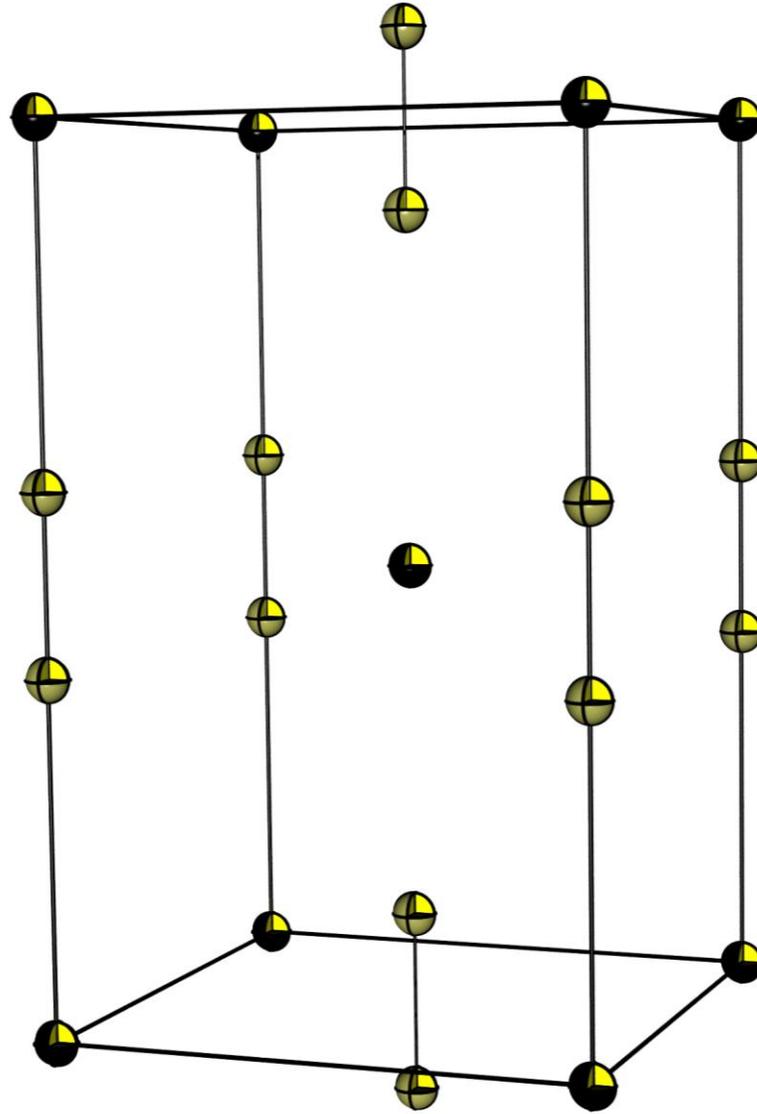


AC III
Übung 4

1) CaC_2

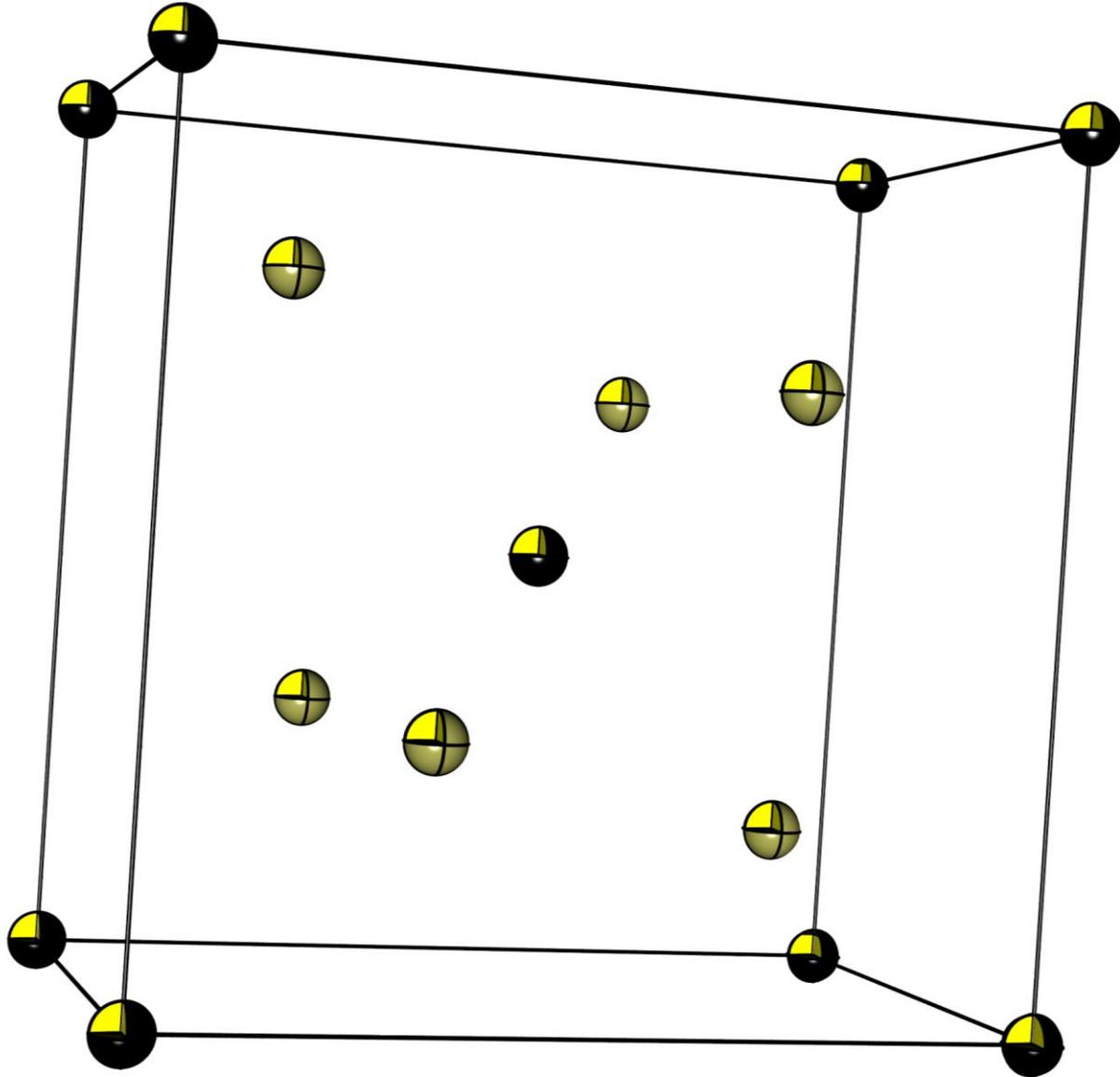
Aufgabe 1.



Jeweils tetragonal innenzentrierte

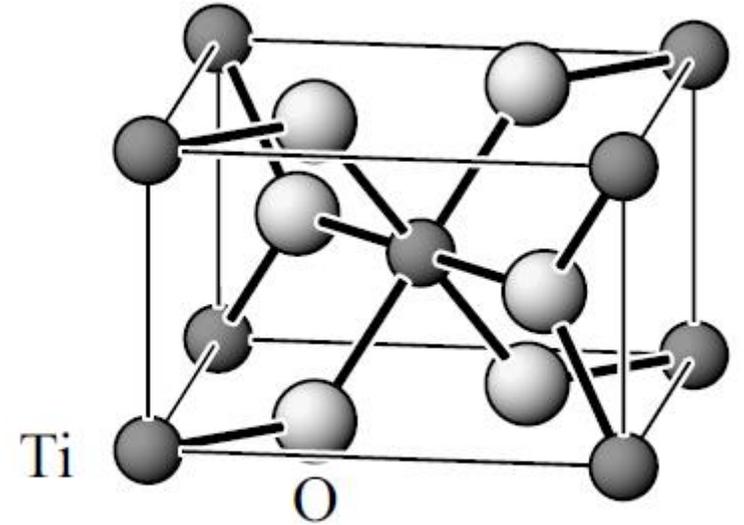
Alle OL besetzt

2) Rutil



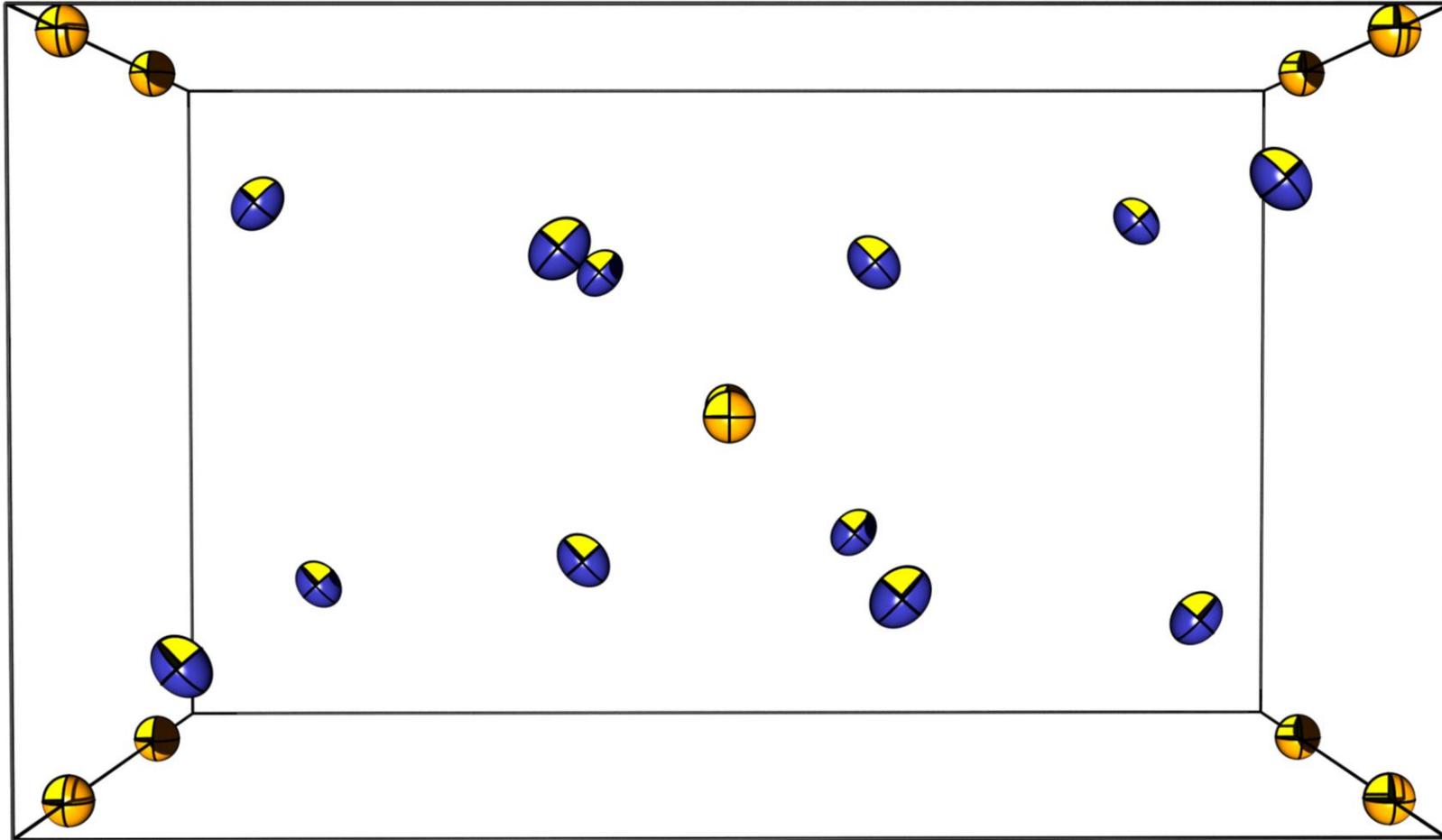
hcp (O^{2-}) + 1/2 Oktaederlücken Ti^{4+}

