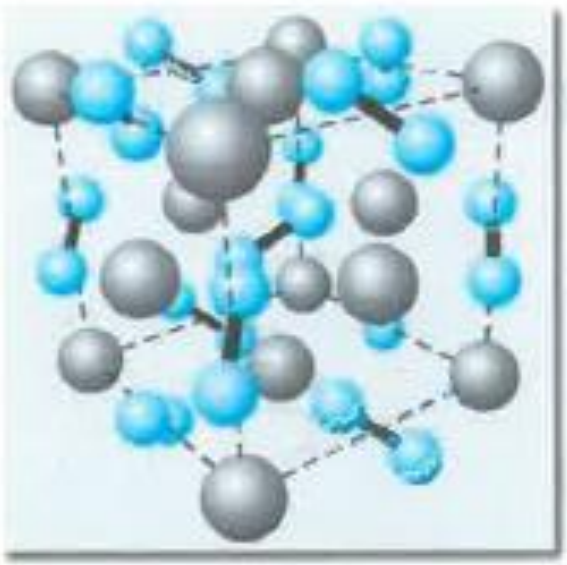
FeS_2-Type Pyrite

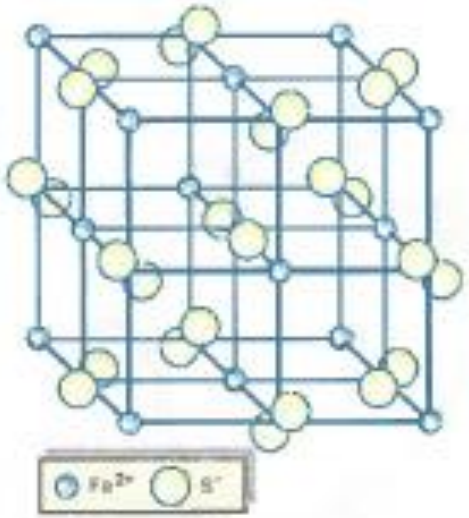
- RuS_2 $PdAs_2$ $(Mn, Fe, Co, Ni, Cu, Zn)S_2$
- OsS_2 $PtAs_2$ $(Mn, Fe, Co, Ni, Cu, Zn)Se_2$
- $RuSe_2$ $FeAs_2$ $(Mn, Fe, Co, Ni, Cu, Zn)Te_2$
- $RuTe_2$
- $FeSb_2$





