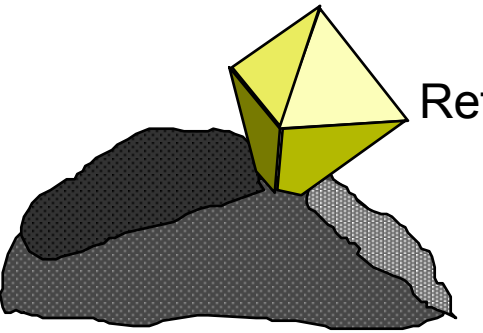
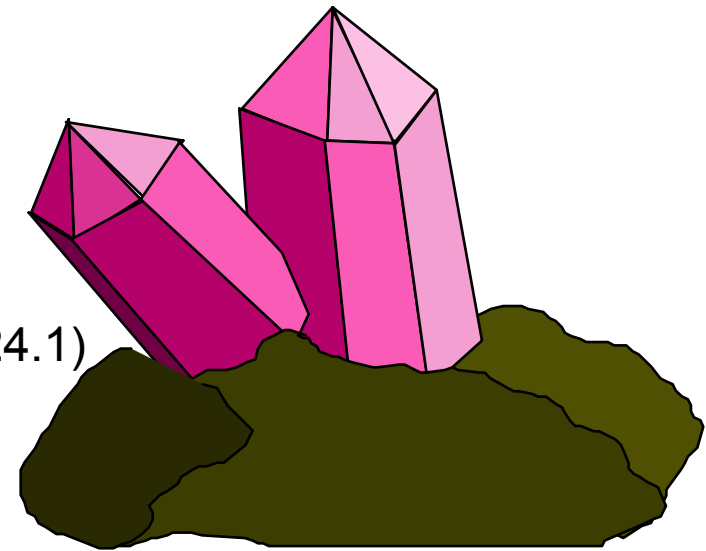
Crystals

Part 1



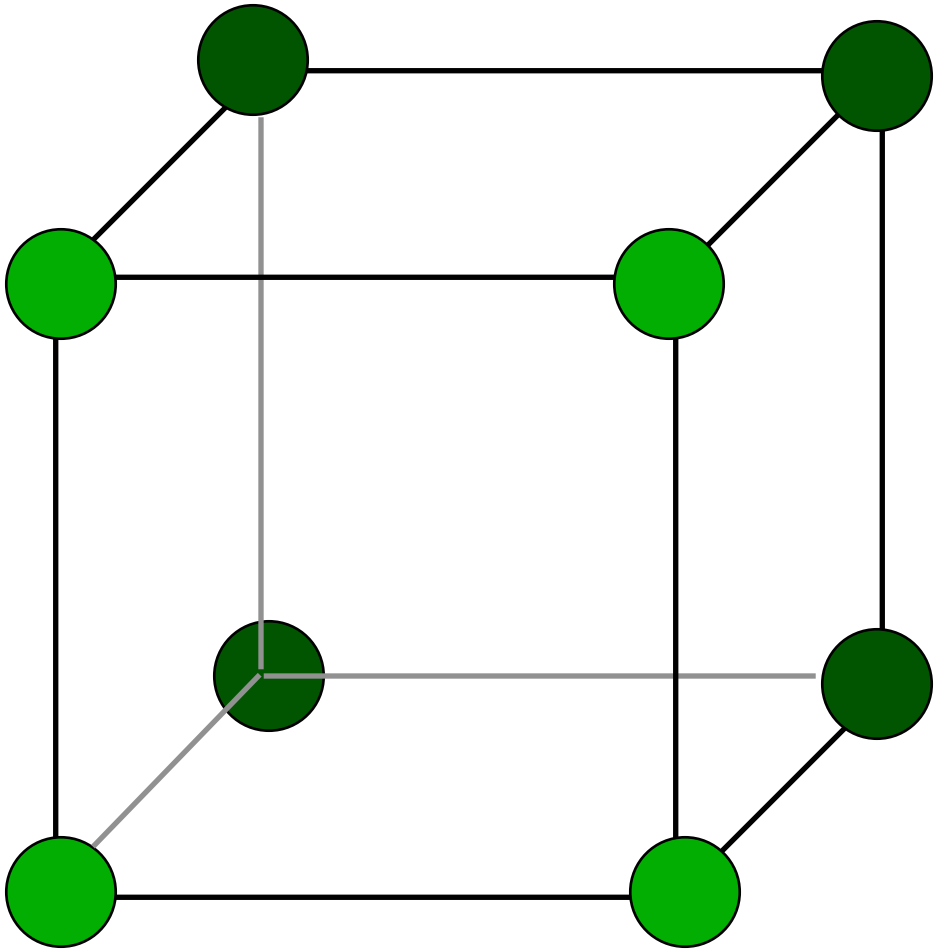
References: Gray: Chapter 6
OGN: Chapter 19 and (24.1)



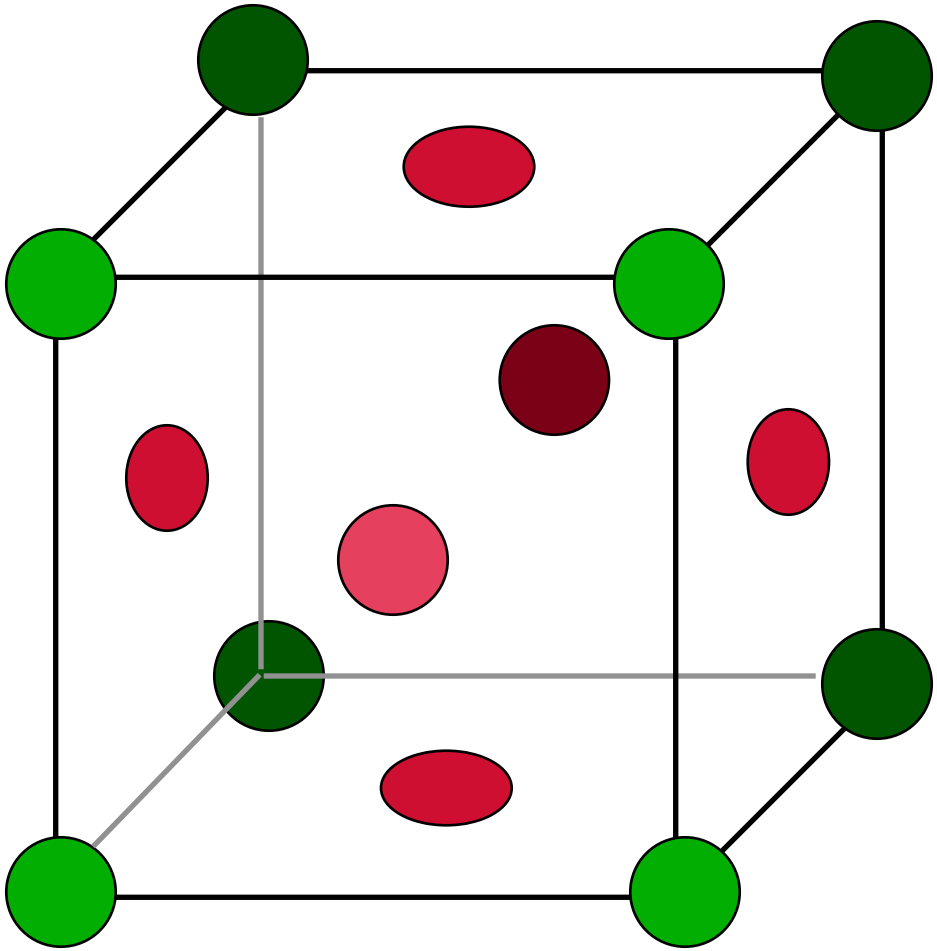
Aspects of Chemical Bonds
⇨ Bonding in Chem 1a ⇦

- Atomic Structure
- Explain Atomic Line Spectra, Galaxies, etc.
- Shapes of Orbitals in Atoms for Bonding
- Ionization Energies and Trends in Chemical Reactivity (e.g., Li^+ vs Li)
- Which Molecules are Likely to Exist and Their Shapes and Reactivities (Ozone, Glo. Warm.)
- Magnetic and Bonding Properties of Molecules (Magnetic Tapes, Disks, etc.)
- Special Properties of Resonance Stabilization
- Directionality of Covalent Chemical Bonds
- Bonding in Solids

A Simple Cubic Lattice



A Face-Centered Cubic Lattice

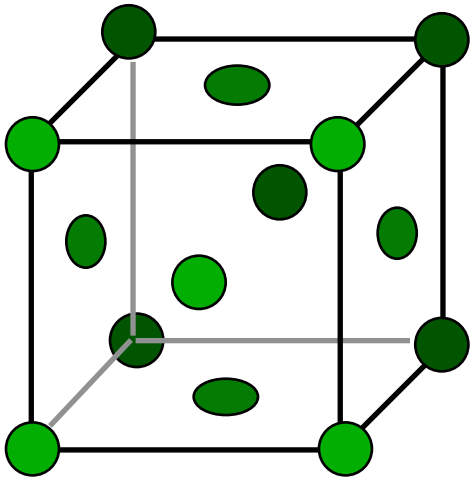


6 Face Atoms 8 Corner Atoms

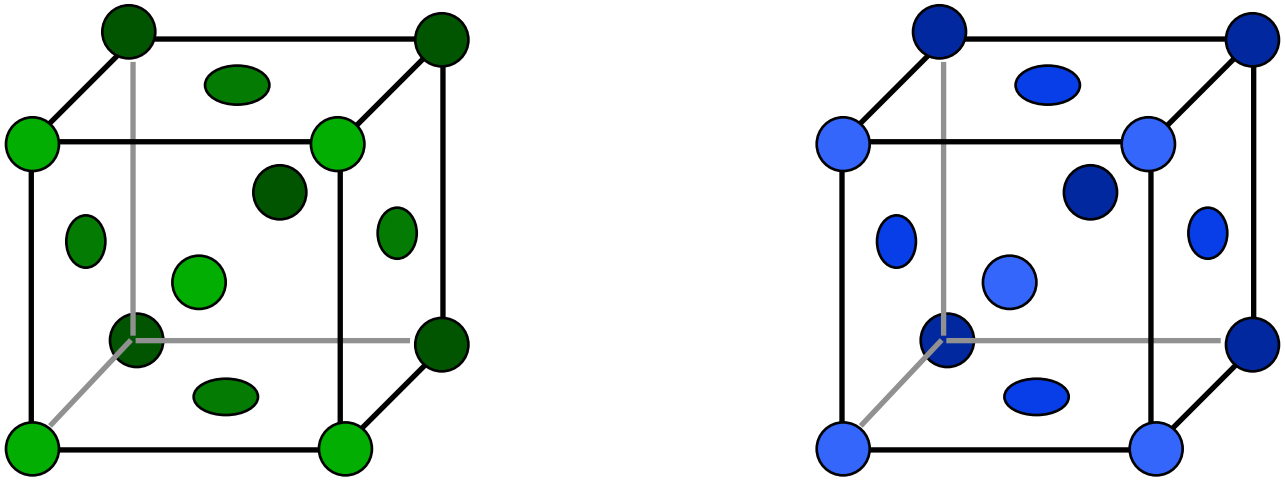
FCC Lattice of Metals and Insulators

- **Metals Are "Closed Packed" Atomic Spheres**
- **Insulators Arise from Binary Compounds with "Holes" Filled in FCC Lattice**