Über 2 Kanten verknüpfte Oktaeder



Rutil-Typ $P4_2/mnm$

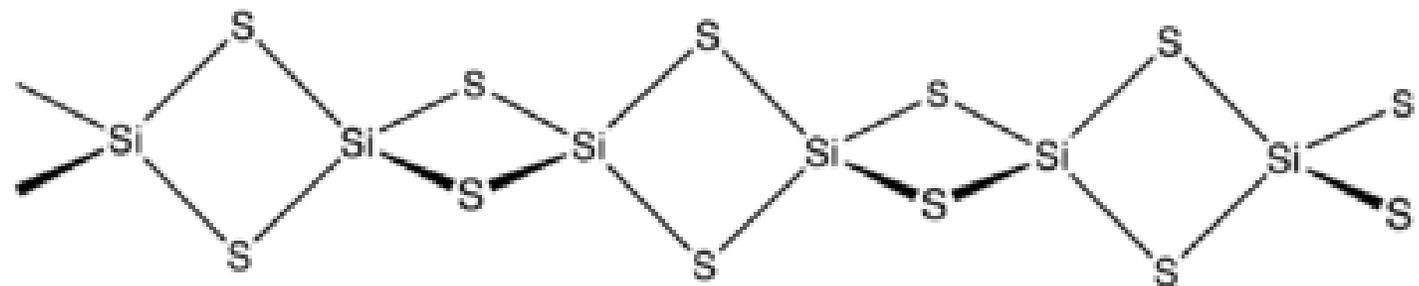
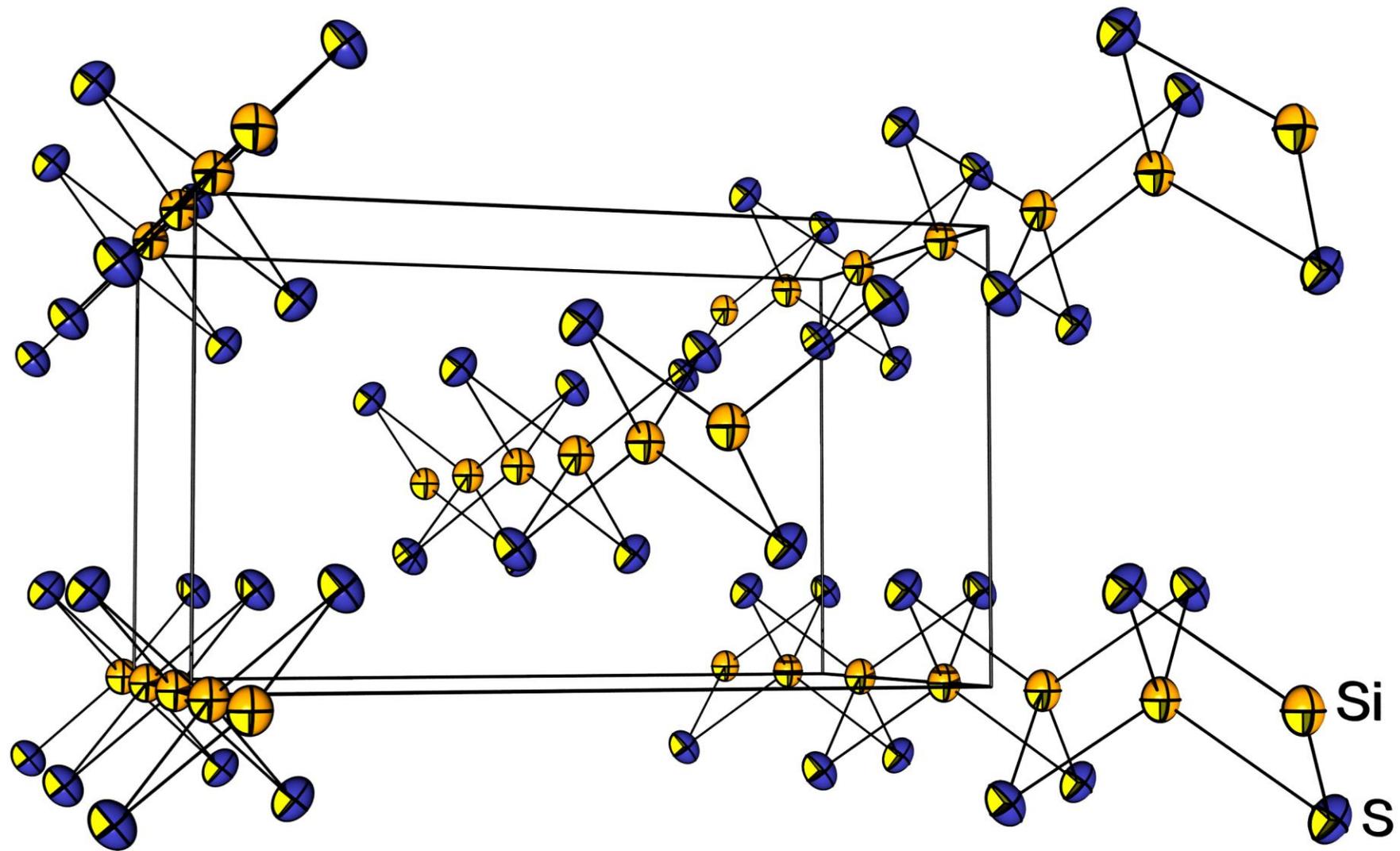
3) SiS₂



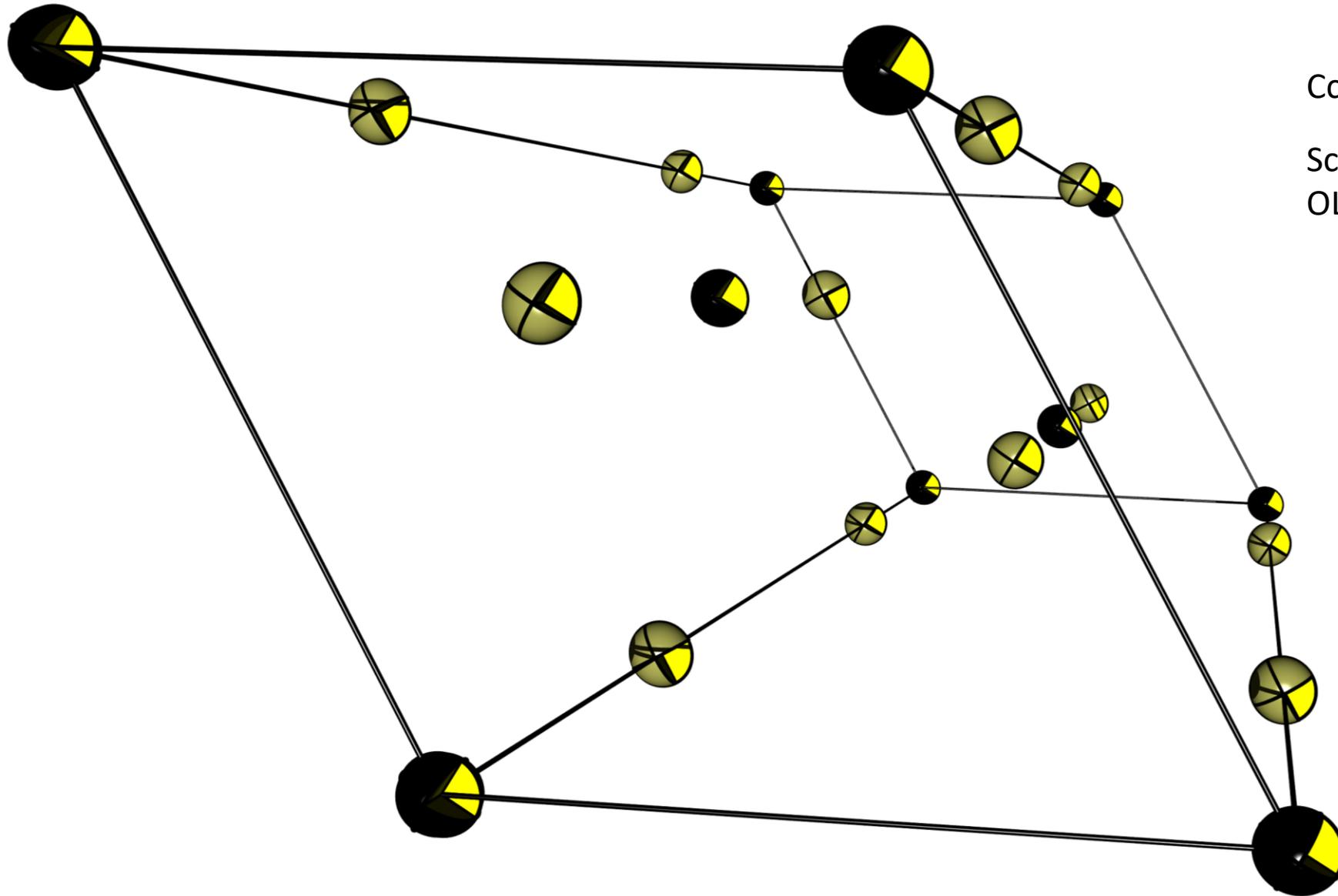
Faserstruktur

Verzerrt ccp (S²⁻) mit ¼
Tetraederlücken mit Si⁴⁺
besetzt

3) SiS₂



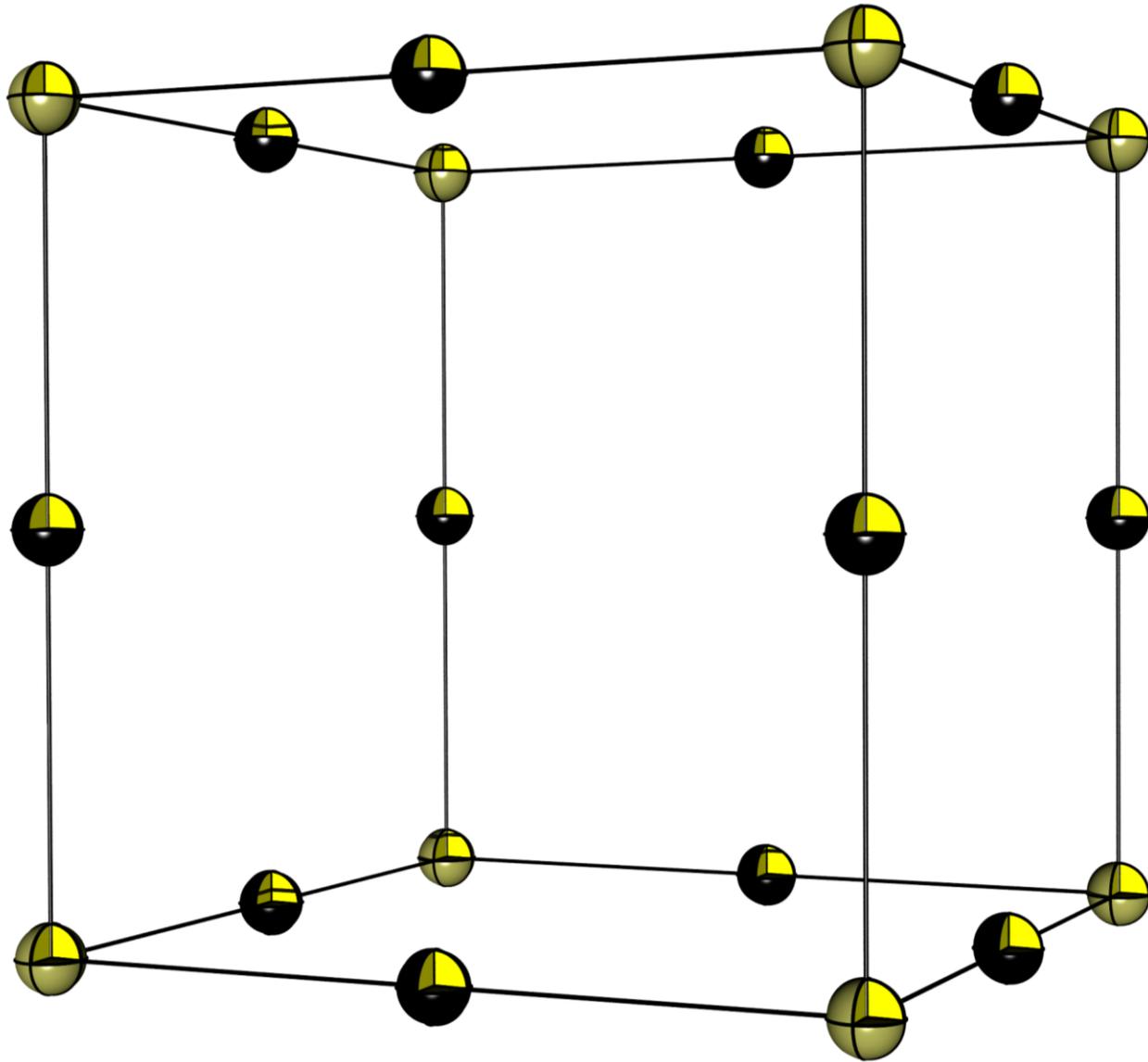
4) CdCl₂



Ccp (Cl⁻) + ½ OL besetzt mit Cd²⁺

Schichtstruktur (Jede 2. Schicht alle OL besetzt)