Fool Structure



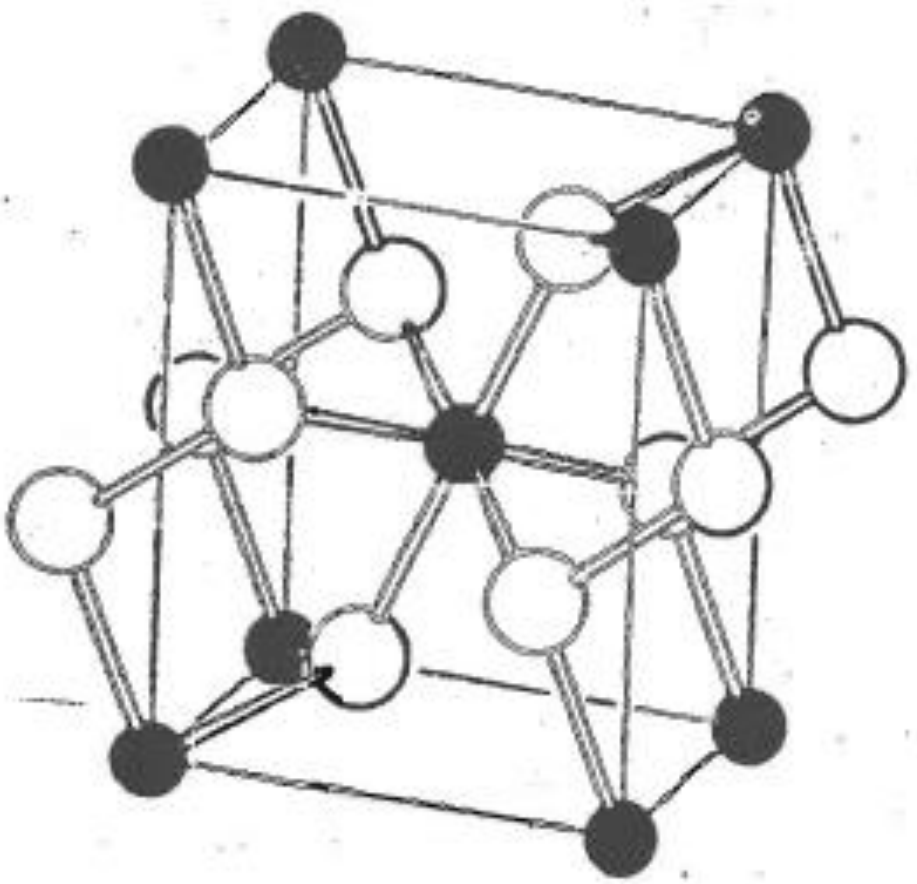


The cubic pyrite structure is related to rock salt…

FeS_2-Type Marcasite

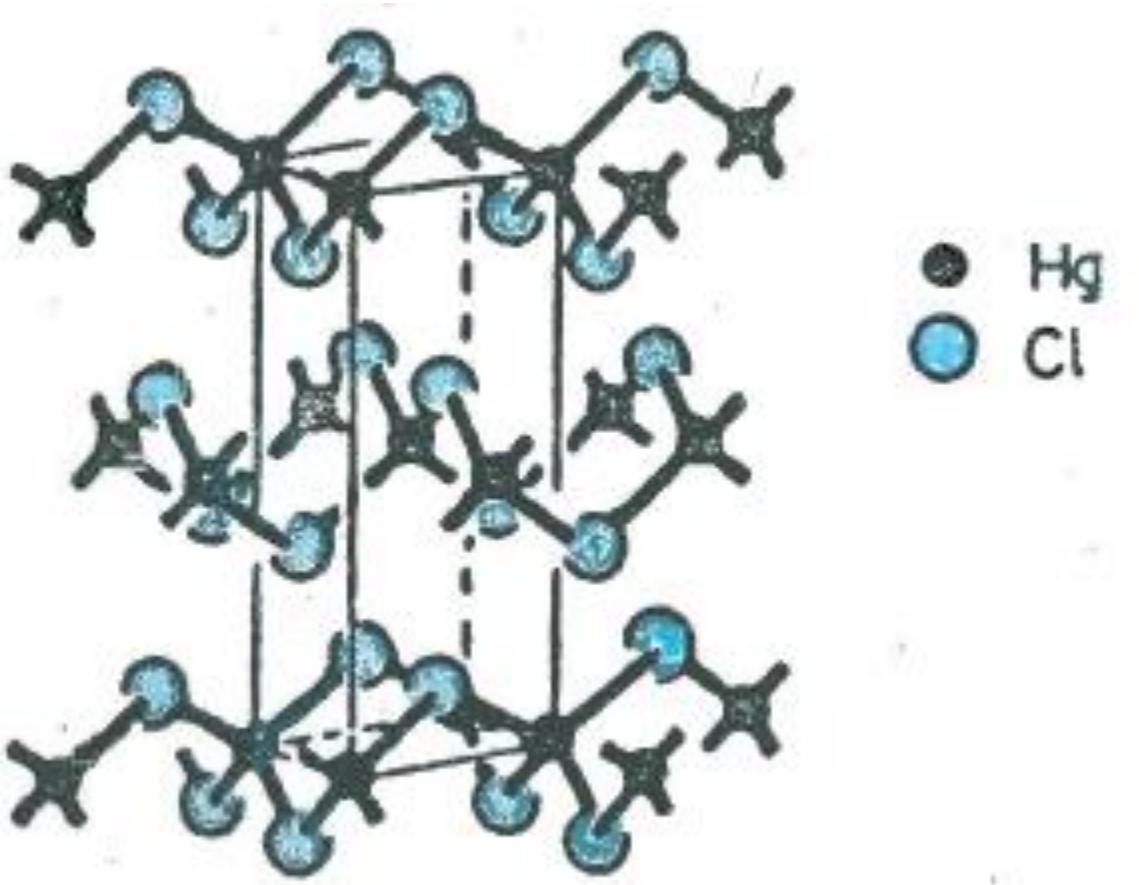
- Modification of the pyrite structure
- PtAs2
- FeSe2
- RuS2
- OsS2, $OsAs_2$
- Fe(SbS)
- Fe(AsS)

