CHAPTER 6

Physical Properties of Minerals

Physical Properties of Minerals

- Physical properties of minerals are controlled by chemical composition and structure

- So, samples of same minerals exhibit the same properties

- Thus physical properties can be used to identify minerals

- Physical properties can be grouped into four categories

Properties based on

1.Mass (density and specific gravity)

2.Mechanical cohesion (hardness, tenacity, cleavage, fracture and parting)

3.Interaction with light (luster, color, streak, lumnescence)

4.Other Properties (magnetism, electrical etc)

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Density

- Density(ρ) : mass (m) per unit volume (v)

$$\rho = m/v \ (g/cm^3)$$

- Specific Gravity (G) = density of a material divided by the density of water at $4°C$

$$G = \rho/\rho_{H2O}$$

is unit less because G is the ratio of two densities.

  – Since the density of water is 1 g/cm^3, the numerical value of density and specific gravity are same in metric system
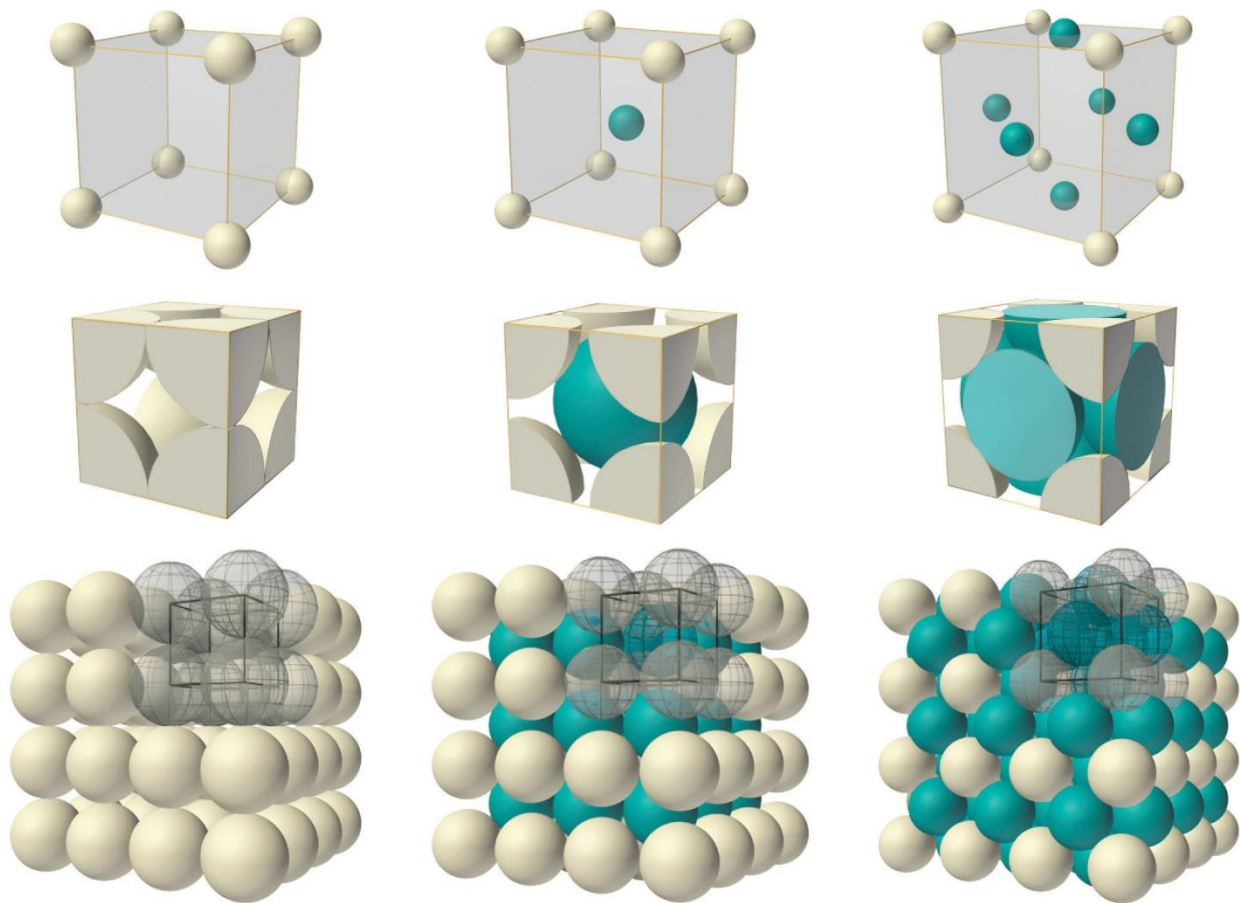
Specific Gravity