A Face-Centered Cubic Lattice

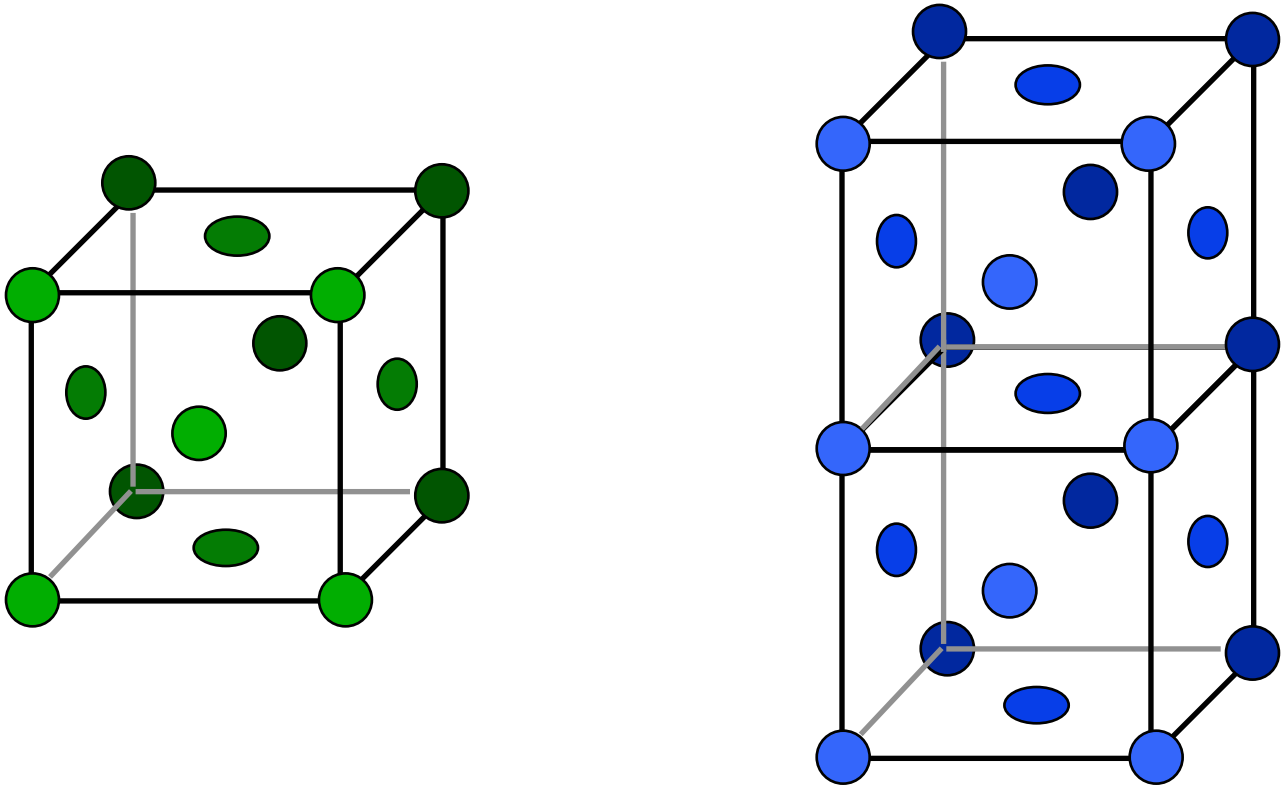


Two Face-Centered Cubic Lattices



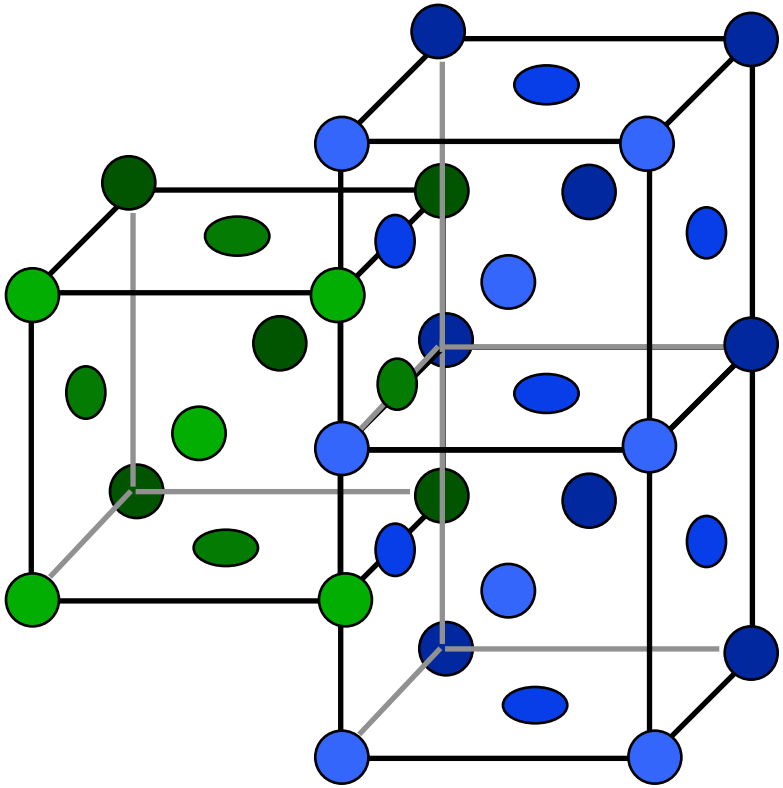
Replicate the Original Lattice

Two Face-Centered Cubic Lattices



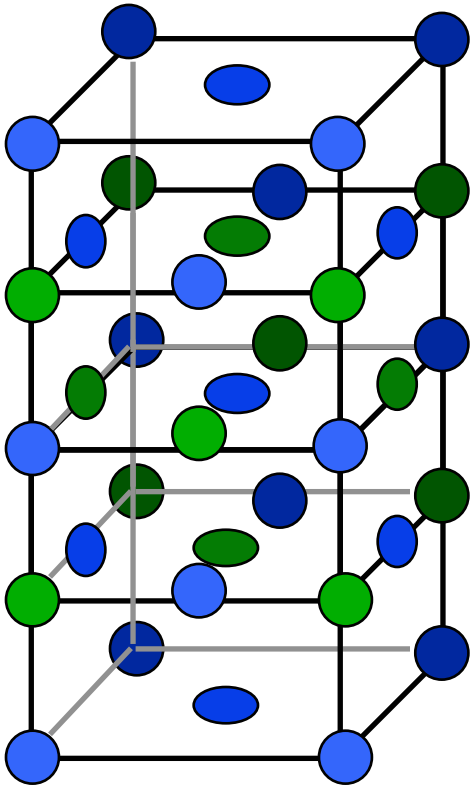
Offset the Lattice by 1/2 An Edge-Edge Distance

Two Face-Centered Cubic Lattices



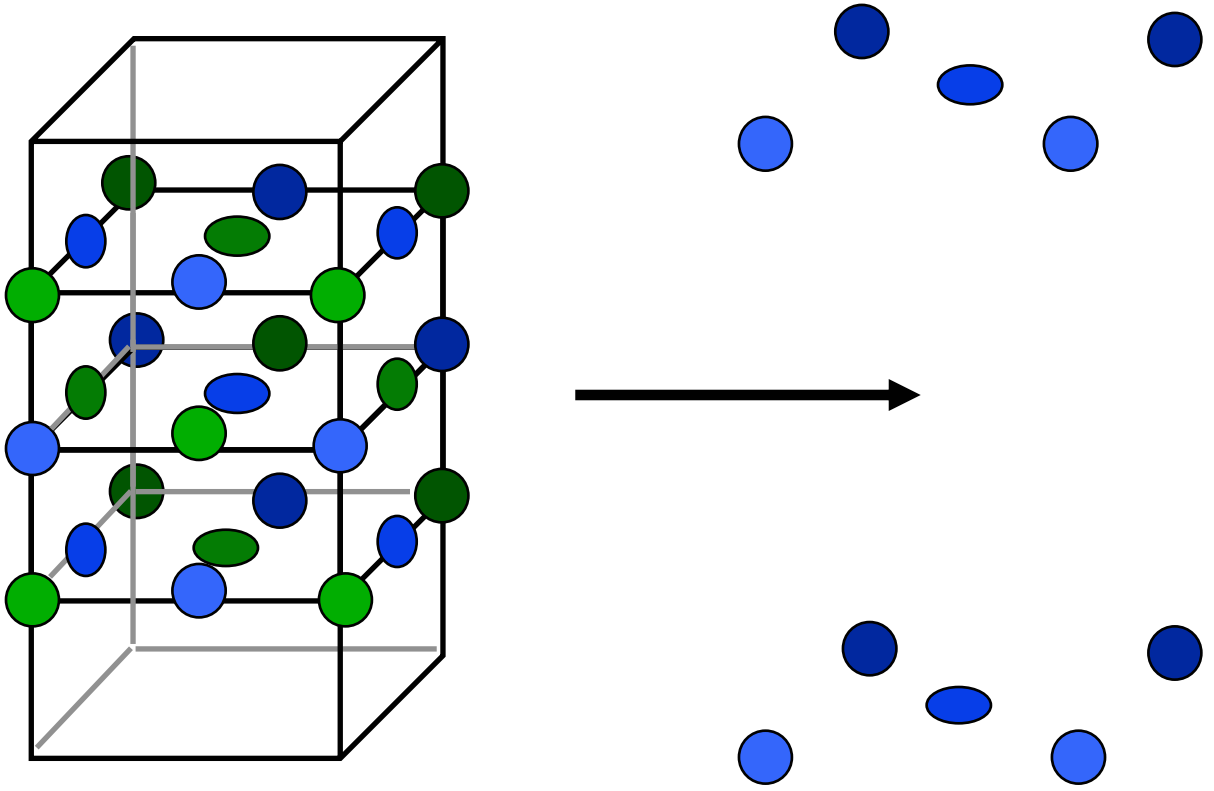
Start to Interpenetrate the Two Lattices

Two Face-Centered Cubic Lattices



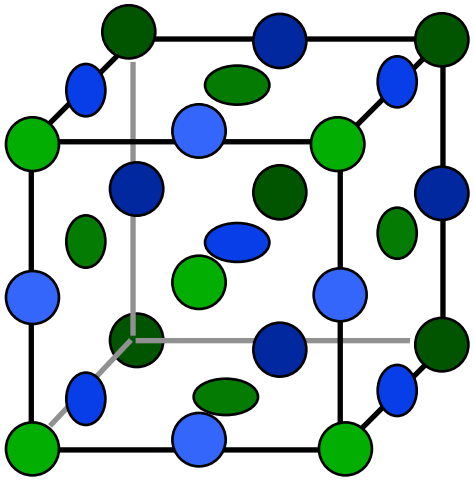
Two Interpenetrating FCC Lattices

A Face-Centered Cubic Lattice



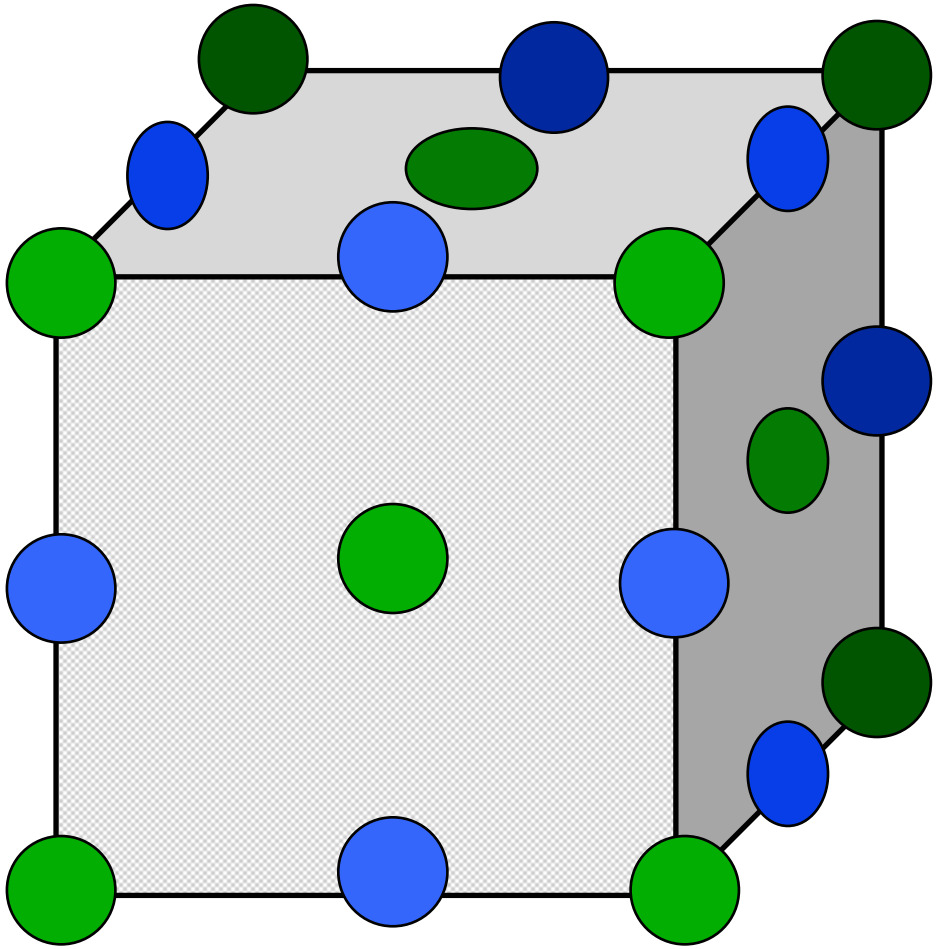
“Chop Off” Top and Bottom Atoms to View Original Unit Cell Volume