etc

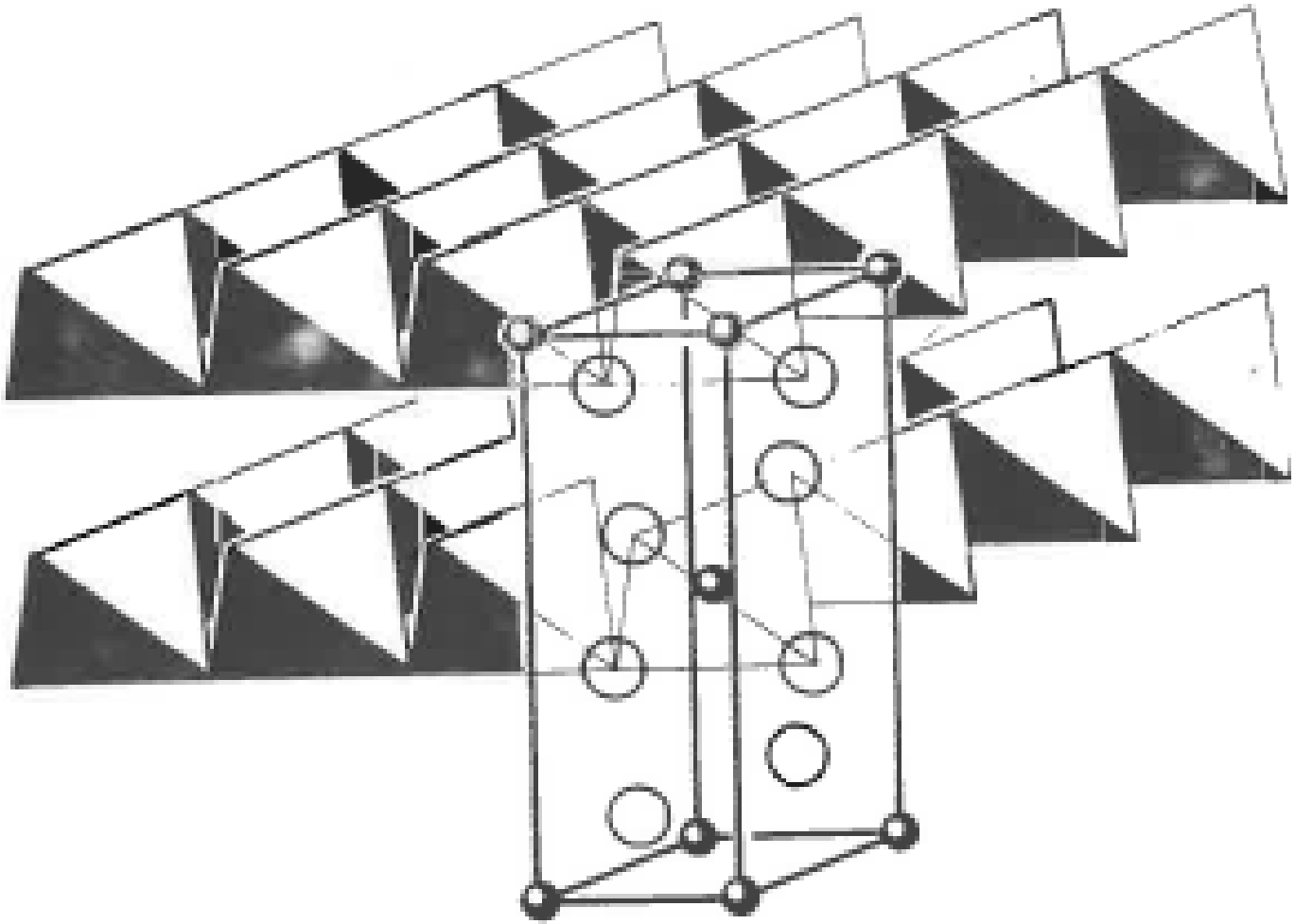


HgI_2-type: Layer structure

- $HgCl_2$
- $ZnBr_2$