- Specific Gravity depends on the chemical composition and how tightly the atoms are packed

- **Packing Index** → how tightly the ions are packed in a mineral:

$$PI = (V_I/V_c) * 100$$

  Where Vc is the unit cell volume and V_I is the actual volume of the ions based on their ionic radii

- Maximum packing index for a close packed structure of uniform spheres is 74% -- most minerals have values between 35 and 74

- Minerals formed at high pressure has higher PI :

  – Kyanite → PI = 60.1 and G = 3.6
    Andalusite → PI= 52.3 and G = 3.1

- G depends on the composition also. Minerals containing elements of high atomic weight have higher ρ and G.

  – In Olivines Fo (Mg2SiO4) : G = 3.26, Fa (Fe2SiO4) : G = 4.39
  – Aromic weights: Fe (56), Mg (24.3)

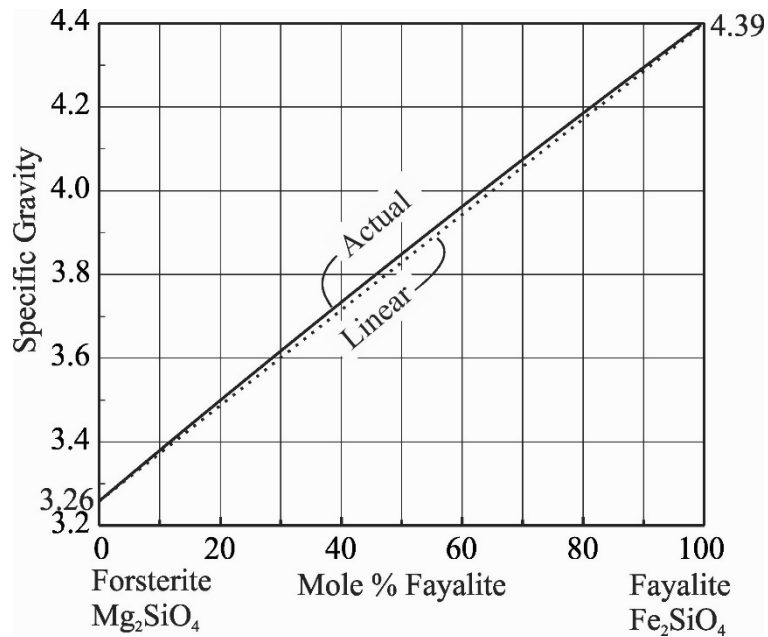(a) Simple cubic   (b) Body-centered cubic   (c) Face-centered cubic

Figure 6.1 Specific gravity of olivine. The dotted line assumes a linear variation in specific gravity between 3.26 for forsterite (Mg_2SiO_4) and 4.39 for fayalite (Fe_2SiO_4). The solid line is the actual specific gravity for intermediate compositions.