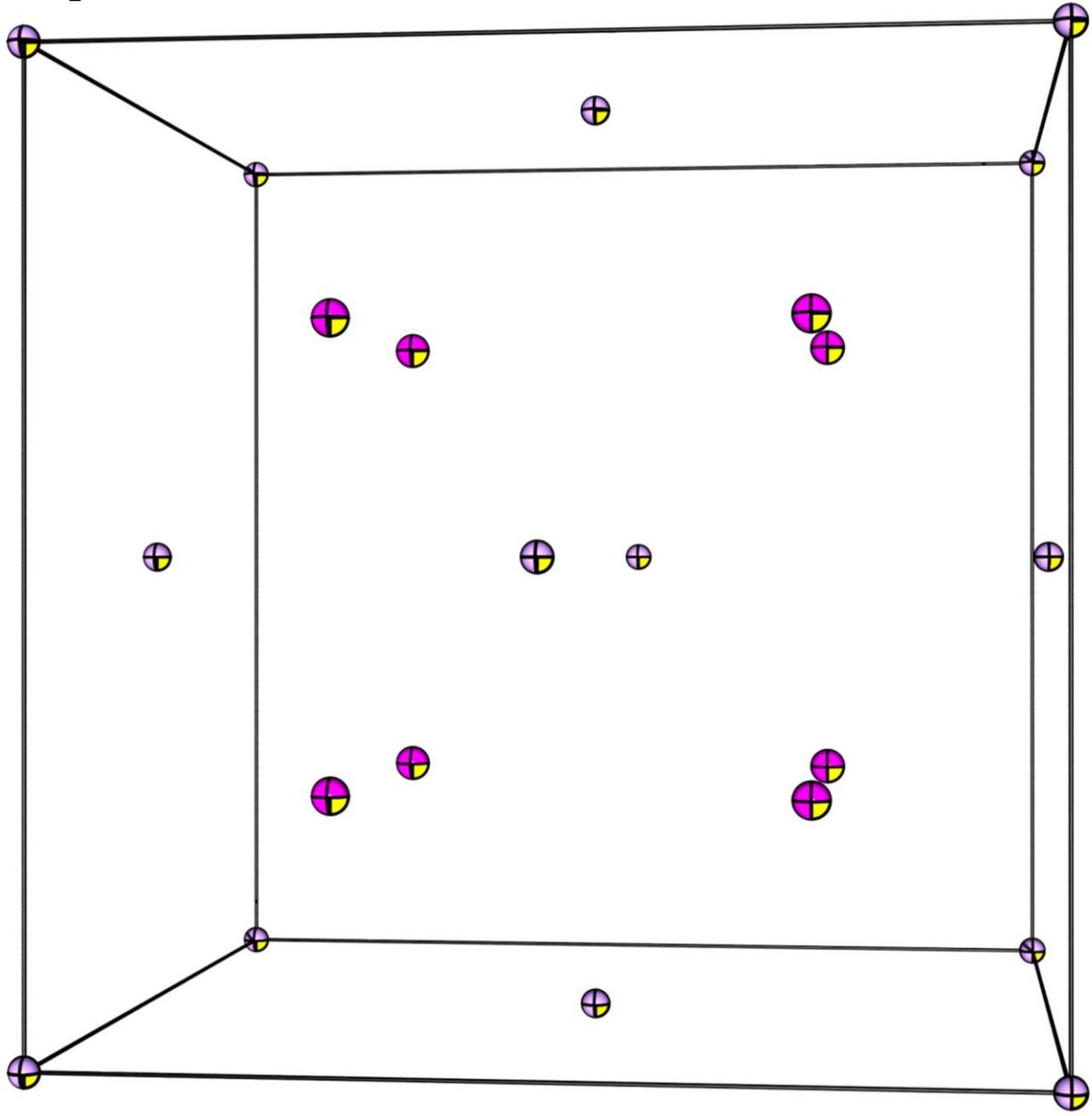
5) ReO_3



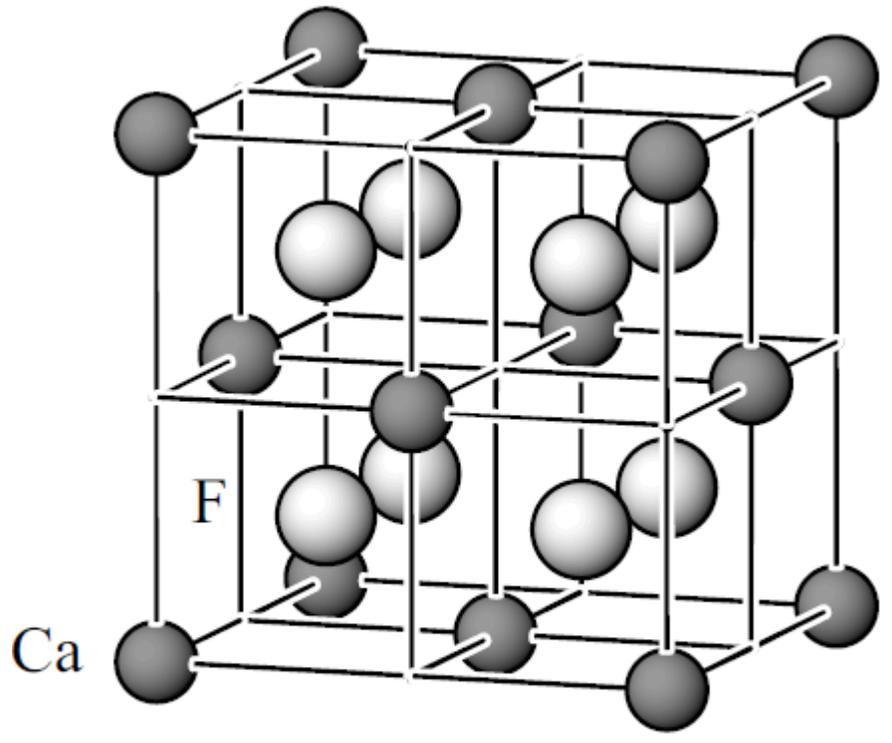
Über alle Ecken verknüpfte O^{2-}
Oktaeder

Kubisch primitiv (Re^{6+})