- $Tl[FeS_2]^-$

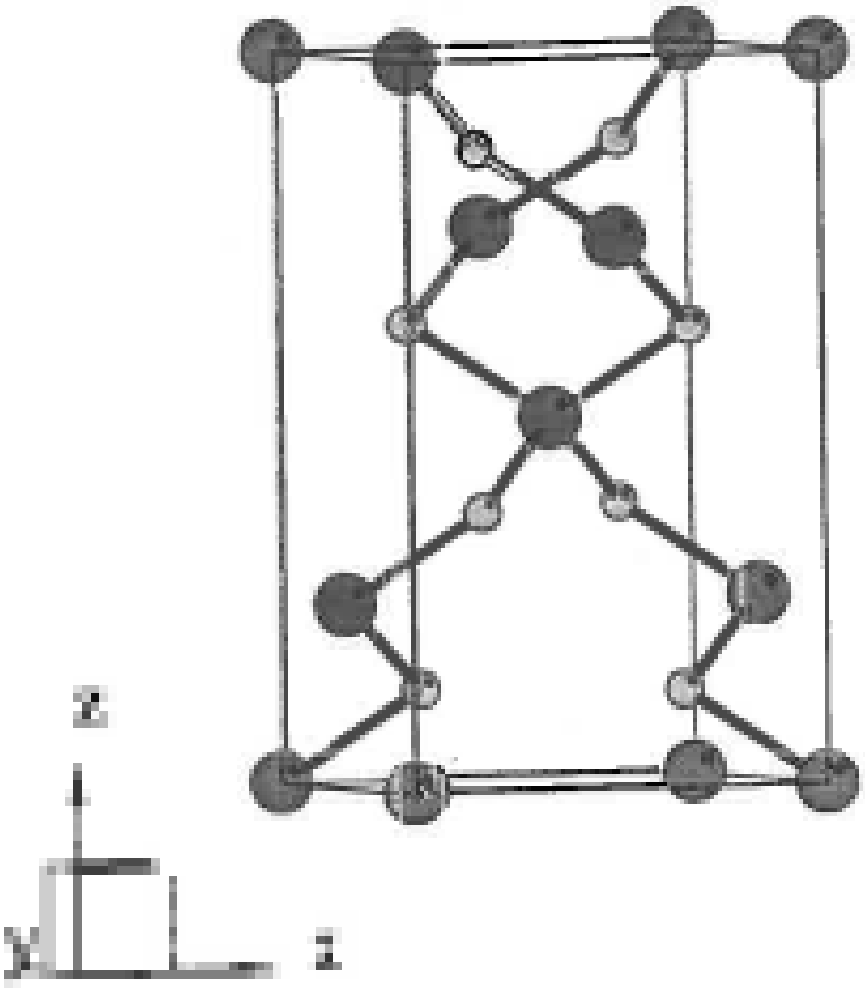


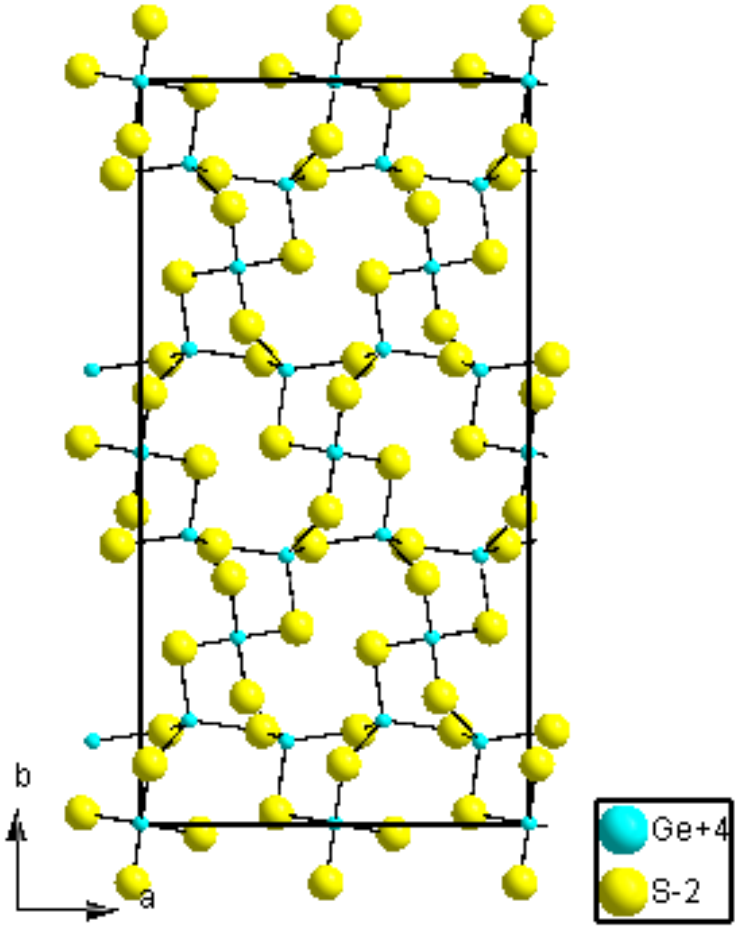