Rock Salt:
Two Interpenetrating FCC Structures



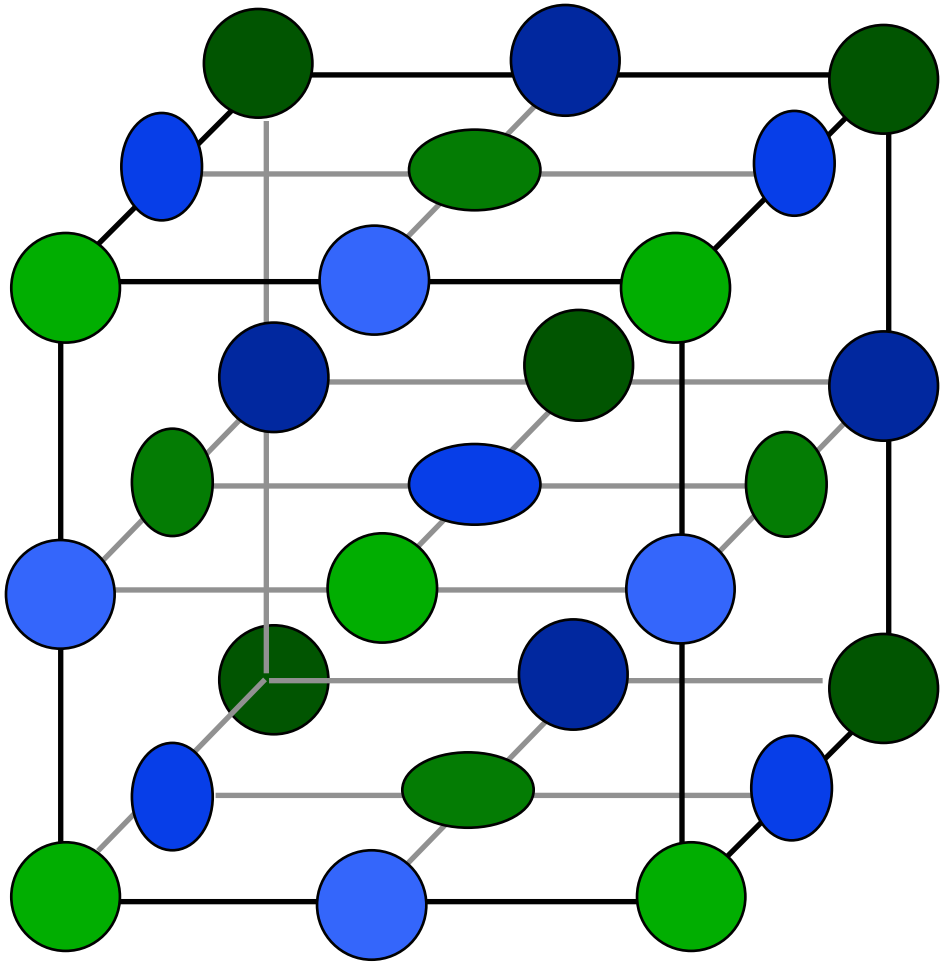
Every Atom Has Six Nearest Neighbors of the Opposite Atom Type with a Locally Octahedral Geometry

Rock Salt:
Two Interpenetrating FCC Structures

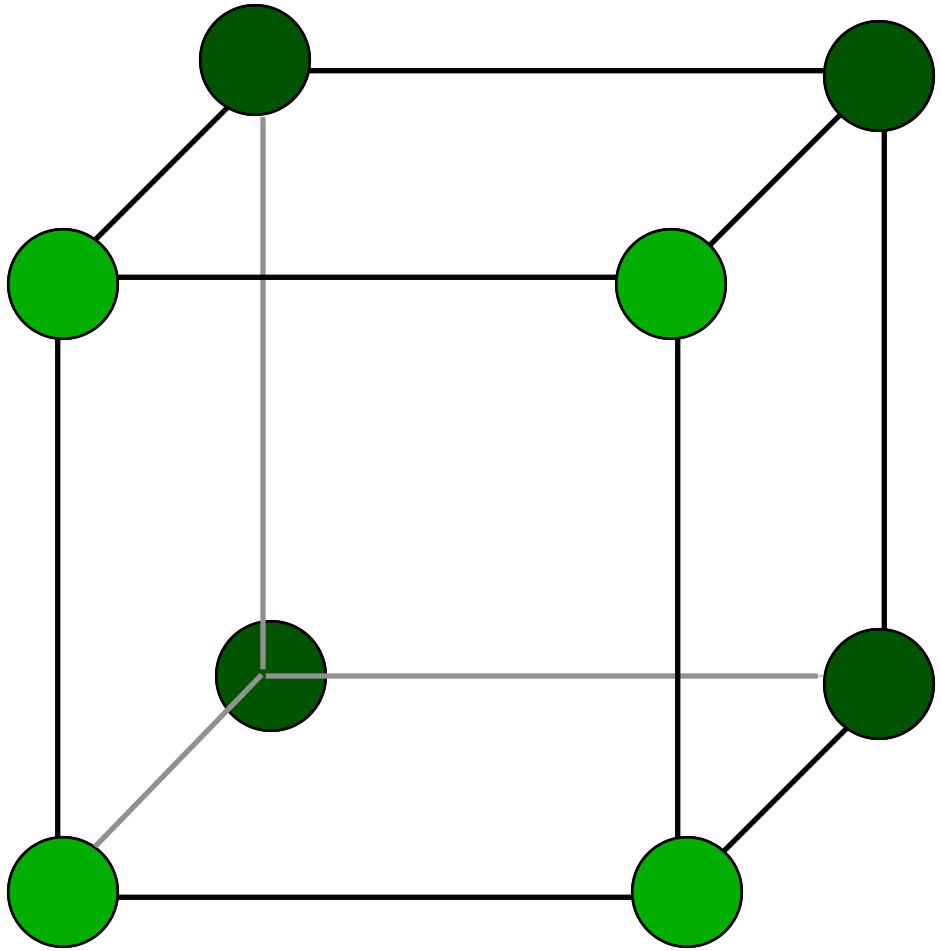


One Can Not See “Through” the Cube in this View

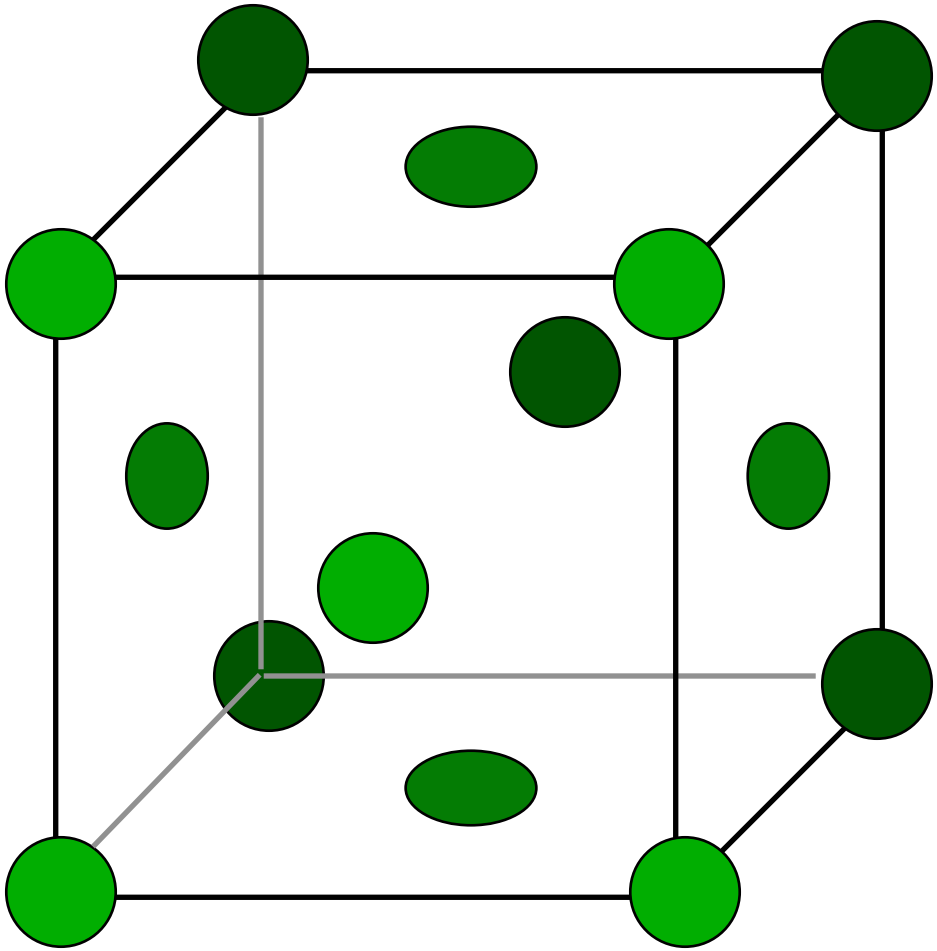
Rock Salt:
Two Interpenetrating FCC Structures