6) CaF₂



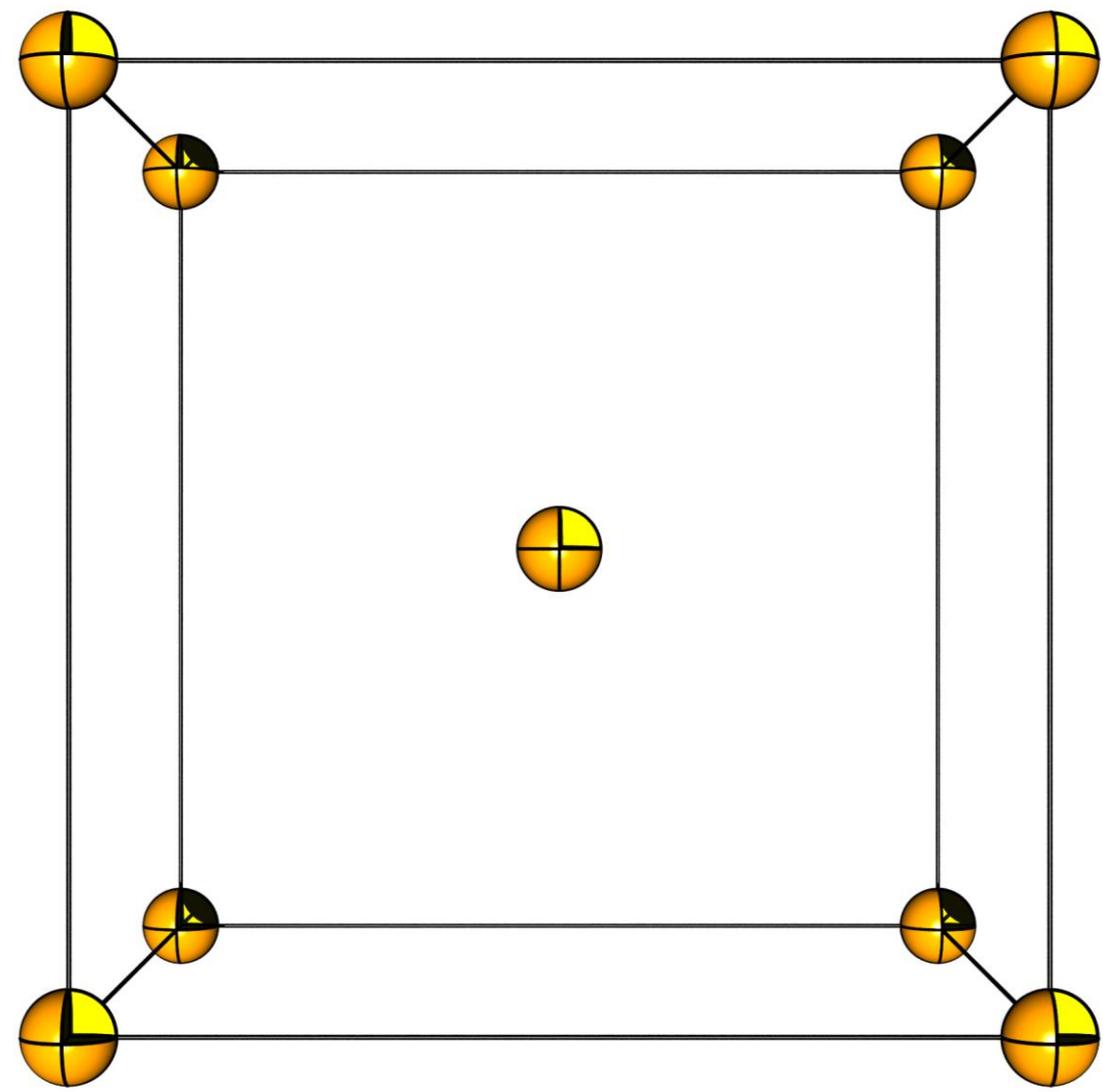
ccp (Ca²⁺) + alle TL mit F⁻ besetzt



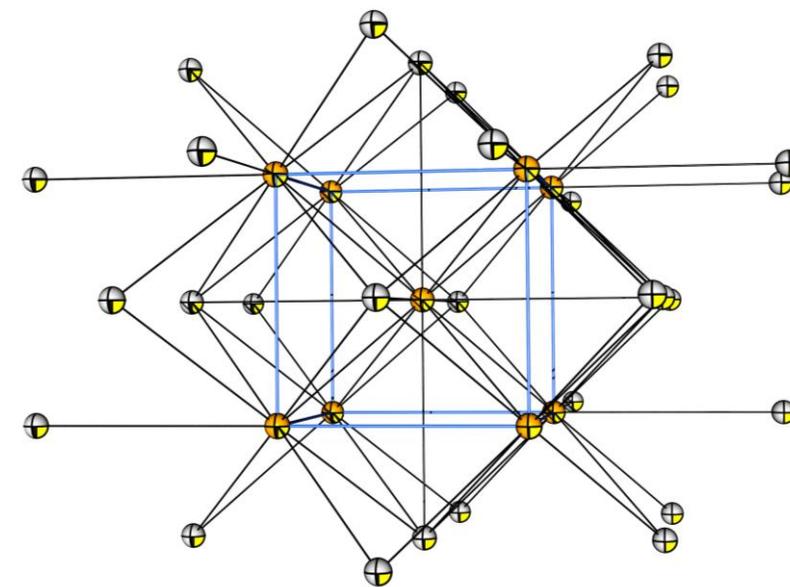
Fluorit-Typ

$Fm\bar{3}m$

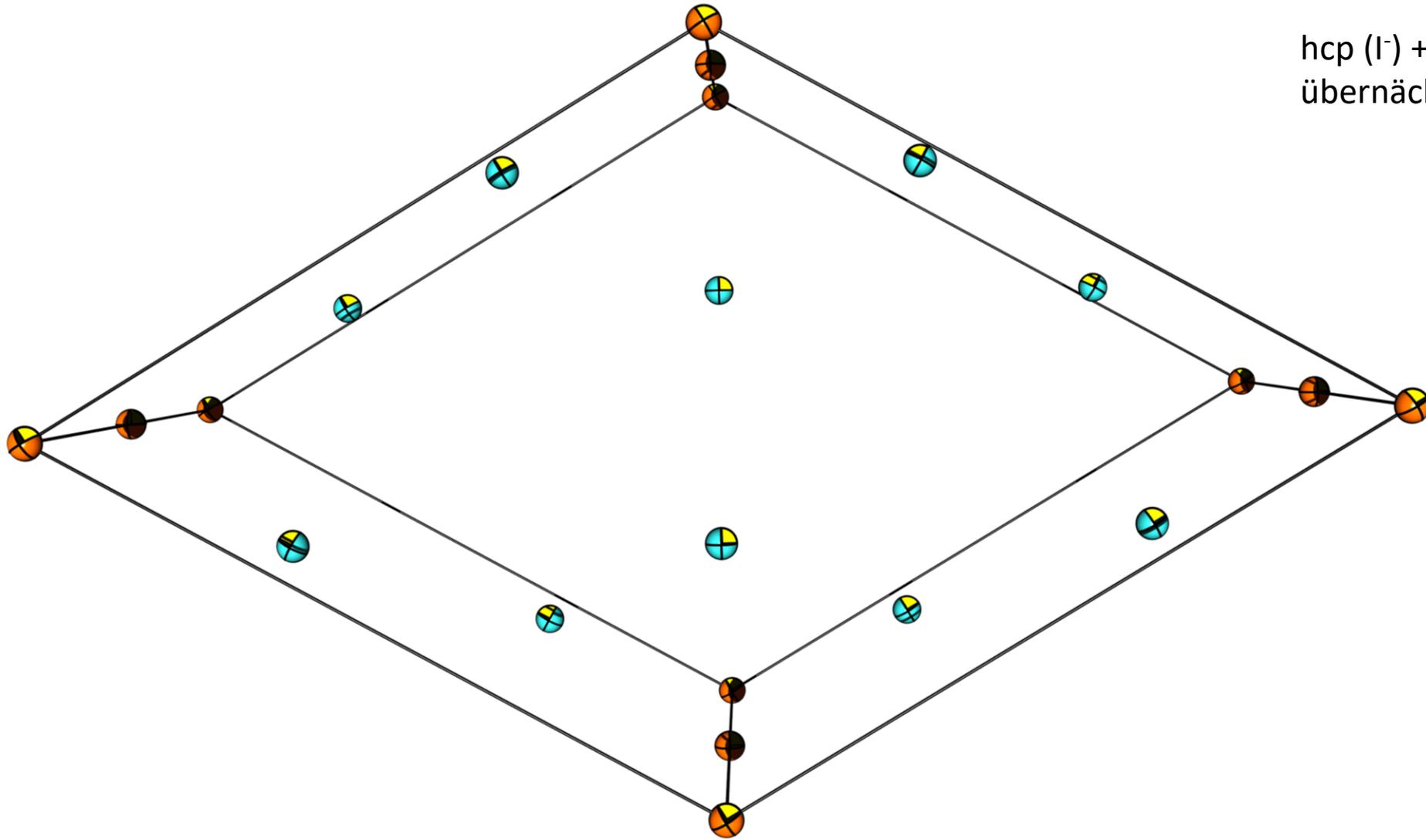
7) W



Kubisch innenzentriert

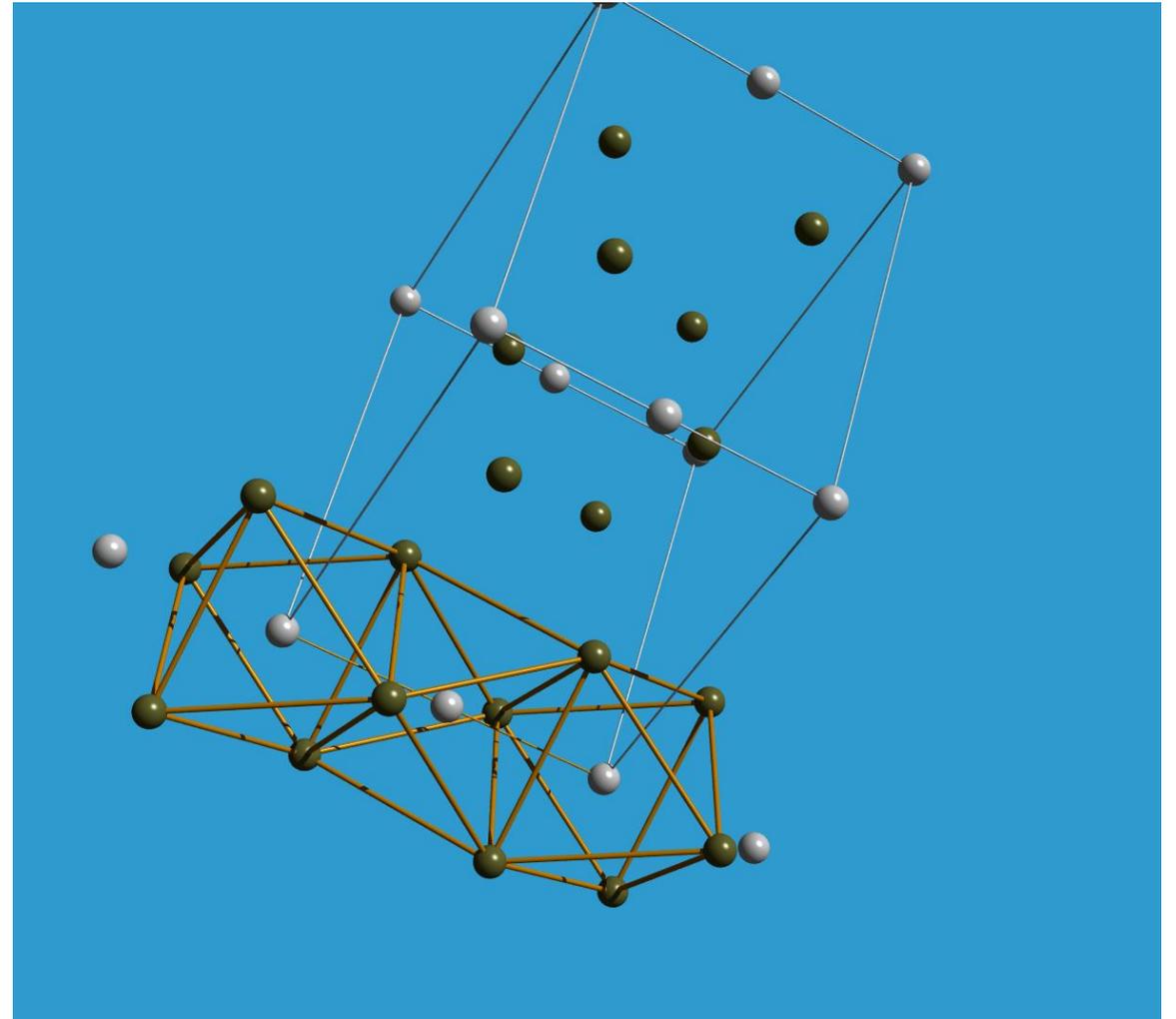
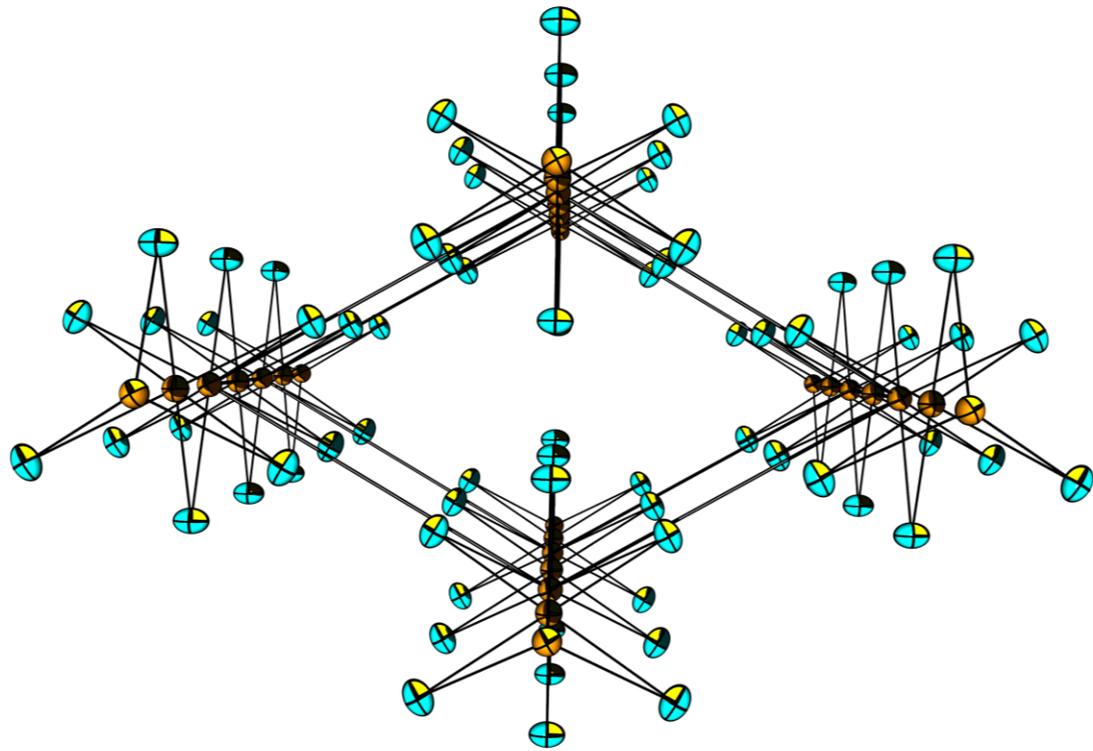