Polyhedral Representation of HgI_2



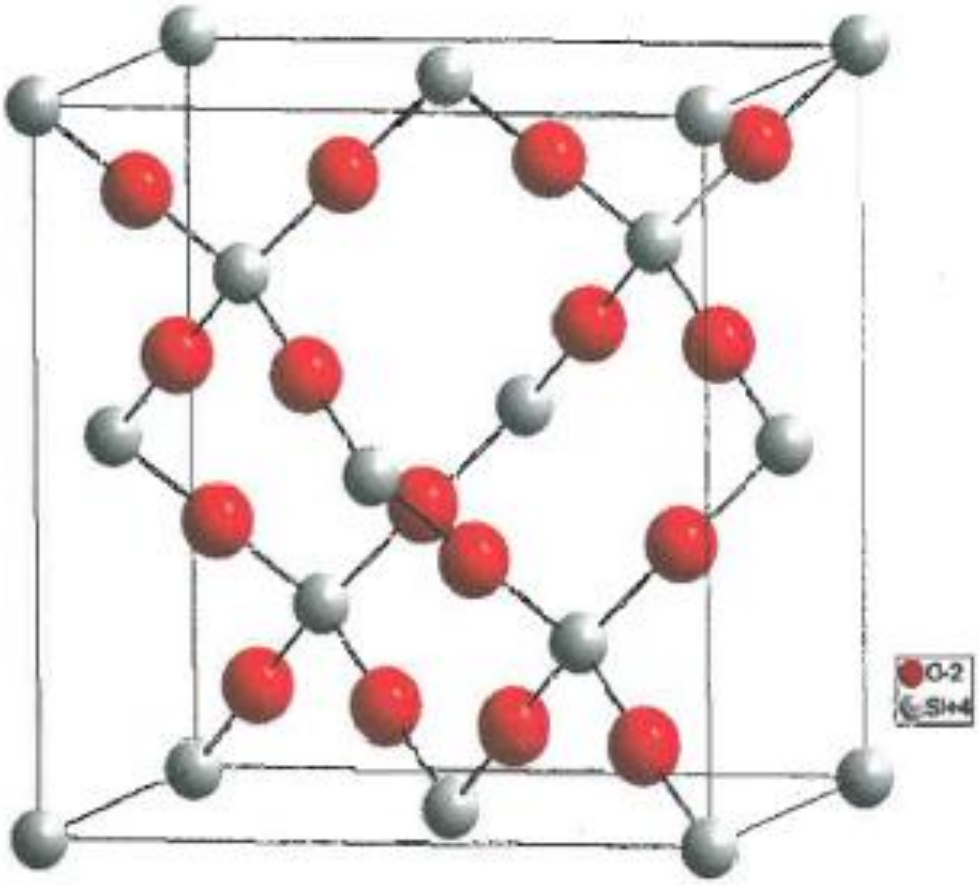
The structure of HgI_2 (red form).