A Simple Cubic Lattice Again

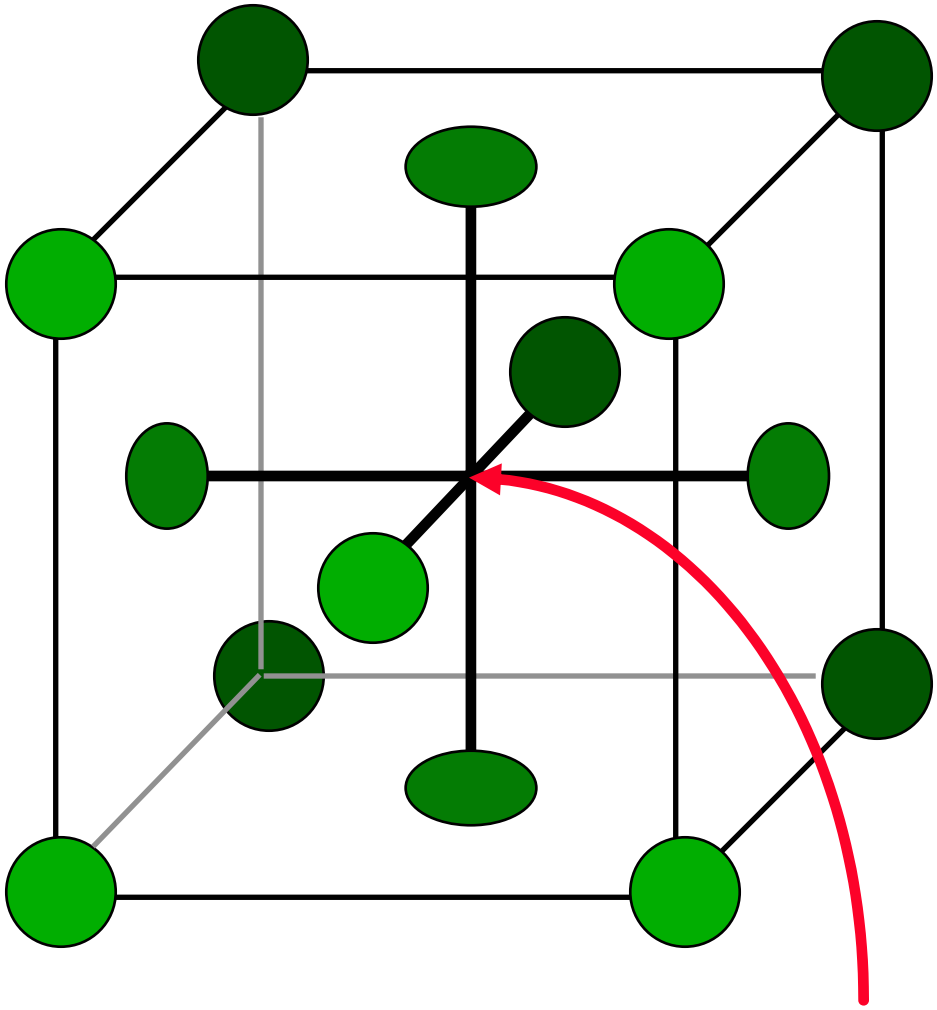


A Face-Centered Cubic Lattice



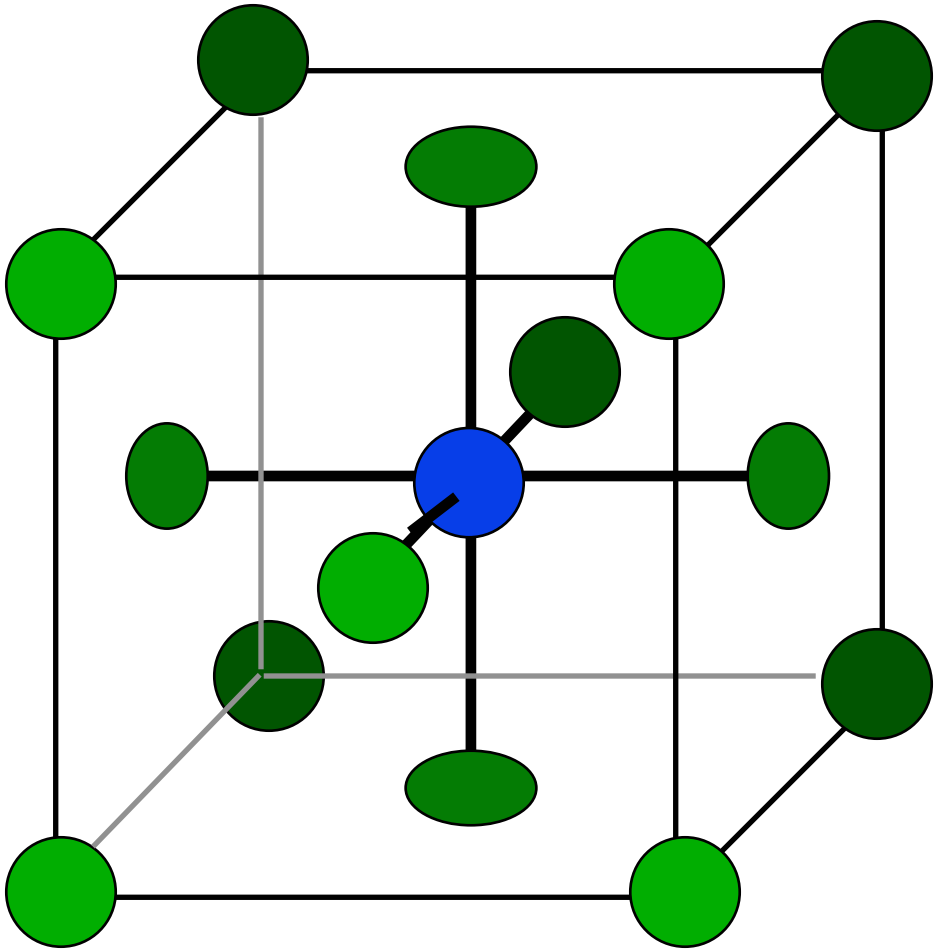
6 Face Atoms 8 Corner Atoms

One Octahedral "Hole" in a Face-Centered Cubic Lattice

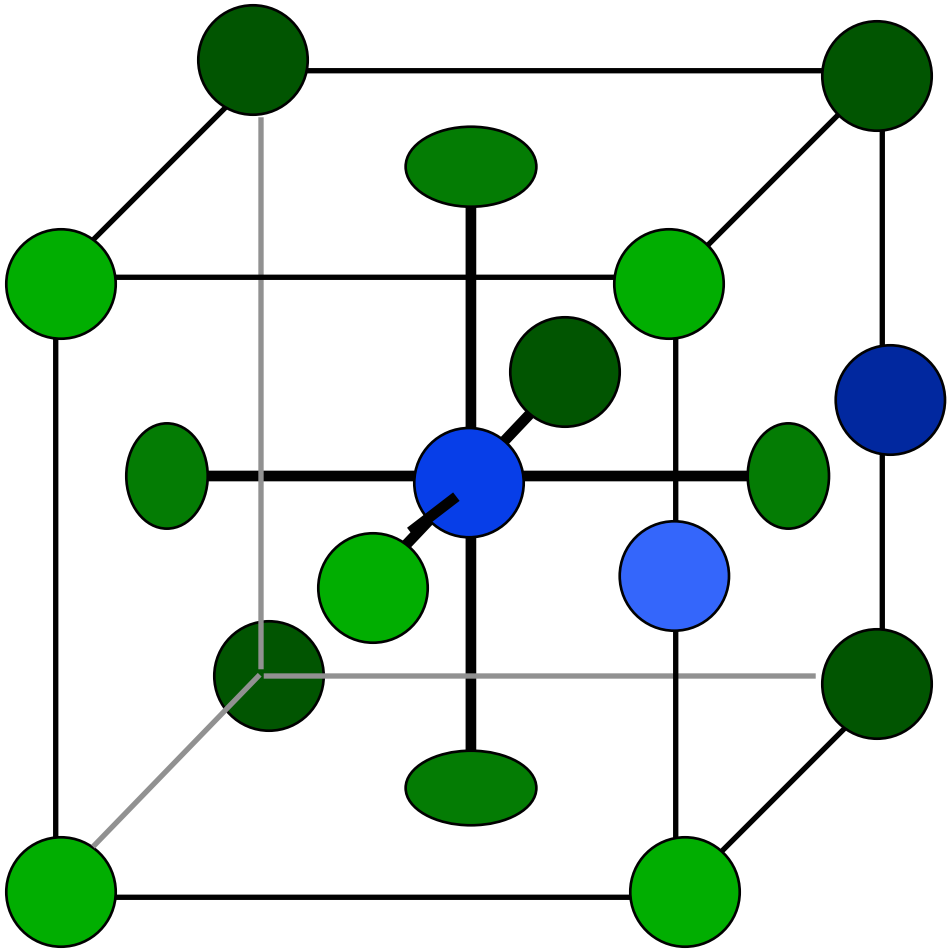


There is a Hole at Center of Unit Cell

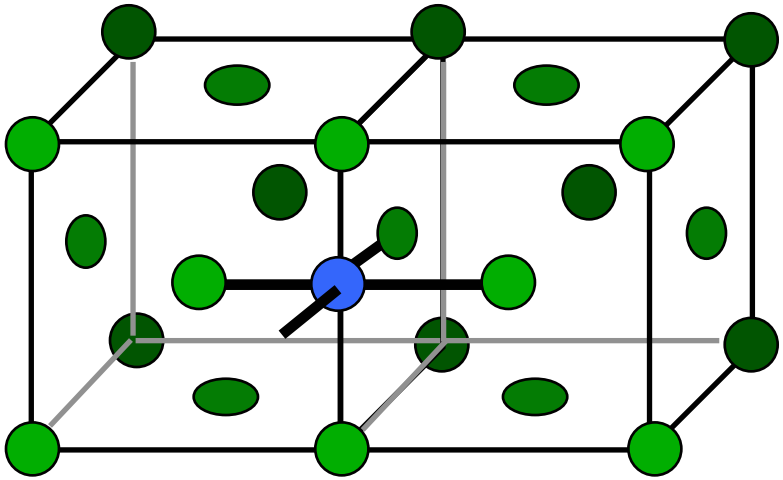
Fill The Unique Octahedral Hole at Center



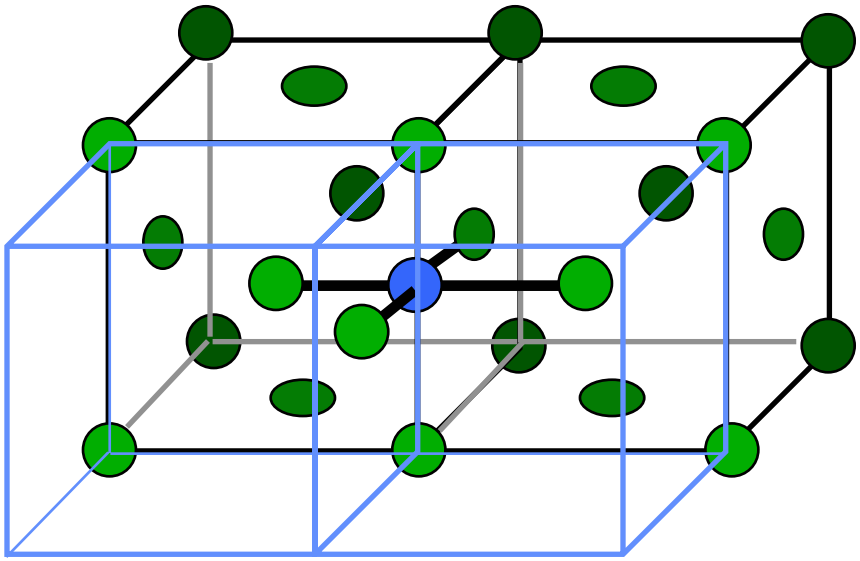
Two of The Octahedral Holes at Edge Midpoints



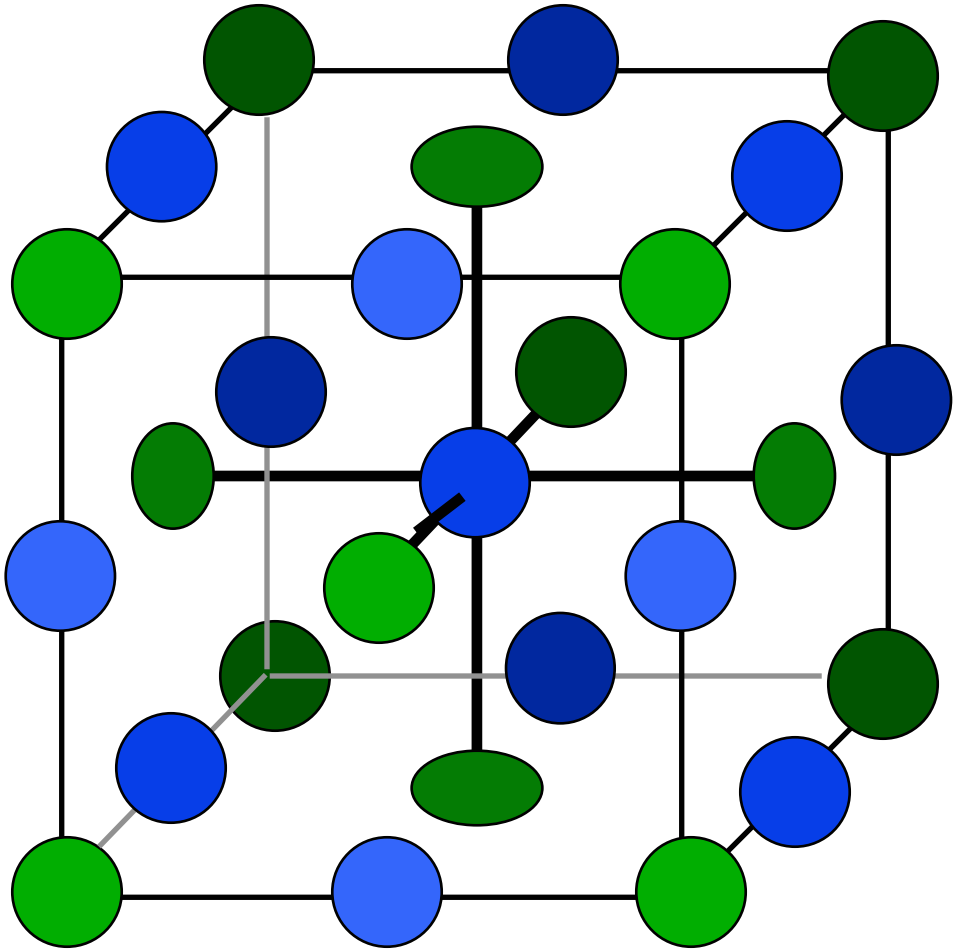
Showing Coordination Around Edge Octahedral Holes