8) ZrI_3

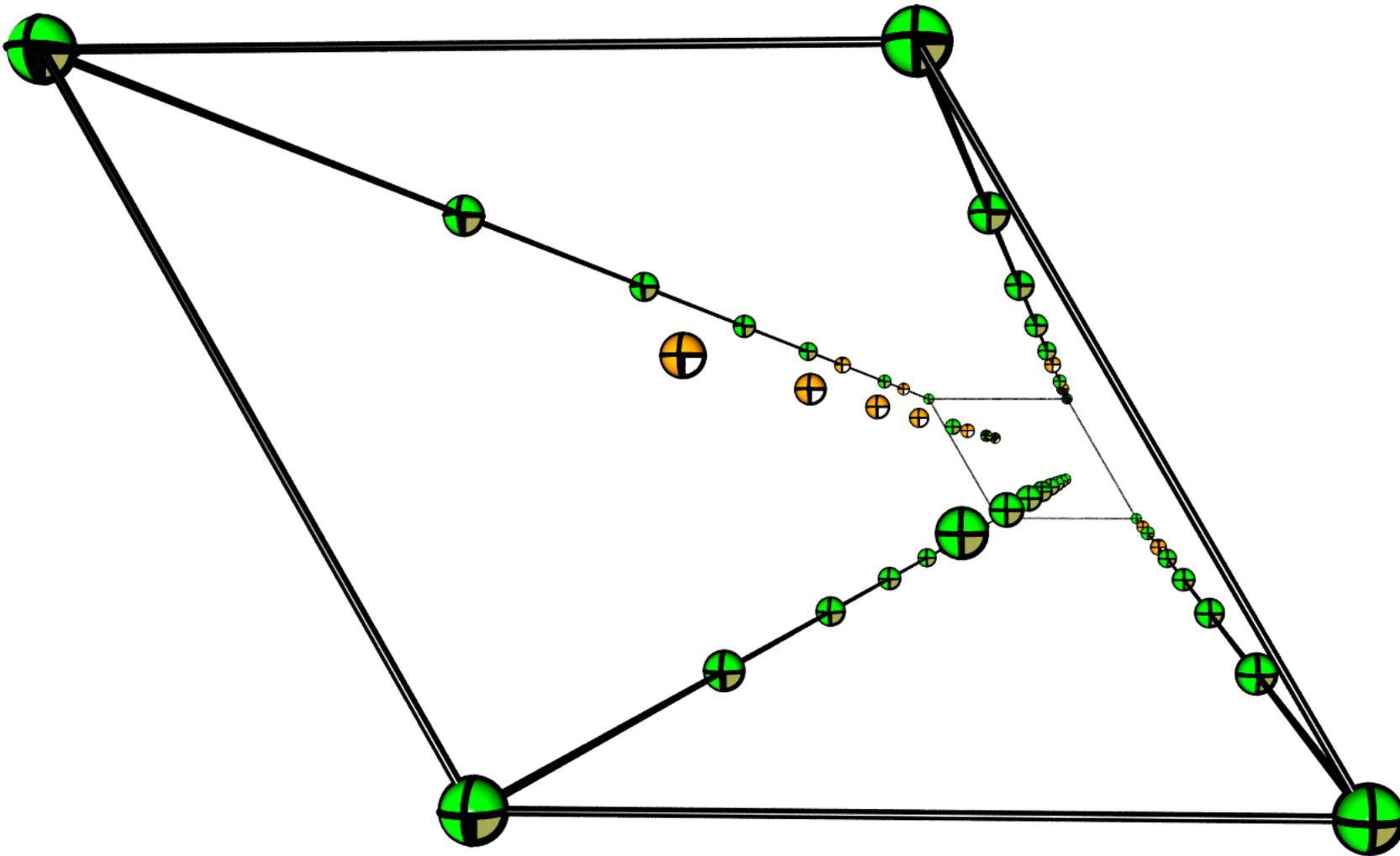


hcp (I⁻) + Zr³⁺ in den OL jeder
übernächsten „Röhre“

8) ZrI_3

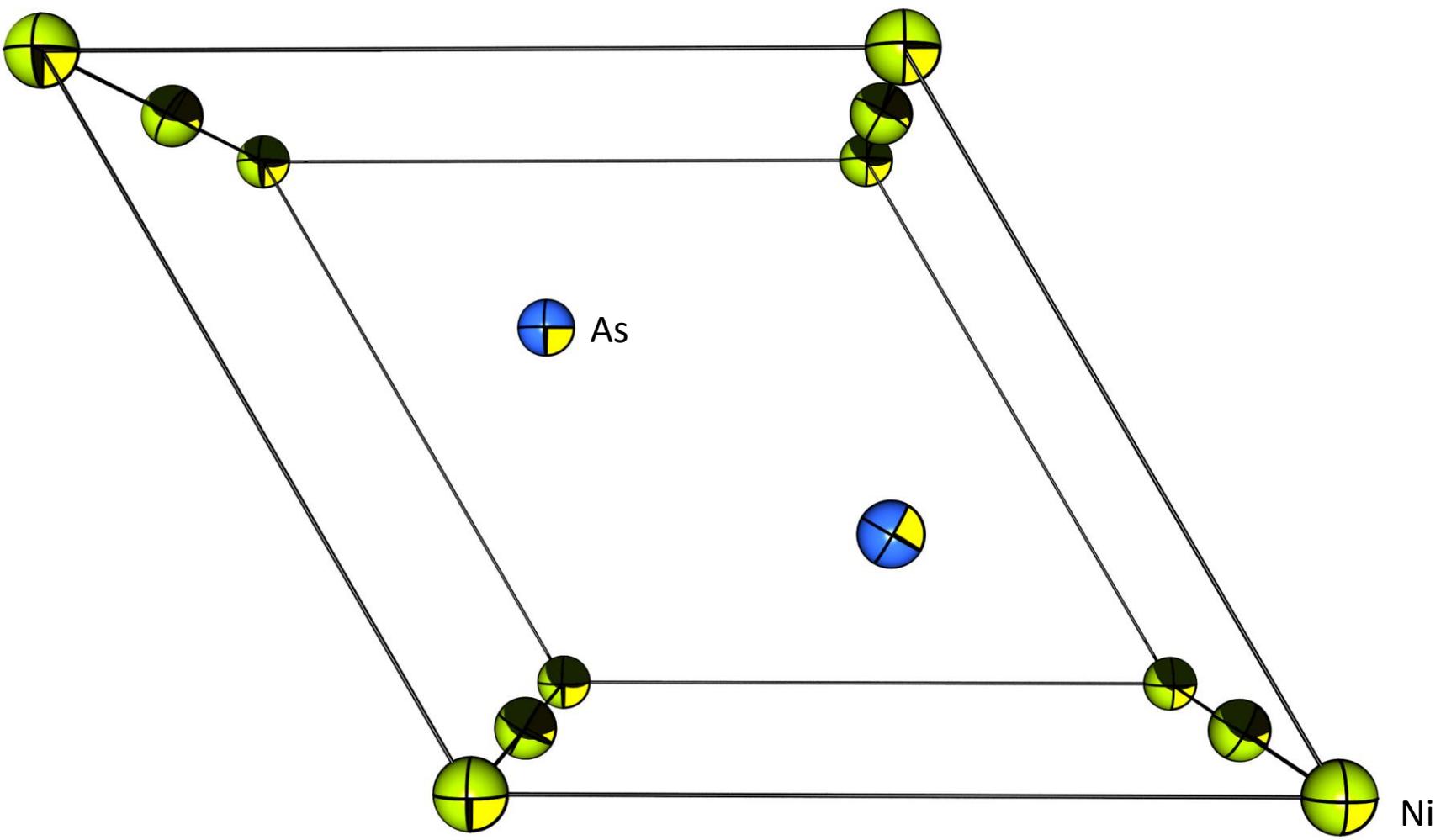


9) CdI_2



hcp (I^-) + $\frac{1}{2}$ OL Cd^{2+} (alle OI in jeder zweiten Schicht)

10) NiAs

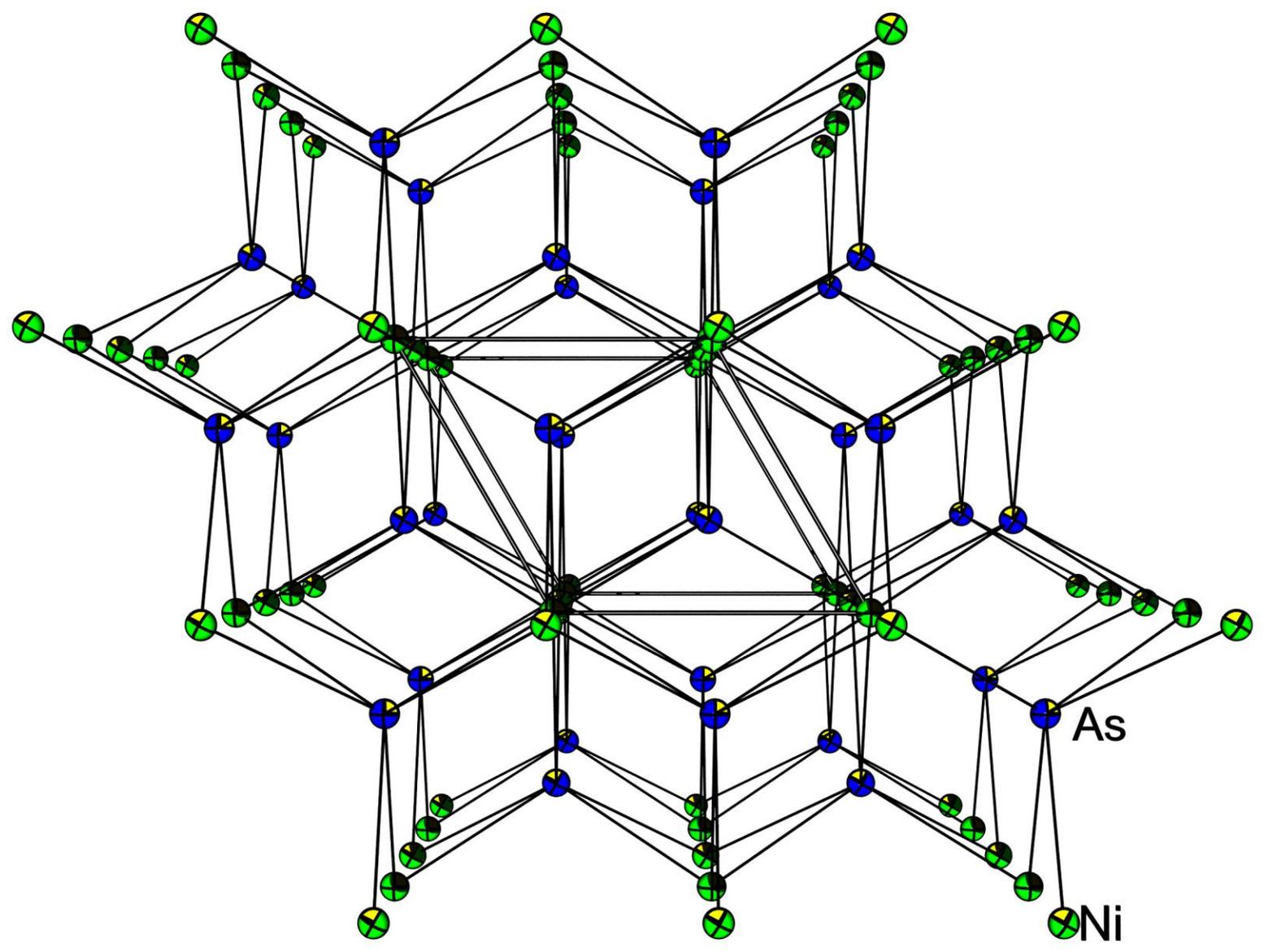


hcp (As^{2-}) + alle OL (Ni^{2+})