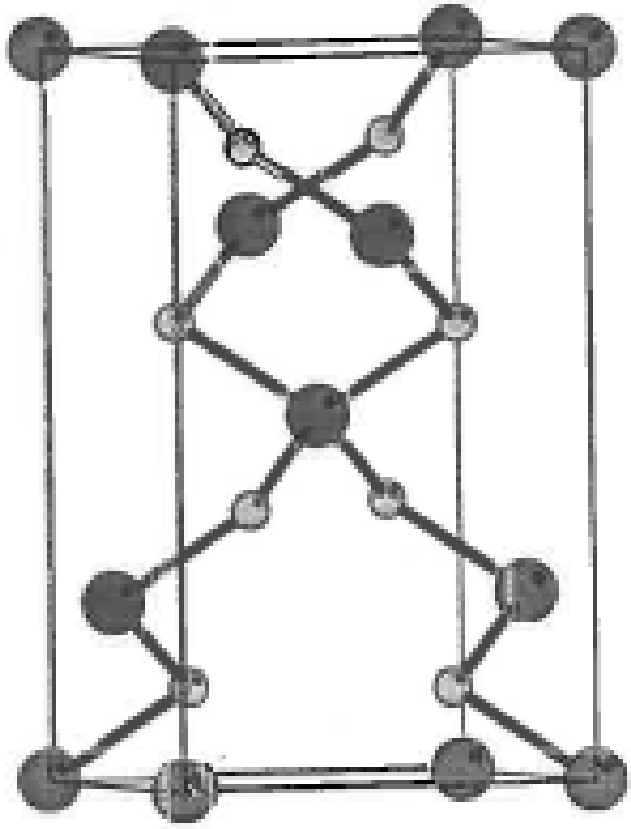
GeS_2



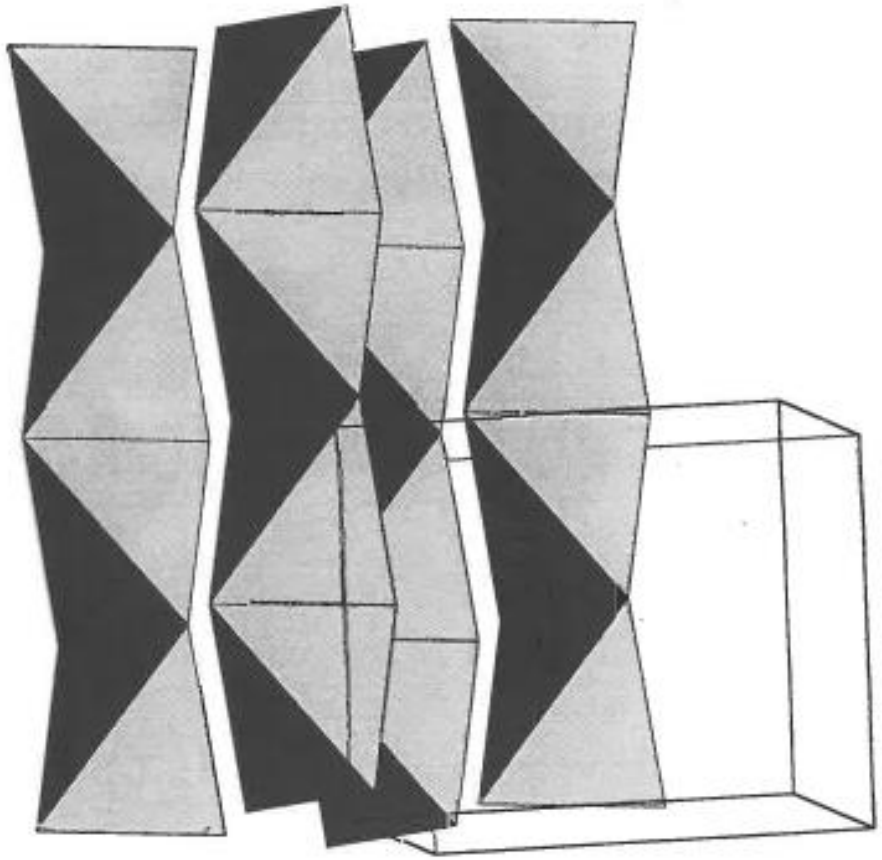


Comparison of SiO_2 and GeS_2