Showing Coordination Around Edge Octahedral Holes



Forming Rock Salt: Fill All of the Octahedral Holes



Fill All of The Octahedral Holes at Edge Midpoints and the Unique Hole in the Center of the Unit Cell

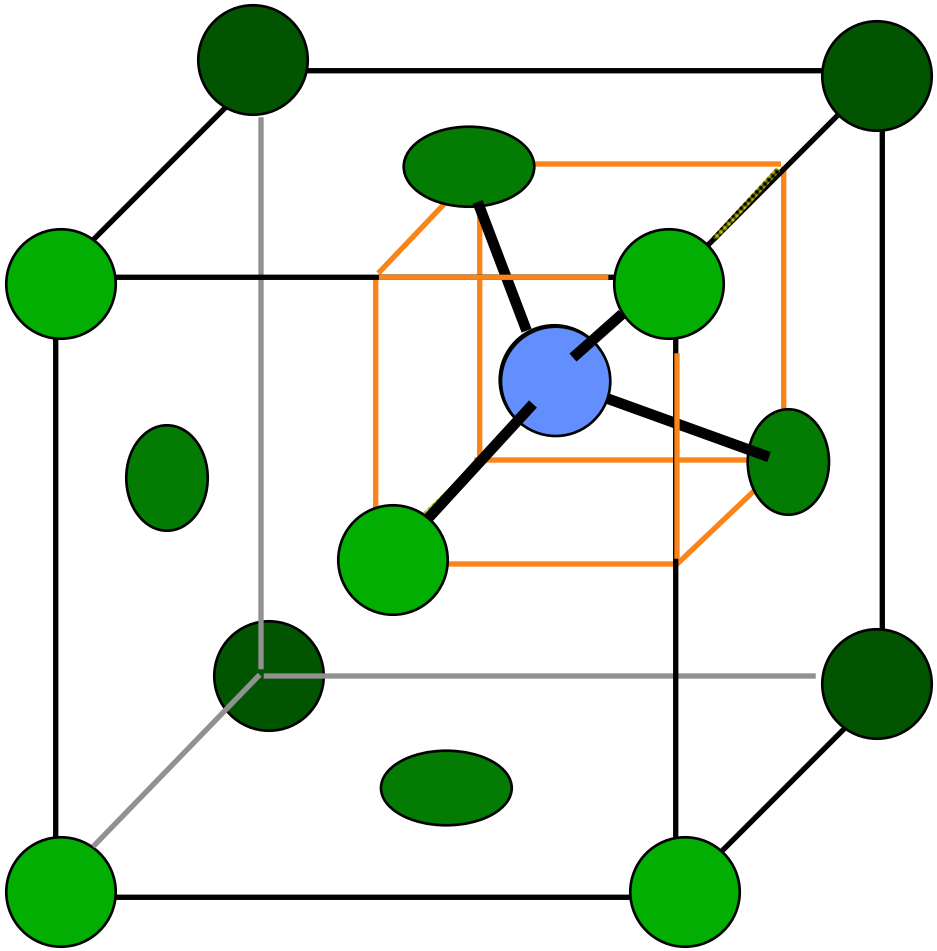
Rock Salt Structure

- Two Interpenetrating FCC Lattices

  or

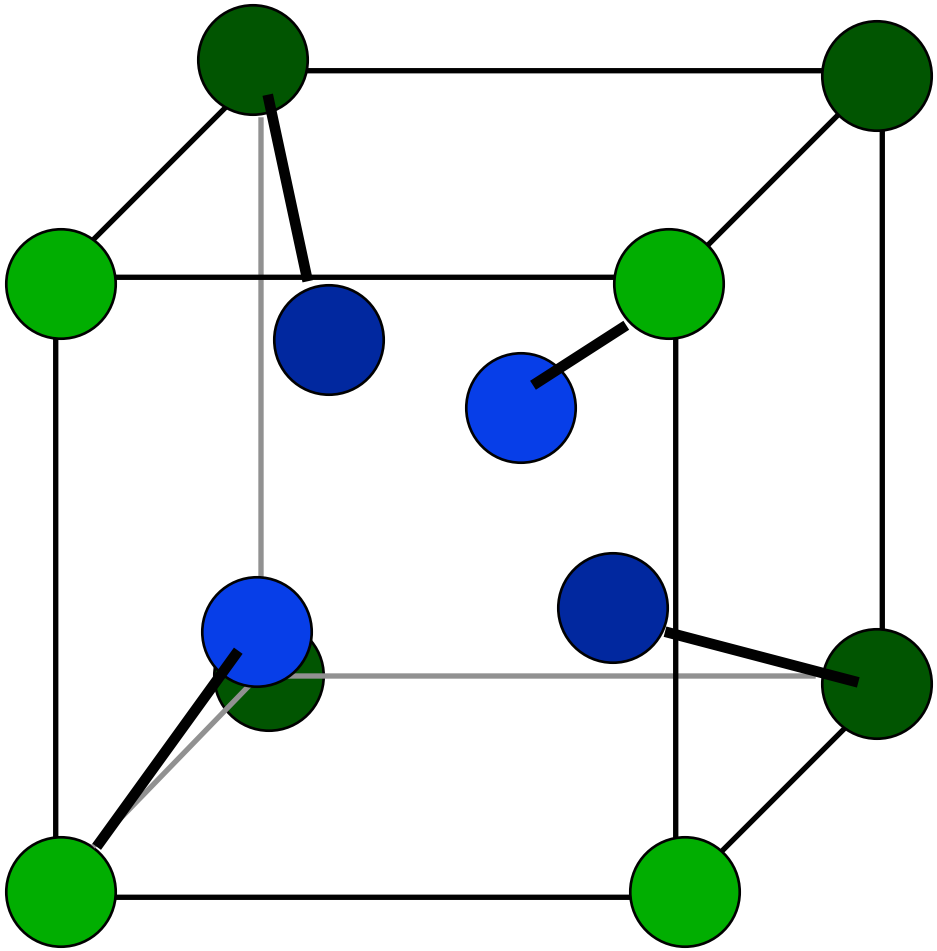
- Fill All Octahedral Holes in One FCC Lattice

Tetrahedral Holes in A Face-Centered Cubic Lattice



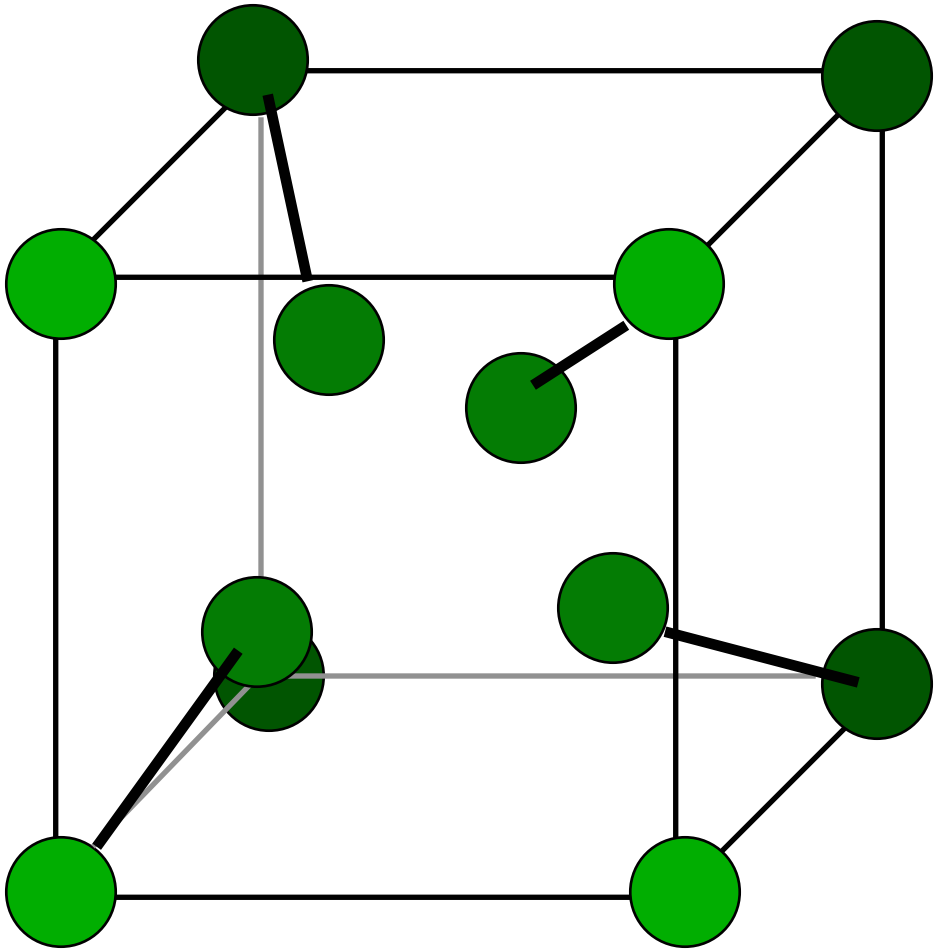
Each Corner (with 3 Face Atoms) Defines One Tetrahedral Hole; Favored by sp^3 Hybrids