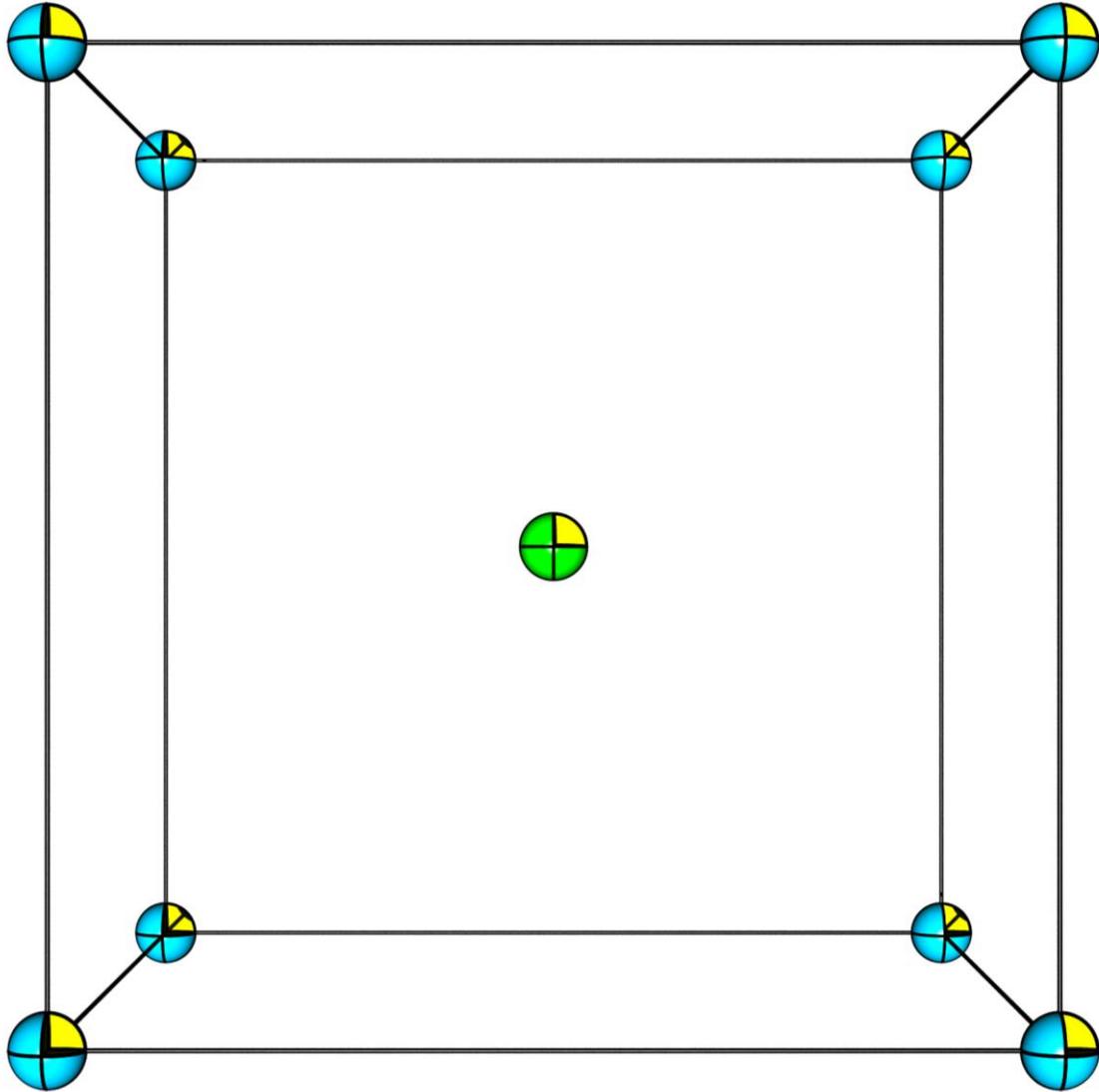
→ Ni_6As Prismen

→ NiAs_6 Oktaeder

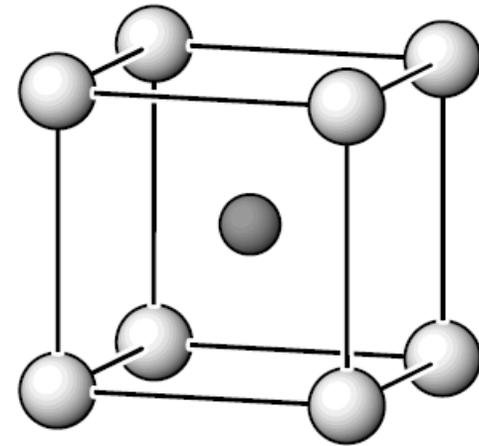
10) NiAs



11) CsCl

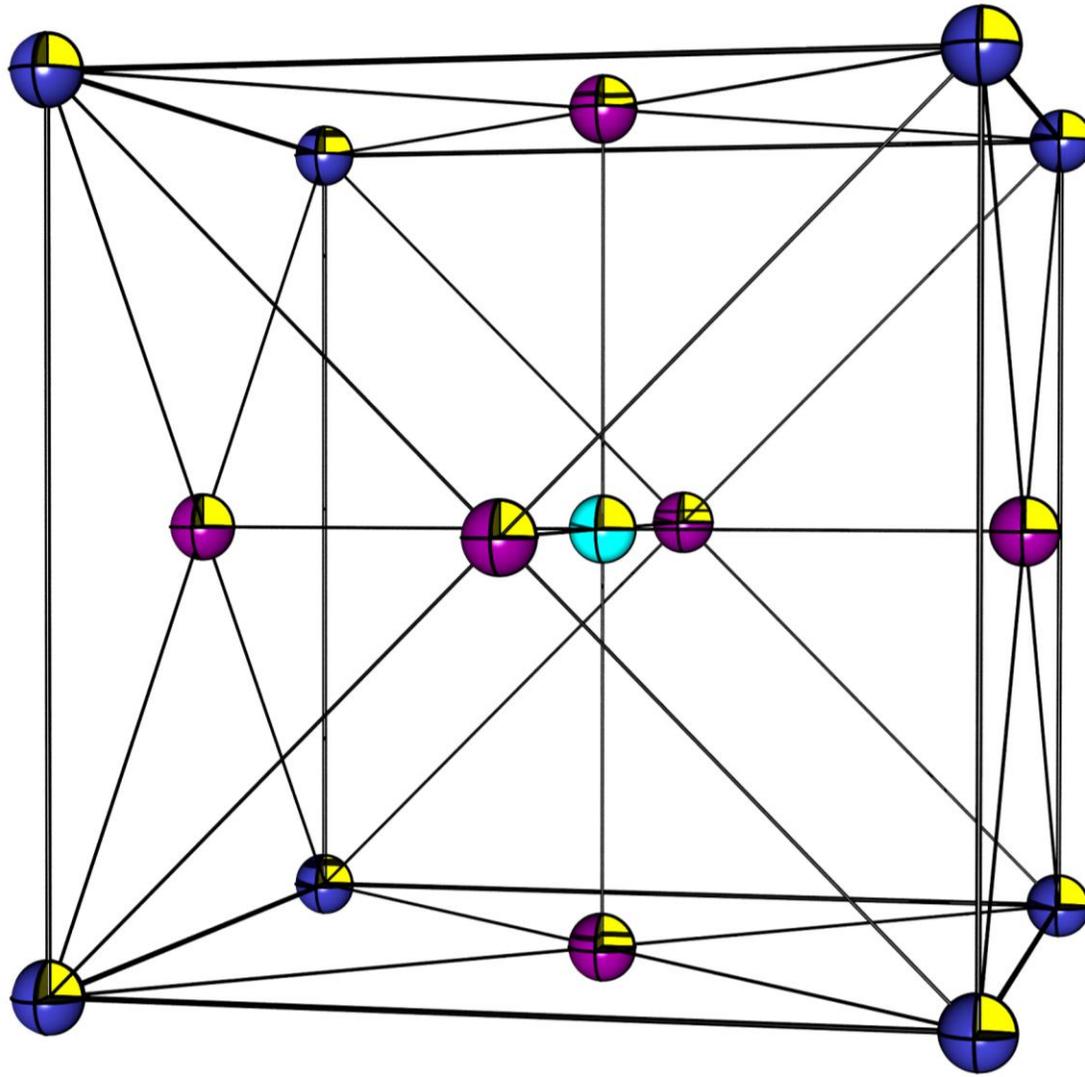


Sich durchdringende einfach
kubische Anordnungen.



CsCl
 $Pm\bar{3}m$

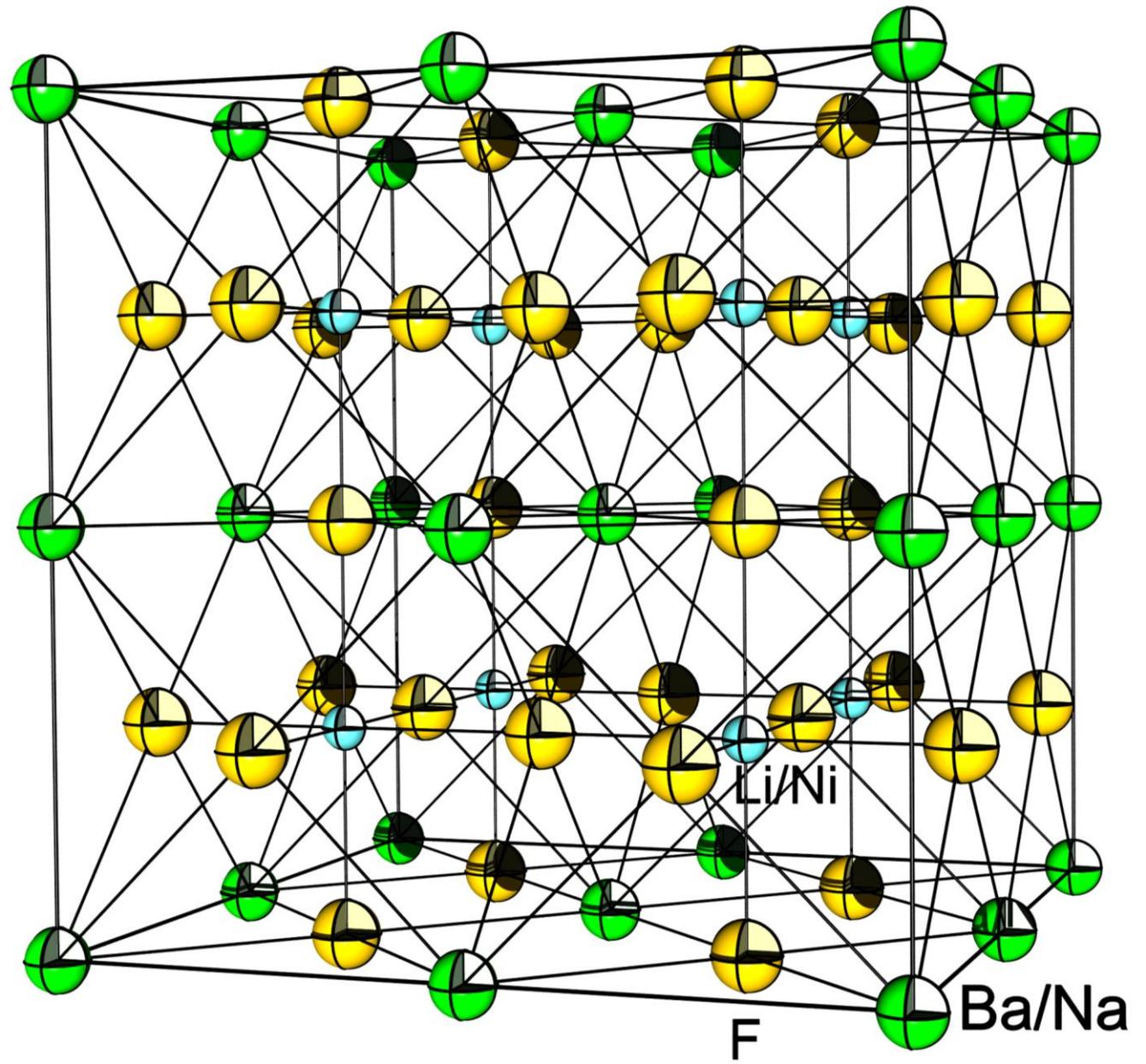
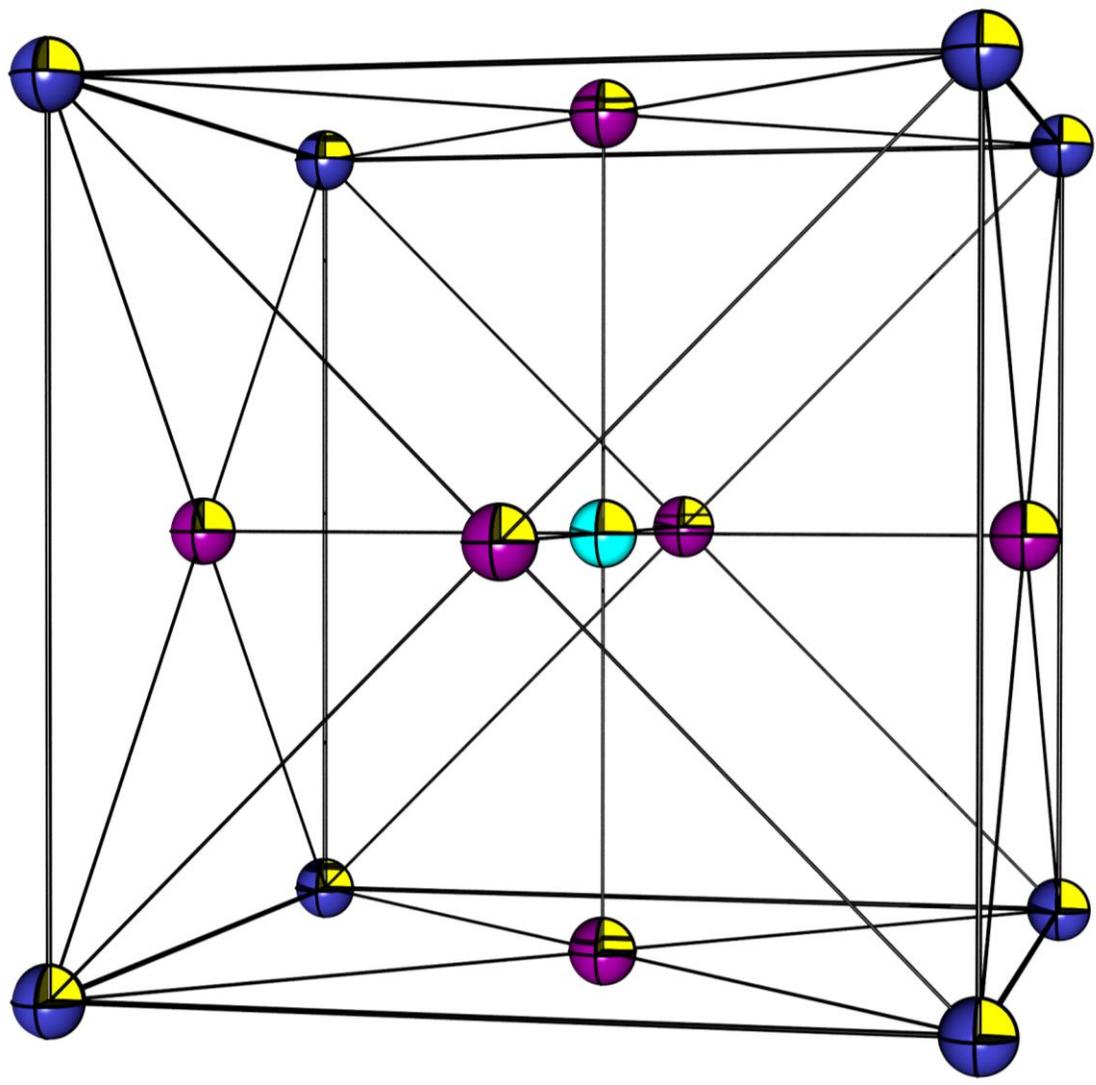
Aufgabe 2.