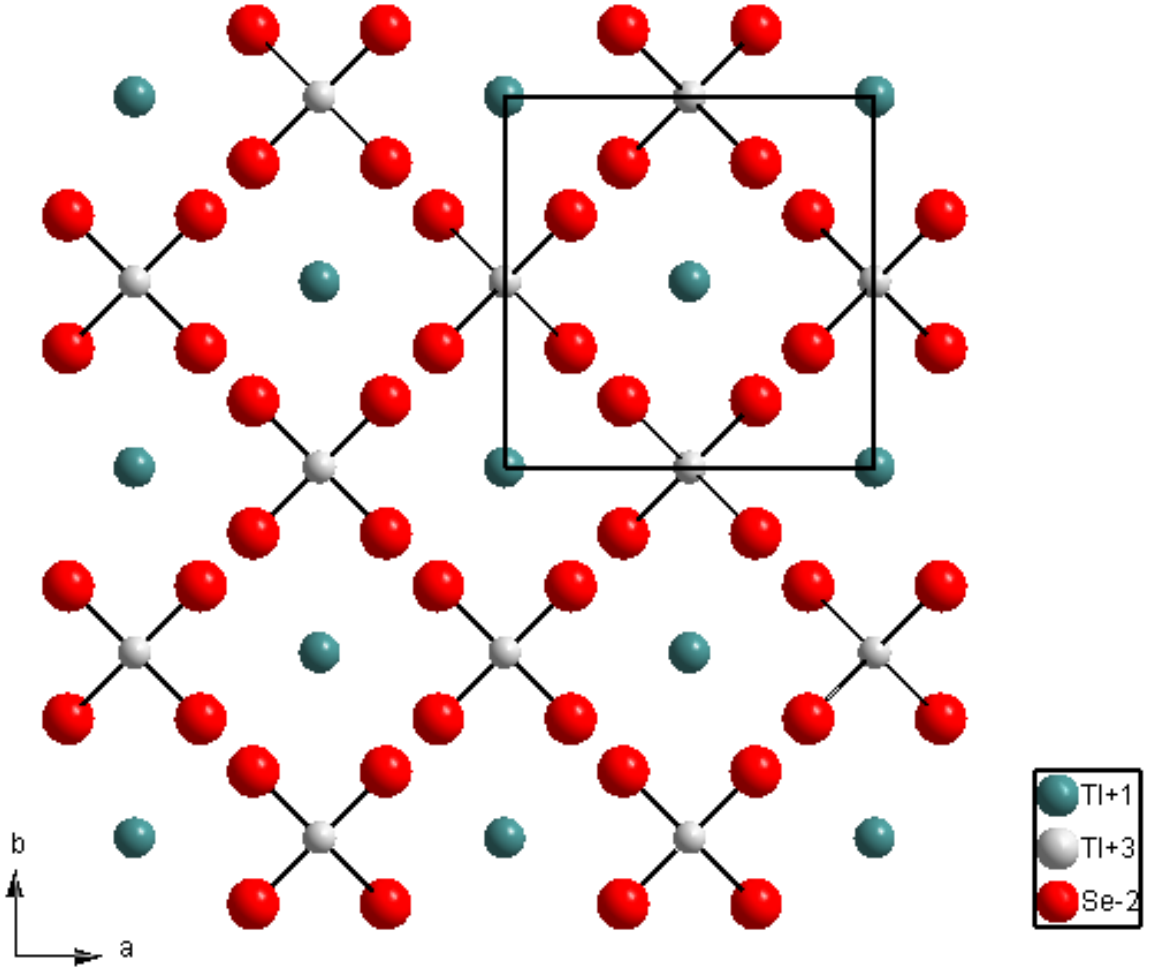




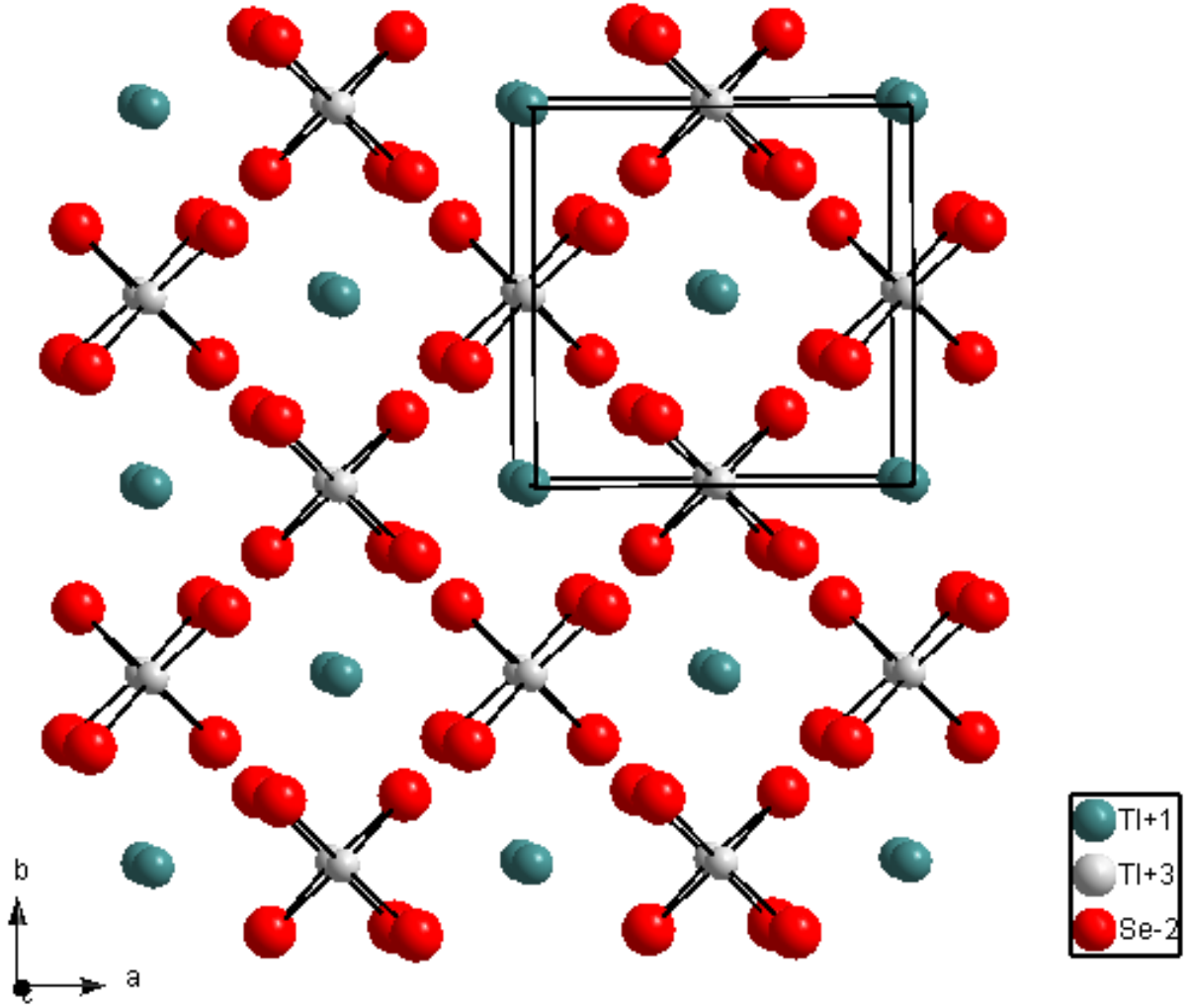
TlSe: The SiS_2-type chains (Tl^{3+})