Filling 1/2 T_d Holes in a FCC Lattice



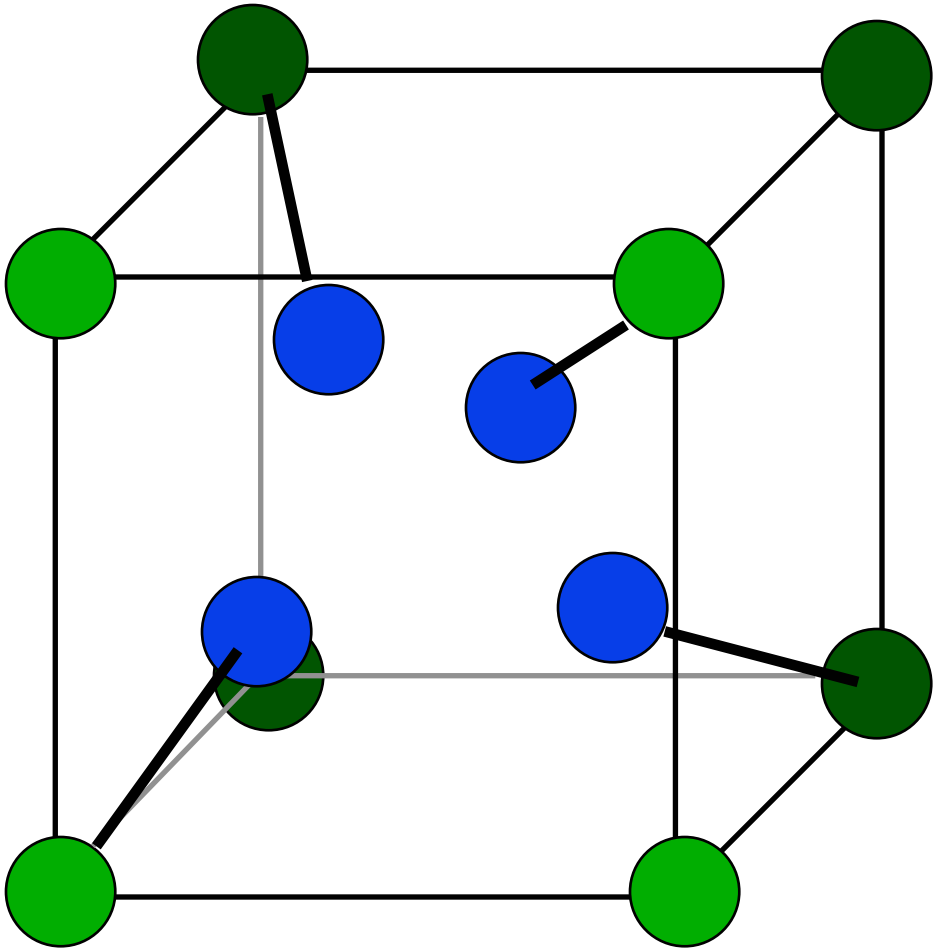
Note: Face Atoms Not Shown For Clarity

Filling 1/2 T_d Holes in a FCC Lattice



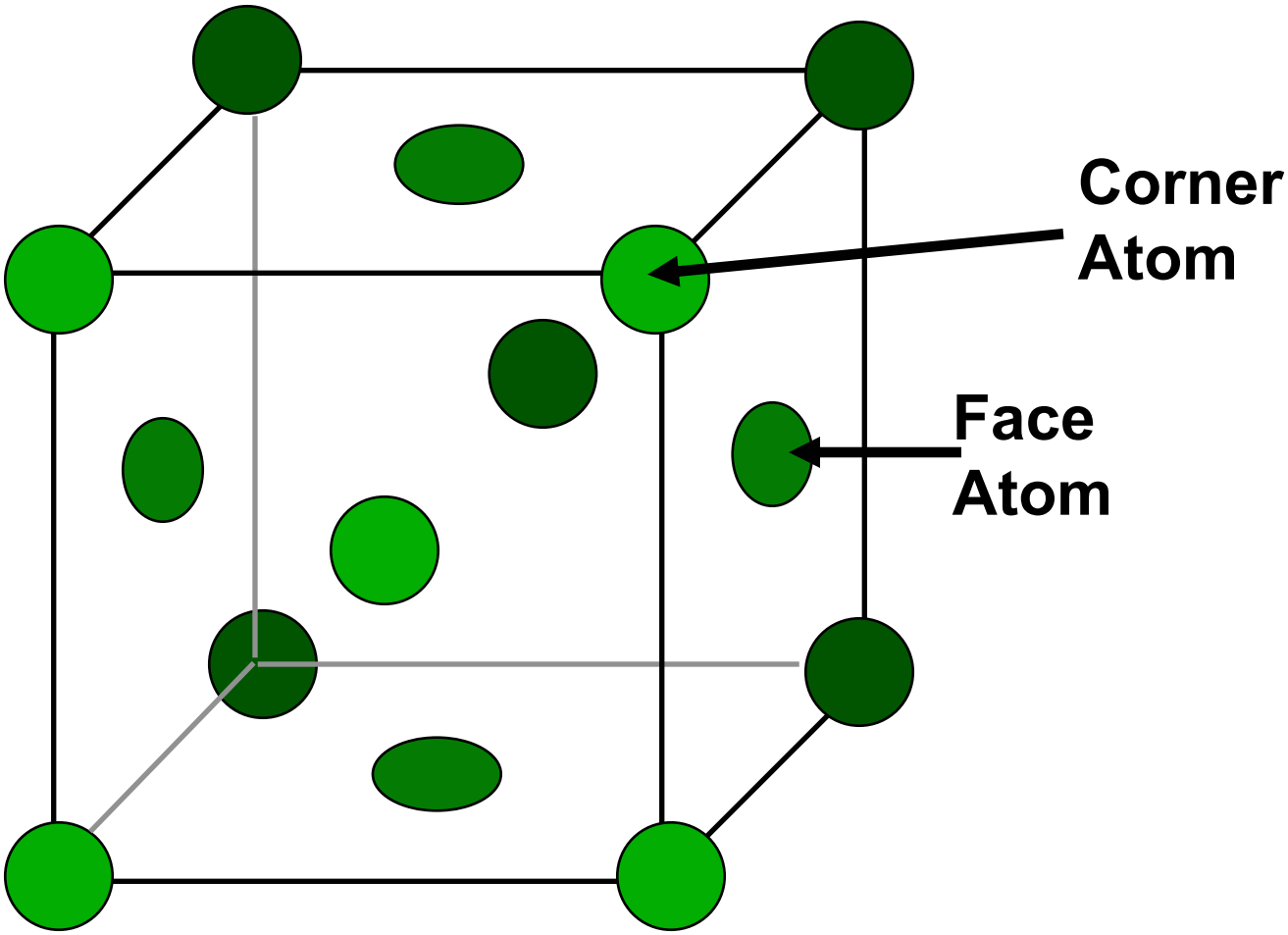
When Atoms Are All Identical, Have Diamond (Si) Structure

Filling 1/2 T_d Holes in a FCC Lattice



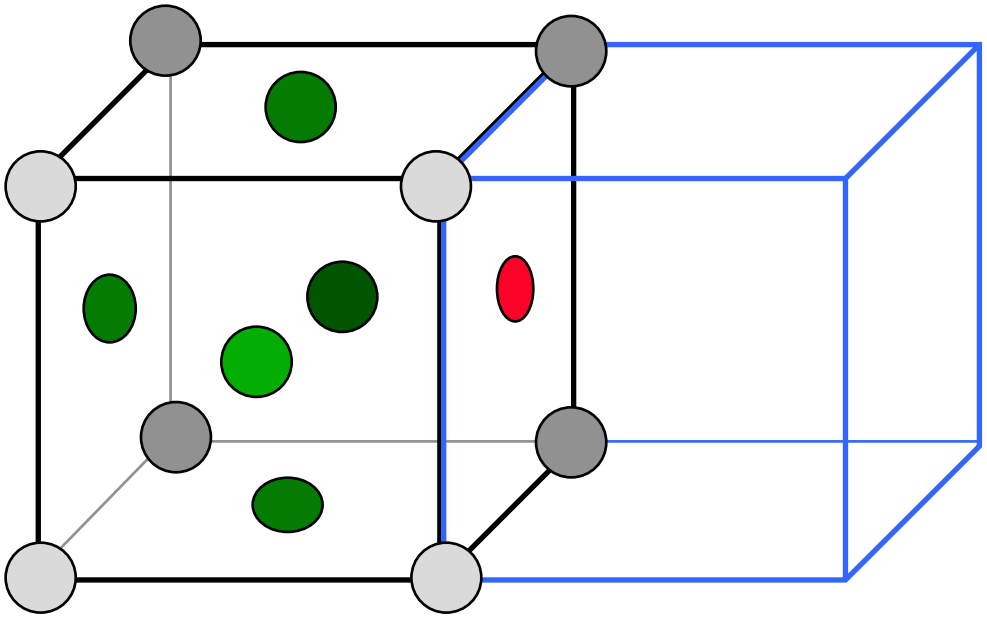
When T_d Atoms are Different than FCC Atoms, Have Zinc Blende (GaAs, InP, etc.) Structure