Measuring Specific Gravity

Jolly's Spring balance:
- Sample is weighed in air (ma) and then weighed while suspended in water (mw).

$$G= ma/(ma-mw)$$

- **Pychnometer**:
- weigh the mineral in air (mm),
- Weigh the bottle filled with water (mw)
- Place the sample in the bottle – close the stopper – the excess water equal to the volume of the sample is expelled – and weigh the bottle+water+sample (ms)
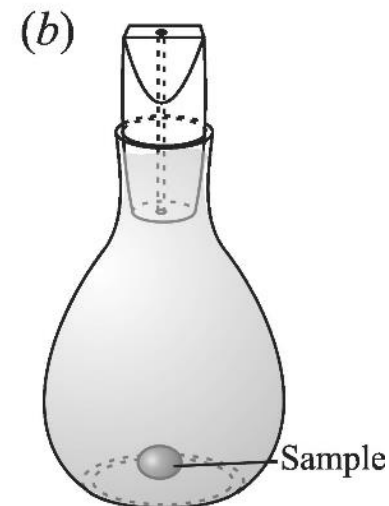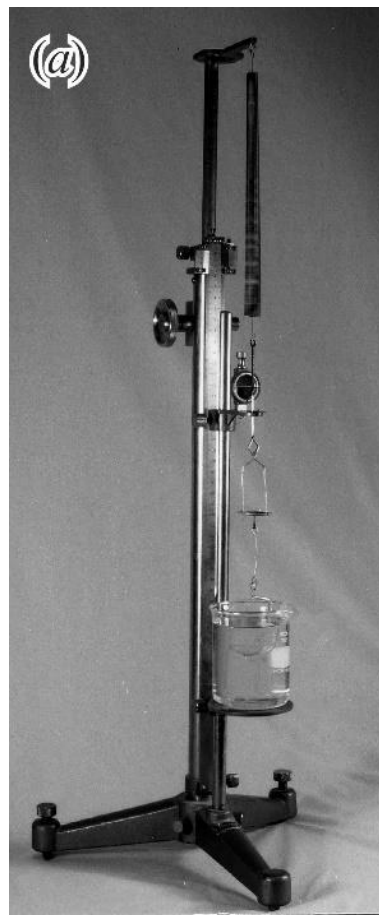
$$G=mm/(ma+mw-ms)$$

Figure 6.2 Apparatus t o measure specific gravity. (*a*) Jolly balance: as ample of a mineral is weighed first in the upper pan and then in the lower pan, which is suspended in water. (*b*) Pychnometer.

Heavy Liquids

- Liquids of varying specific gravity is used to separate minerals of different densities.
    - Di-iodo-methane (methylene Iodide) (3.3)
    - Lithium Metatungstate (3.1)
    - Bromoform (2.9)
- These liquids can be diluted with acetoneor alcohol to form liquids of lower densities
- Small glass cubes (density cubes) of varying density is used to determine the density of any intermediate liquid

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Properties Related to Mechanical Cohesion

Mohs Scale of Hardness

Hardness	Mineral		Mnemonic
1	Talc		**T**all
2	Gypsum	Finger Nail (2+)	**G**irls
3	Calcite	Copper Penny (3)	**C**an
4	Fluorite		**F**lirt
5	Apatite	Knife Blade (5)	**A**nd
6	Orthoclase	Window Glass (5.5)	**O**ther
7	Quartz	Steel File (6.5)	**Q**ueer
8	Topaz		**T**hings
9	Corundum		**C**an
10	Diamond		**D**o

- Moh's scale is not linear
- Can vary according to crystallographic directions: Kyanite has hardness of 5 parallel to length of the crystal and 7 right angles to it. Such variations is quite common in non-isometric systems. Halite, though isometric, is also harder at angle to the cleavage traces.