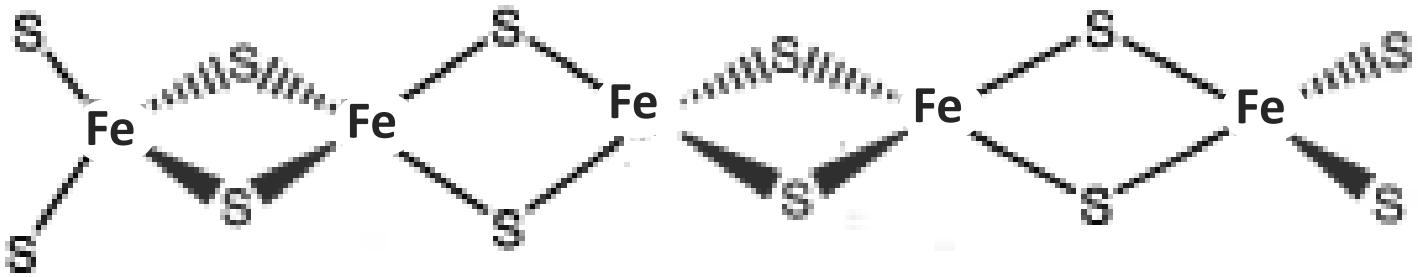
TlSe: The SiS_2-type chains (Tl^{3+})



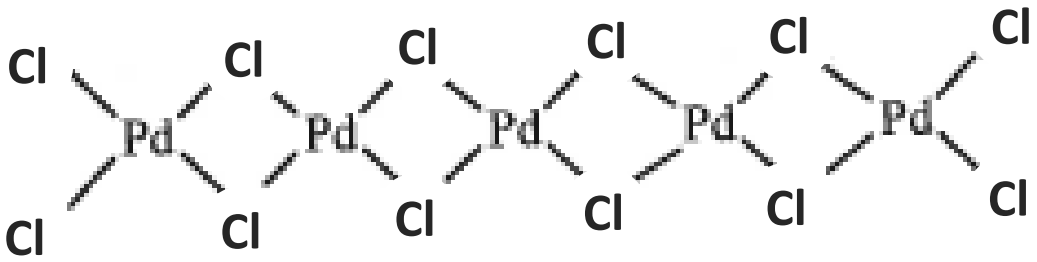
TlSe: The SiS_2-type chains (Tl^{3+})



$K^+[FeS_2]^-$ $K_2[SiP_2]$ $Ba[FeS_2]$



$PdCl_2$-type: One-dimensional



$K_2[PtS_2]$ $Na_2[PdS_2]$

SiO_2-Crystobolite

Triymite

PdS_2-type

- $PdSe_2$ •PdSSe • PdPS

Structure derives from making 3D marcasite 2D