A Face-Centered Cubic Lattice



How Do We Determine Stoichiometry?
Consider Face and Corner Atoms Separately

Face Atoms in a FCC Lattice

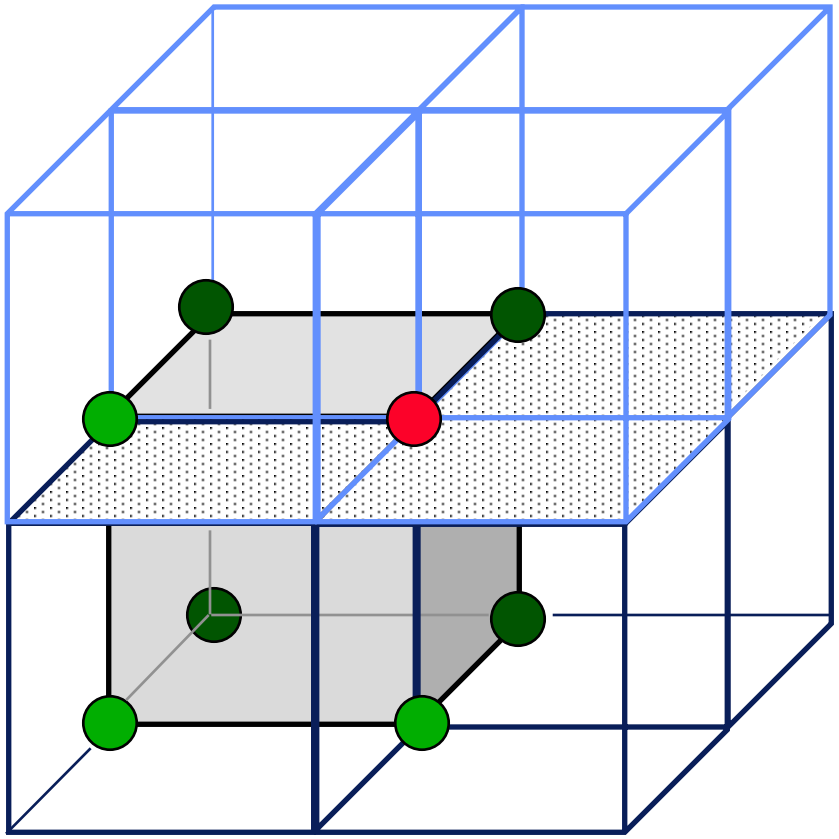


Face Atoms Are Shared Between 2 Unit Cells

So Each Face Atom Counts as 1/2 for Each Unit Cell

6 Face Atoms per Unit Cell * 1/2 = 3 Atoms/Unit Cell

Corner Atoms in a FCC Lattice

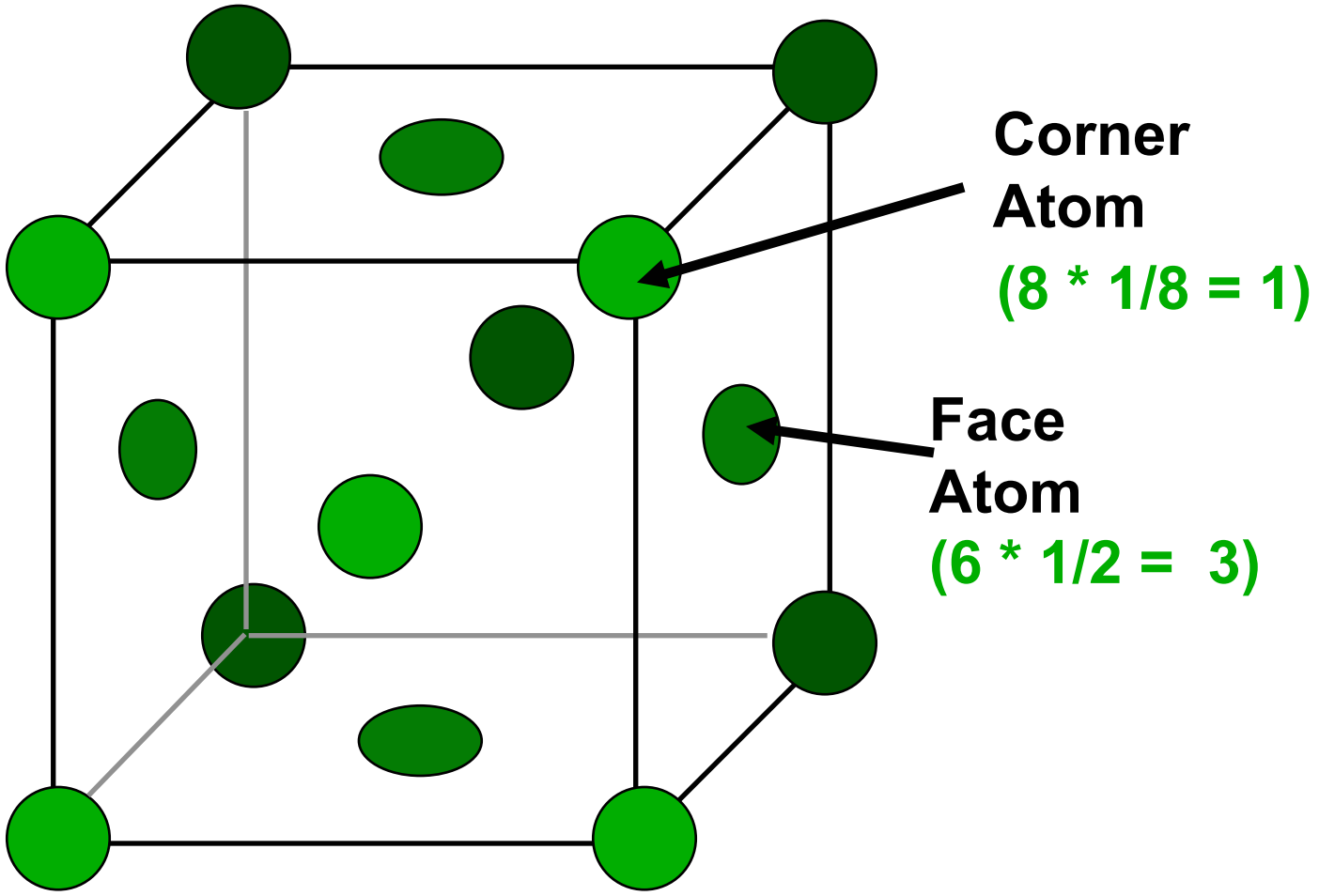


Corner Atoms Are Shared Between 8 Unit Cells

So Each Face Atom Counts as 1/8 for Each Unit Cell

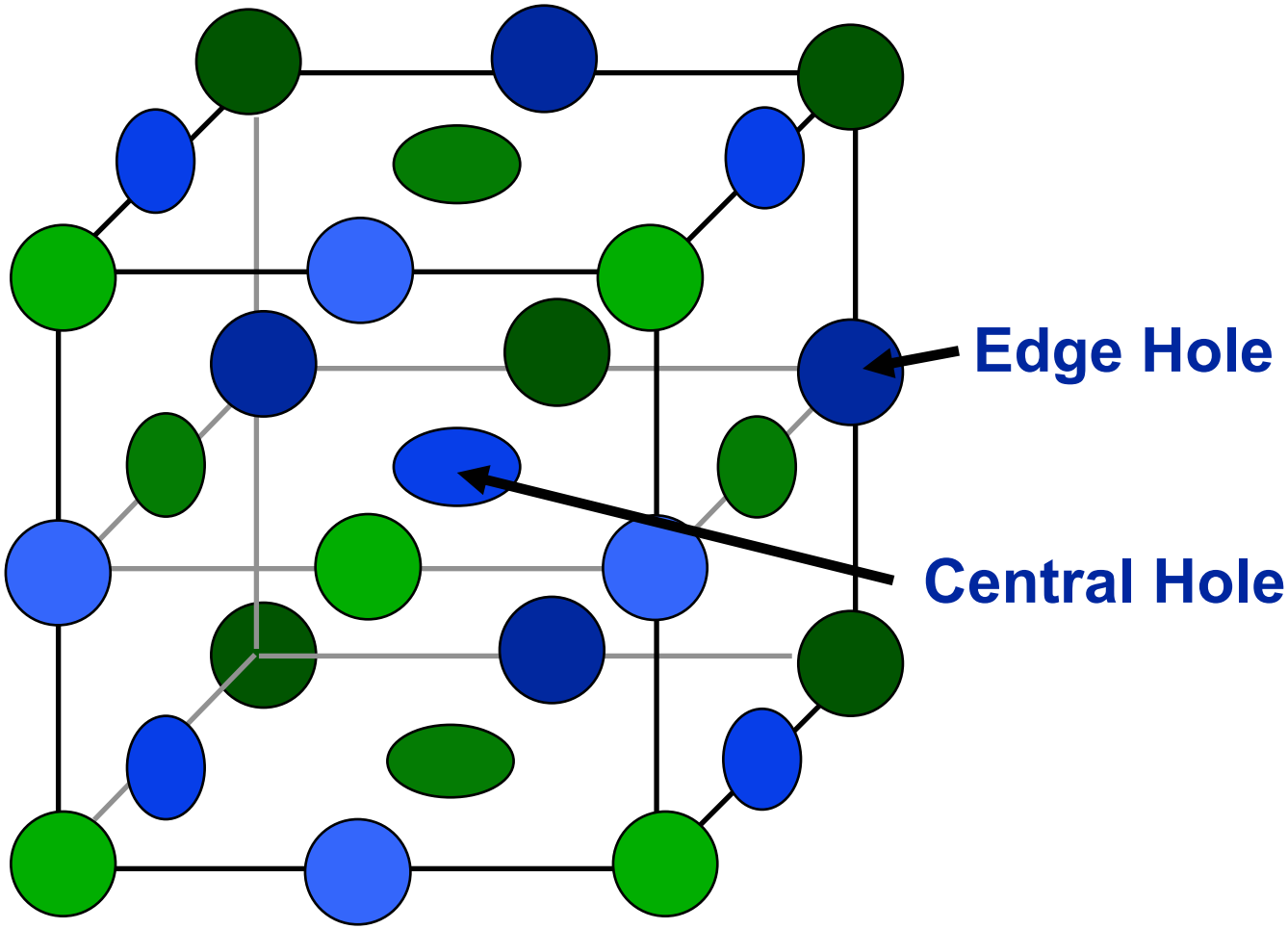
8 Corner Atoms in a Unit Cell * 1/8 = 1 Atom/Unit Cell

A Face-Centered Cubic Lattice



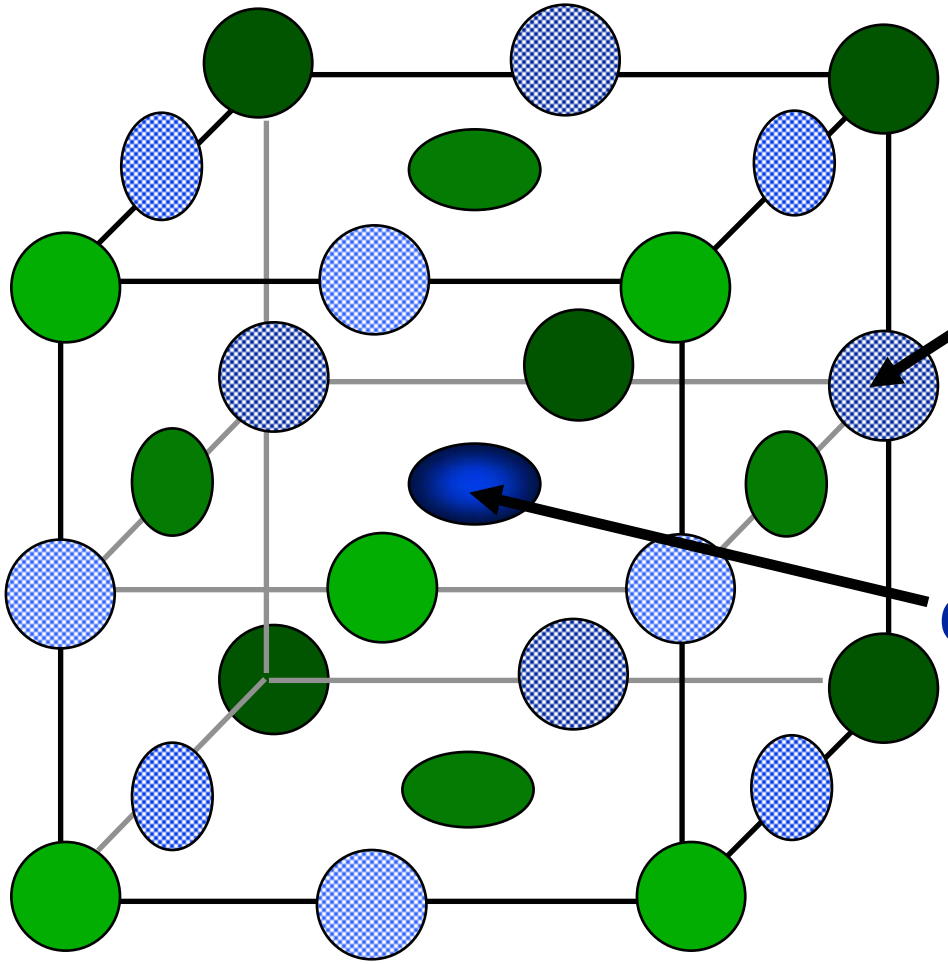
3 Face Equivalents and 1 Corner Equivalent =
4 Total Atoms/Unit Cell From the FCC Lattice

Octahedral Holes in FCC Lattice: Rock Salt



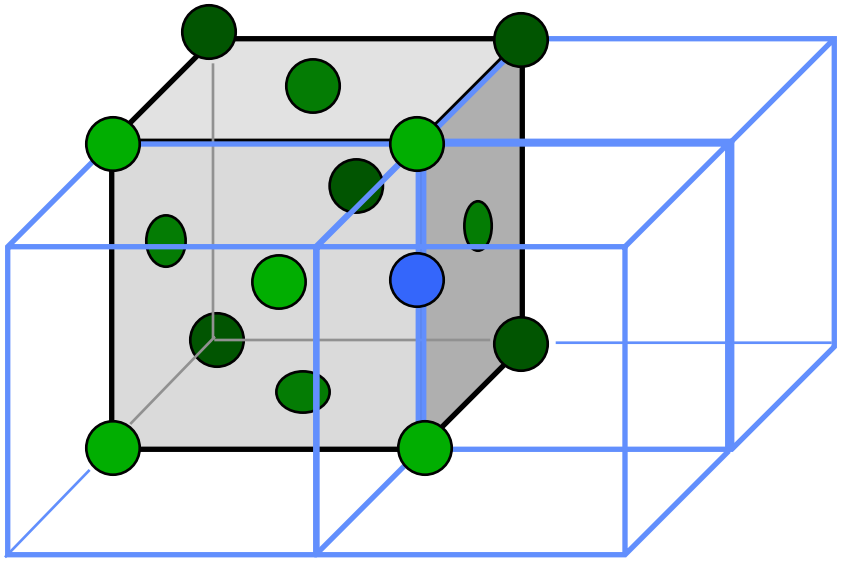
Now We Will Consider the Contribution of "Holes"/Unit Cell

Octahedral Holes in FCC Lattice: Rock Salt



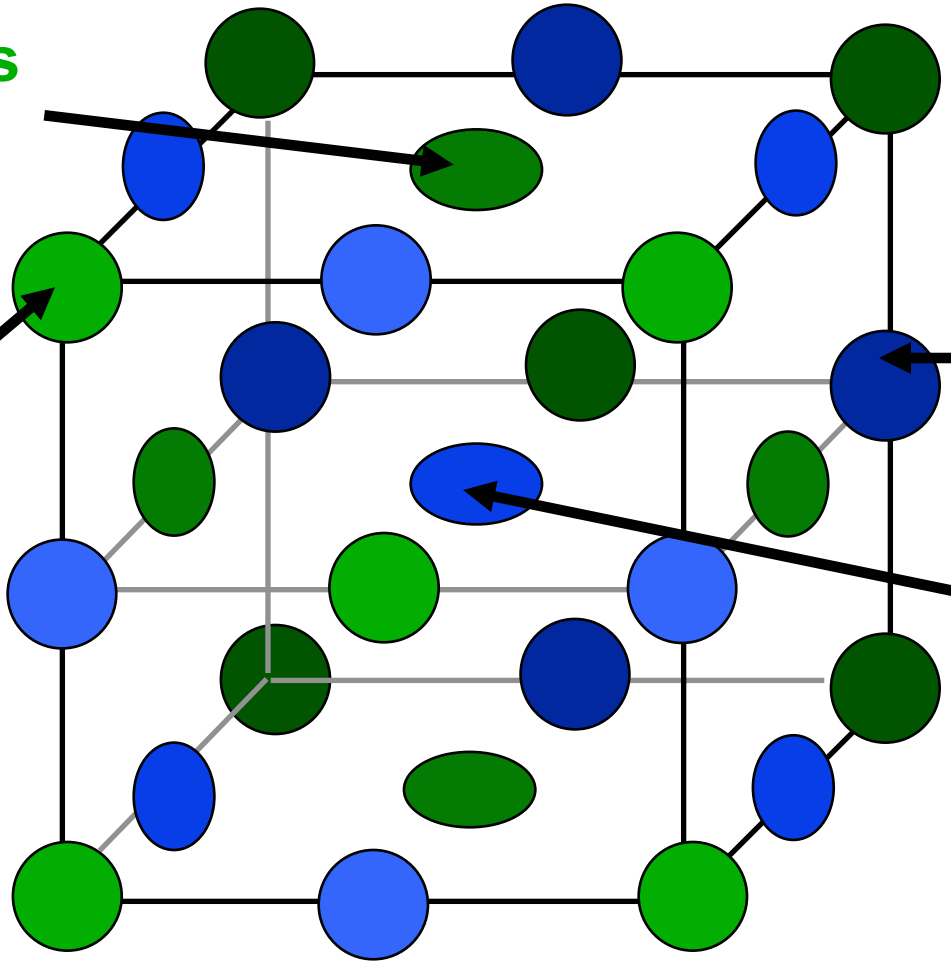
What About Edge Atoms? (12 Total Edge Atoms)