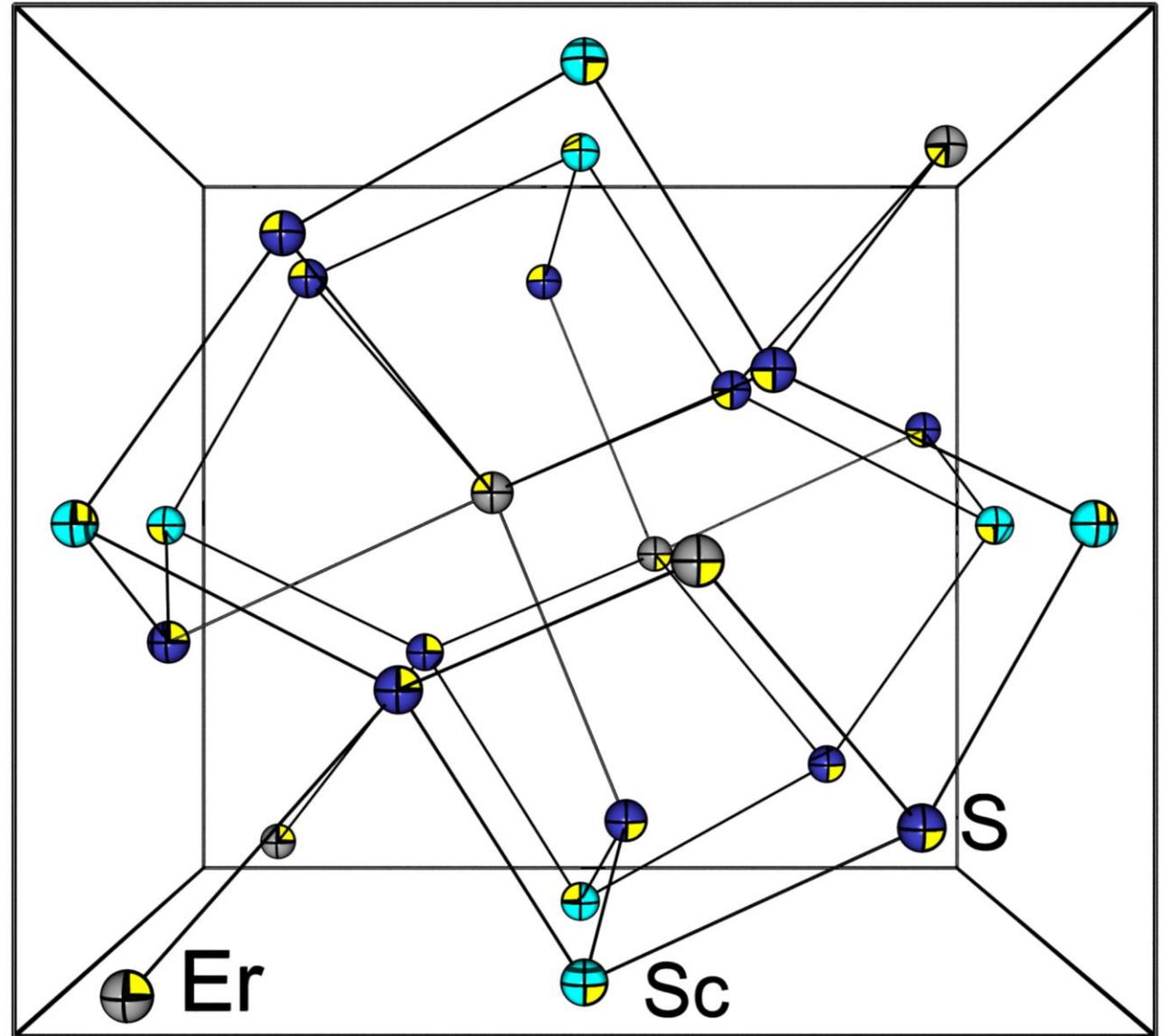
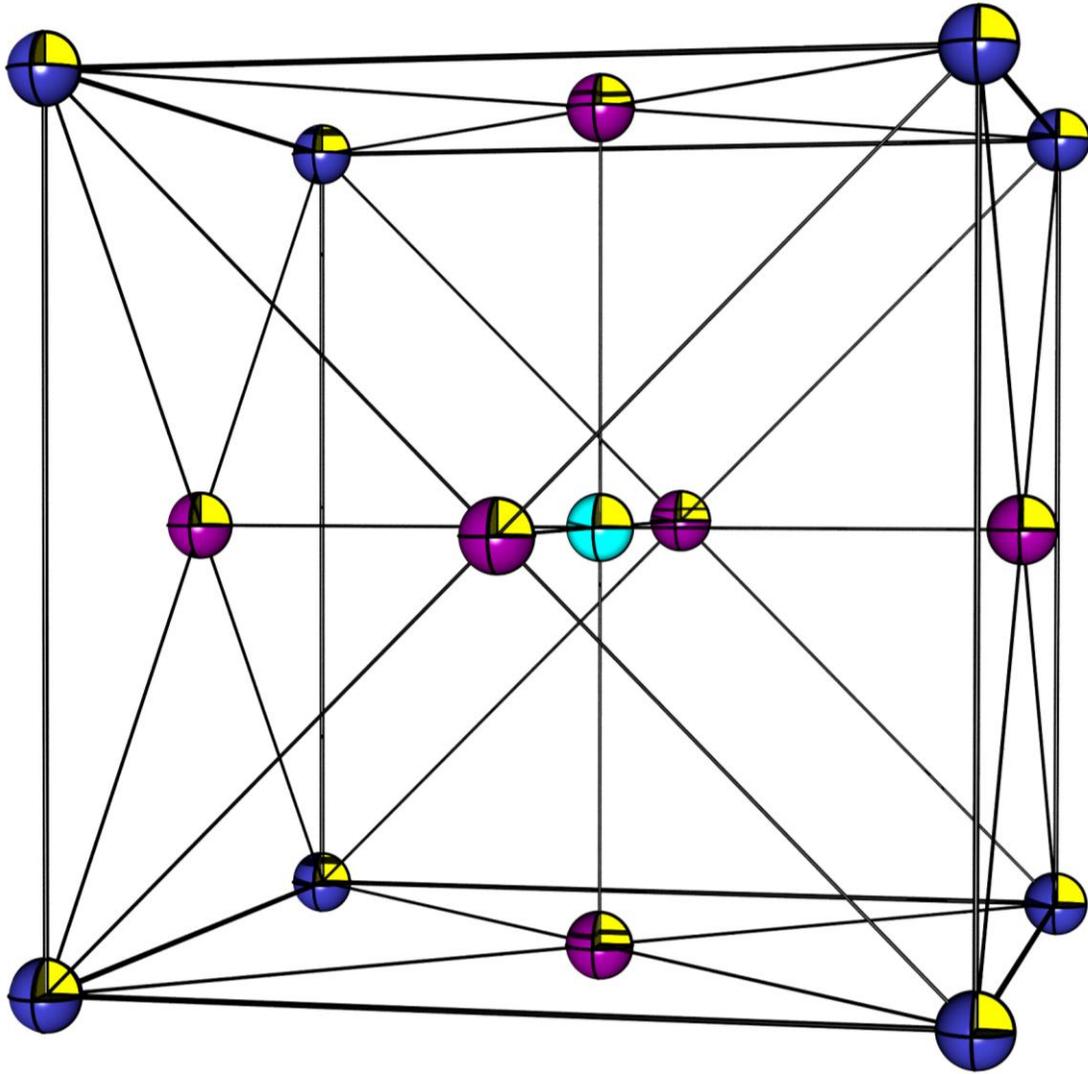
ccp (O^{2-})
+ $\frac{1}{4}$ OL (Ti^{4+})
+ Ca^{2+} Kuboktaederlücke

Perowskite $SrTiO_3$

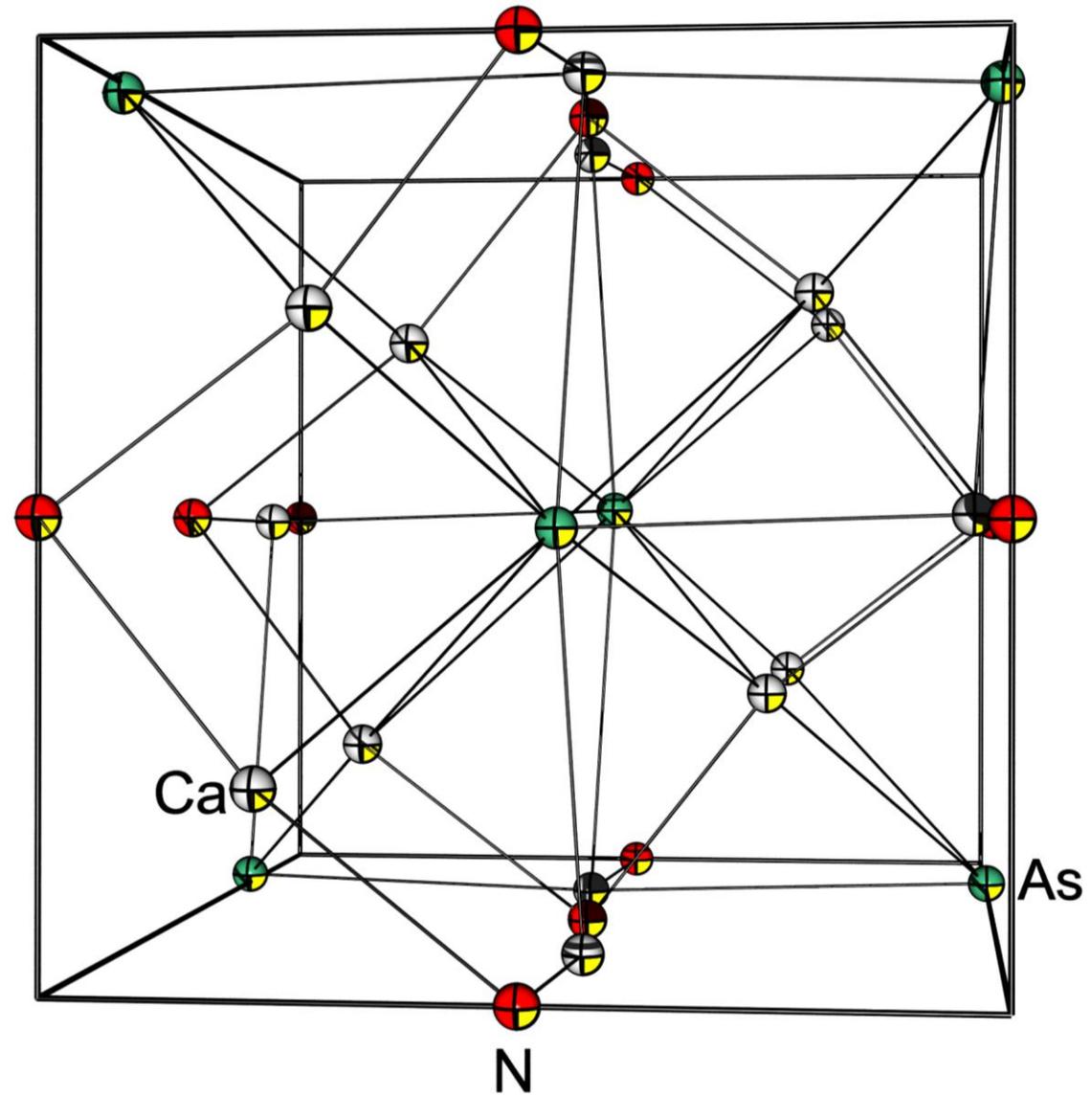
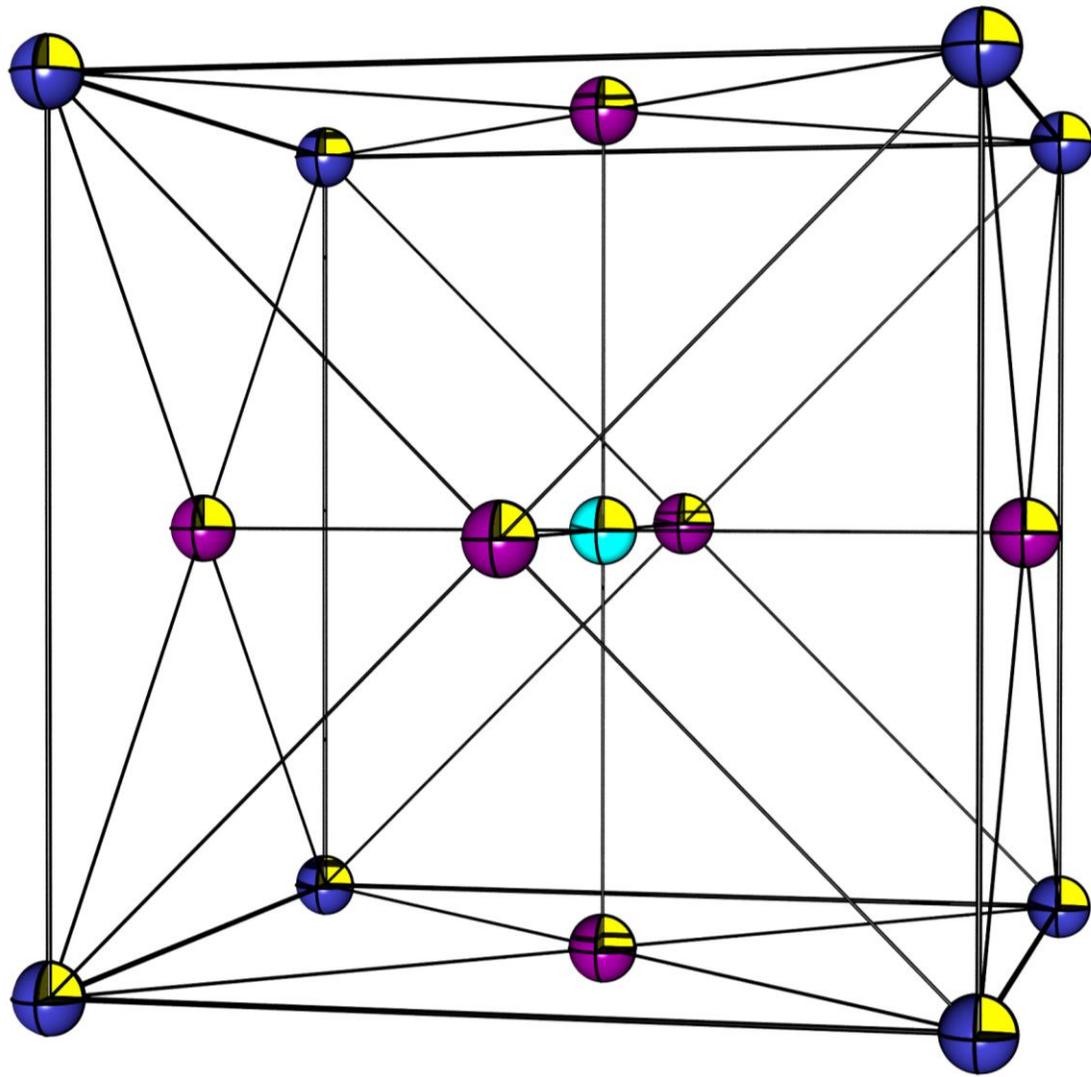
a) Überstruktur durch alternierende Na/Ba Besetzung
/Zusätzlich statistische Ni/Li Besetzung