Edge Atoms in a FCC Lattice



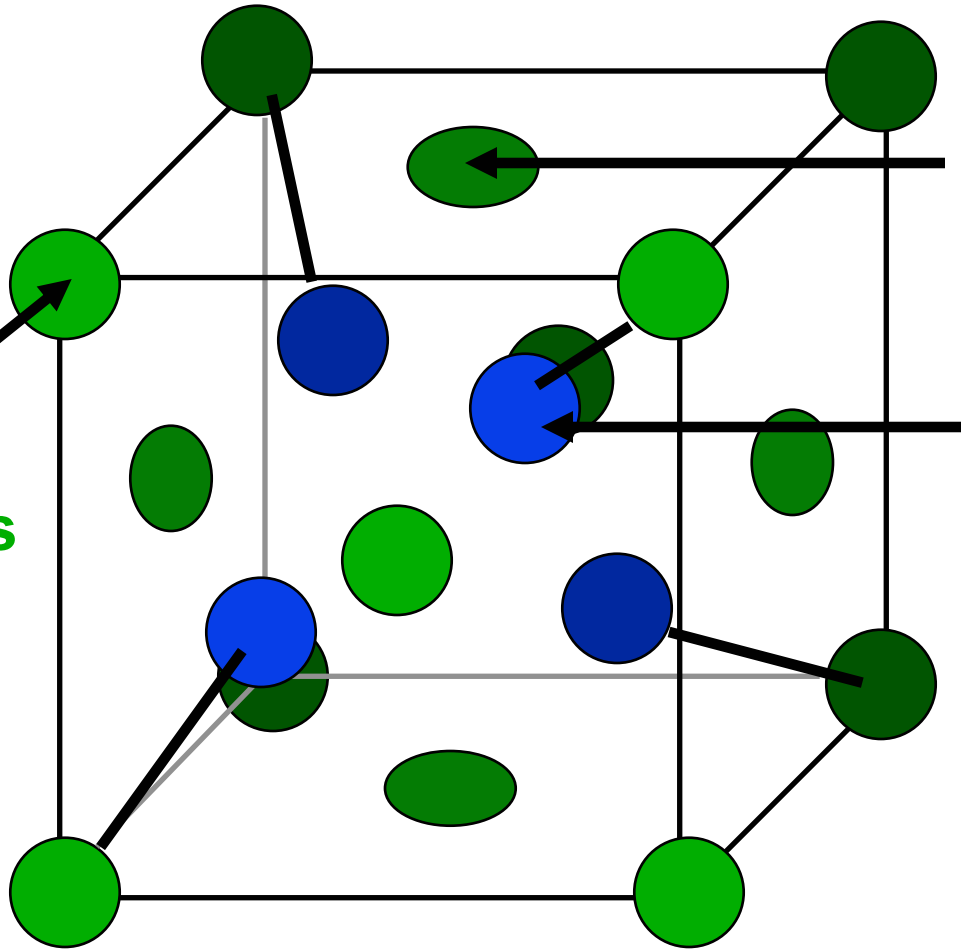
Edge Atoms Are Shared Between 4 Unit Cells
So Each Edge Atom Counts as 1/4 for Each Unit Cell
12 Edge Atoms per cell * 1/4 = 3 Edge Atoms/Unit Cell

Stoichiometry of Rock Salt



4 Total Lattice Atoms: 4 Lattice Holes
1:1 Stoichiometry (NaCl)

Stoichiometry of Zinc Blende



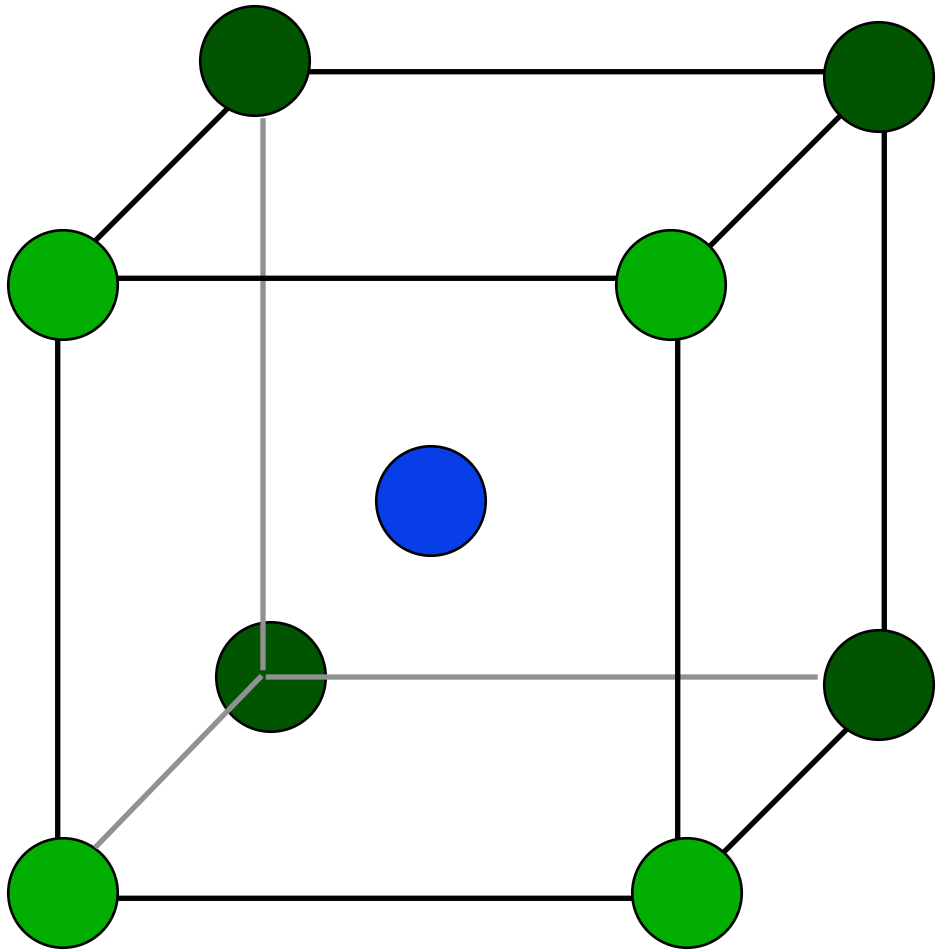
Face Atoms
(6 * 1/2 = 3)

T_d Holes
(4 * 1 = 4)

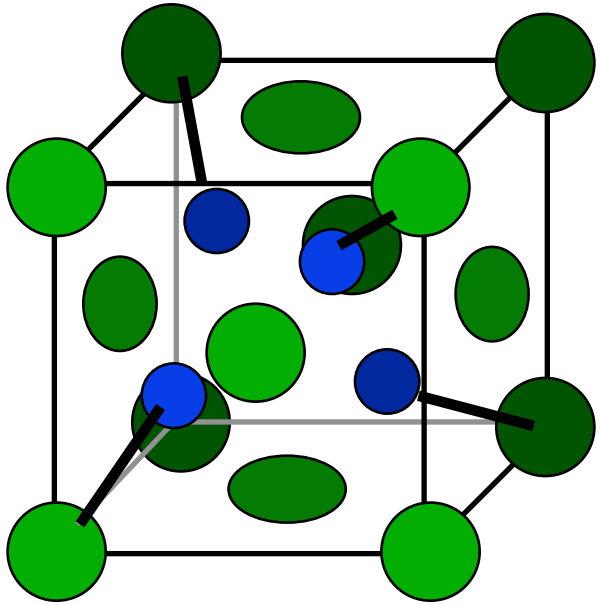
Corner Atoms
(8 * 1/8 = 1)

4 Lattice Atoms: 4 Tetrahedral Holes
1:1 Stoichiometry (GaAs, InP, CdS, ZnS)

Body Centered Cubic Lattice

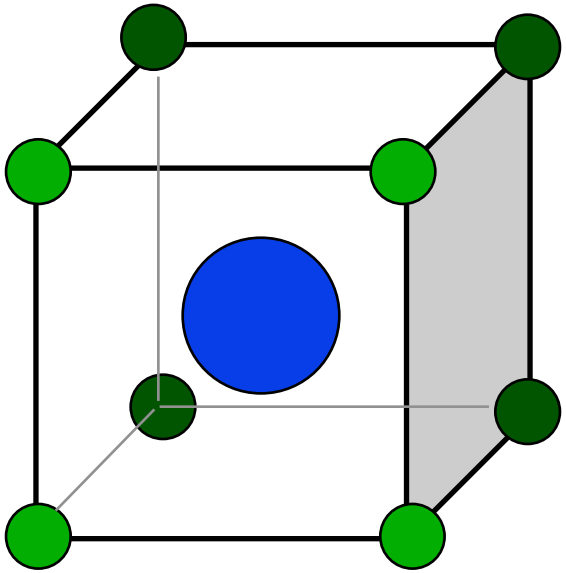


1 Extra Atom at Center of Unit Cell; 1:1 Also

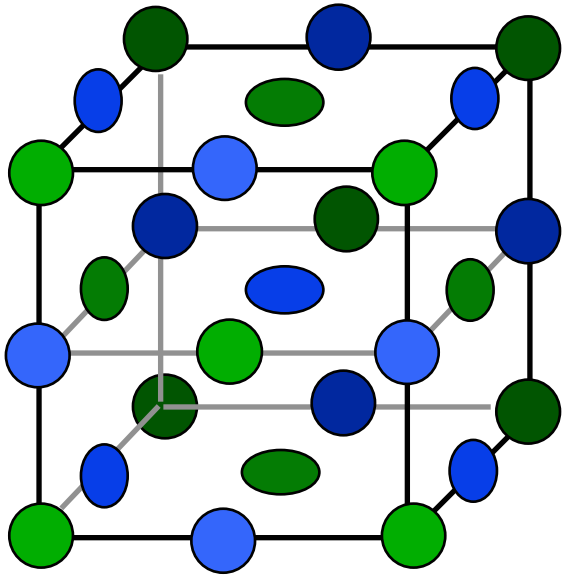


ZnS
(Smallest Cation/Anion)

CsCl
(Biggest Cation/Anion)



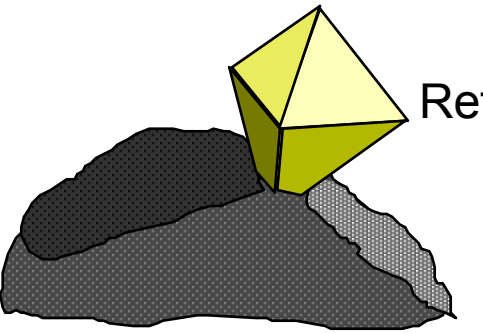
NaCl
(Intermediate Cation/Anion)



END

Crystals

Part 1



References: Gray: Chapter 6
OGN: Chapter 19 and (24.1)