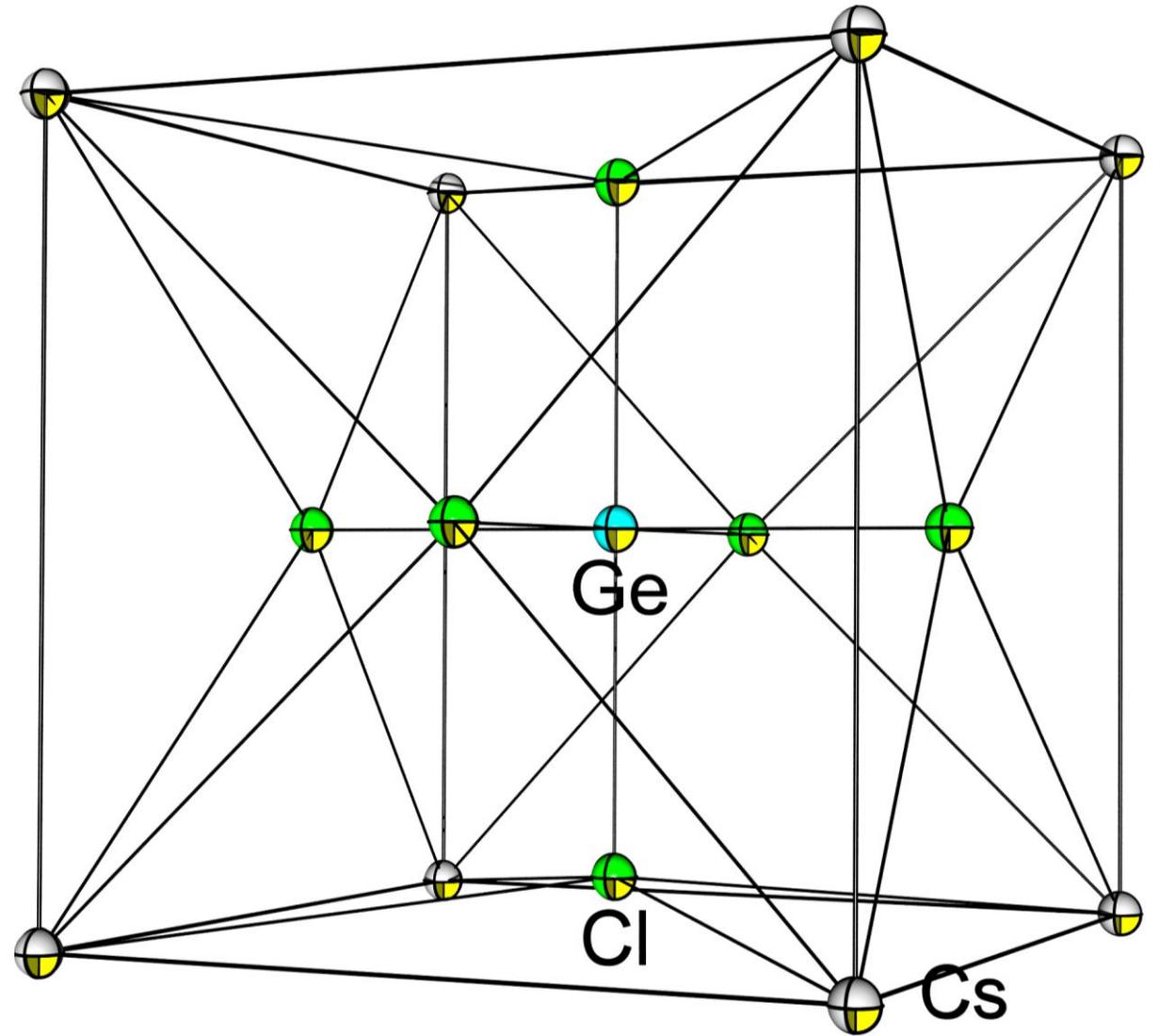
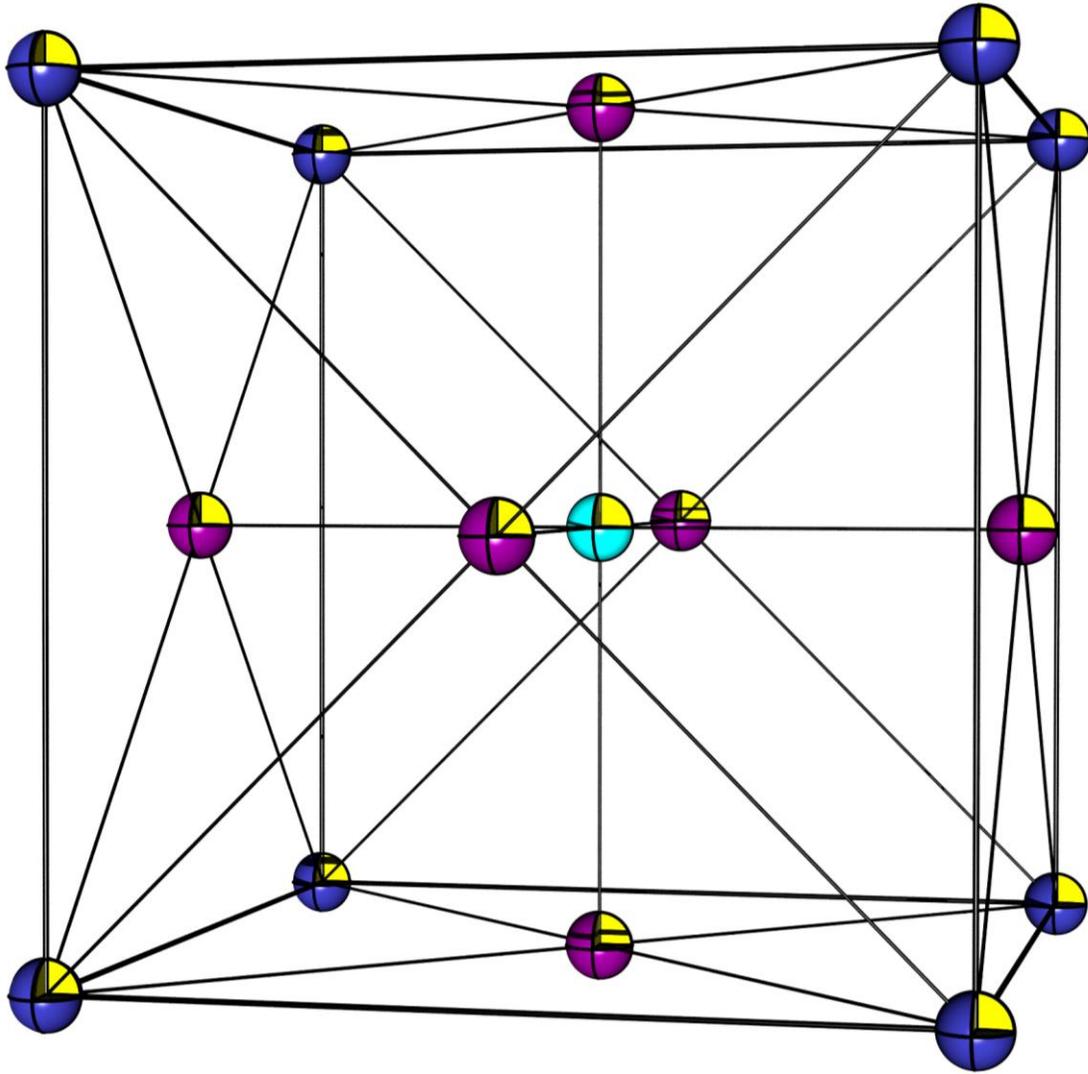
b) extreme Verzerrung – trotzdem noch Perowskit
genannt



c) anti-Perowskit



d) Ge anisotrop entlang $[1\ 1\ 1]$ verschoben, dadurch molekularer GeCl_3 Charakter



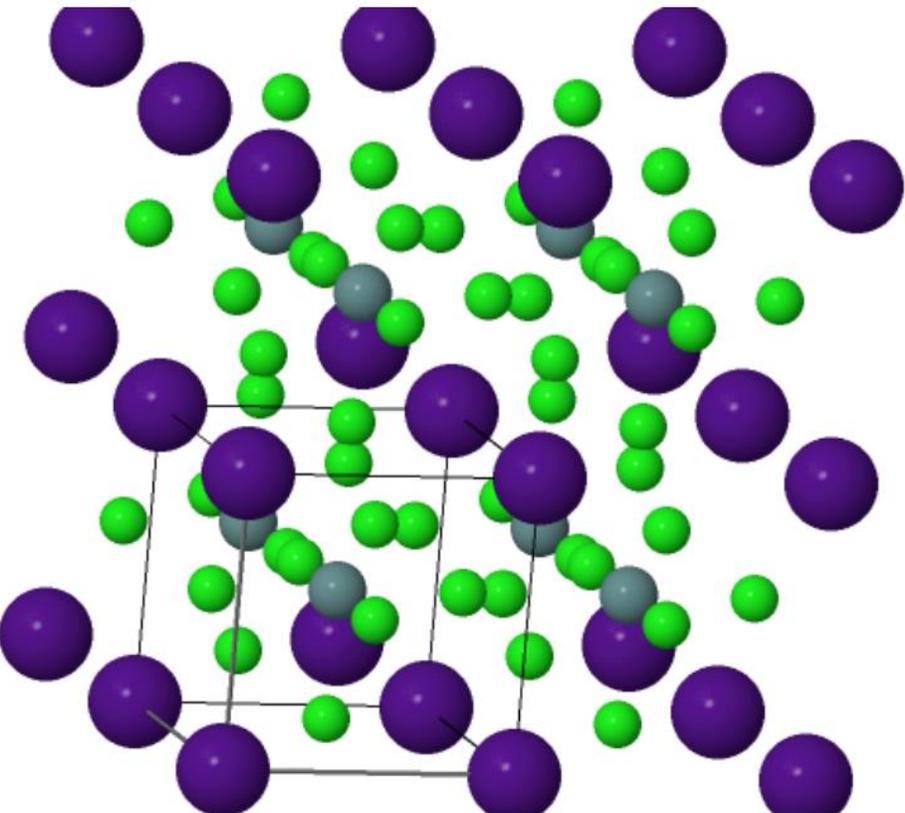
d)

ICSD - Details on Search

https://icsd.fiz-karlsruhe.de/display/details.xhtml

Coll. Code: 23122, Cs (Ge Cl3) - 1965 Christens ...

HM: $P m \bar{3} m$ #221
a=5.475Å
b=5.475Å
c=5.475Å
 $\alpha=90.000^\circ$
 $\beta=90.000^\circ$
 $\gamma=90.000^\circ$



ICSD

Align Explore Coordination Unitcell Distance/Ionic Radii Display Properties Display Content

a: b: c: Apply Unitcell

Save As Default Restore Defaults Reset To System

e) Verzerrung durch Oktaederverkippung