Quantitative Hardness:

- Indentation hardness: : load is applied to a plunger with a diamond tip placed on a polished mineral surface

- The depth of the indentation is checked with a microscope and is proportional to the mineral's hardness
- **Vicker's hardness:** uses a square pyramid shaped indenter

- **Vicker's hardness number (VHN) =**

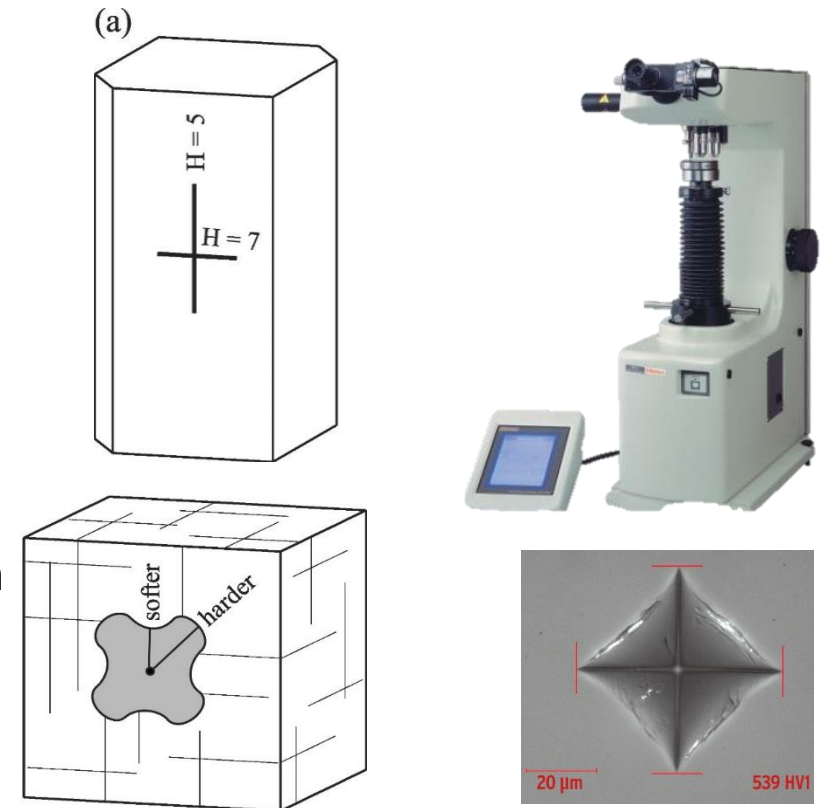Load applied/ surface area of the indentation

Figure 6.3 Variation of mineral hardness with direction.
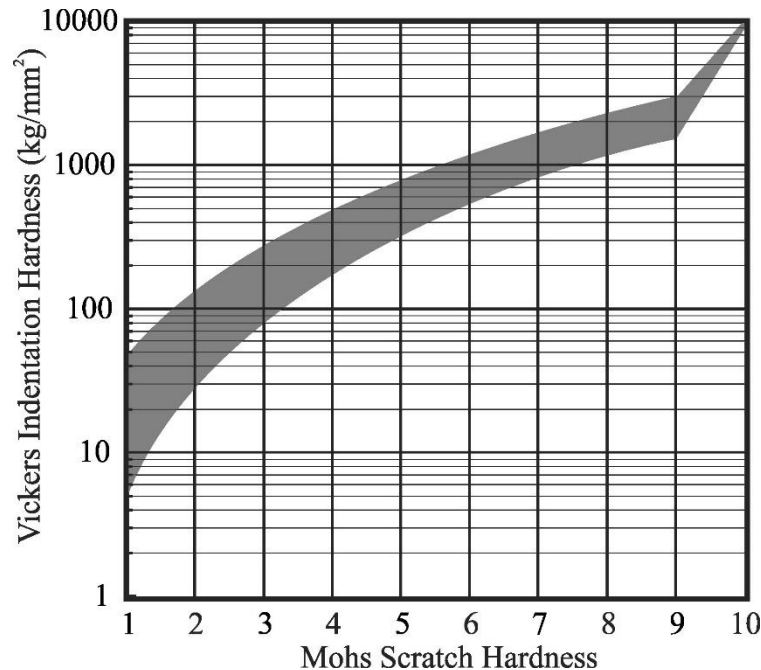
Figure 6.4 Approximate range of Vickers indentation hardness (shaded) as a function of Mohs scratch hardnes.

- Note the difference between hardness of 9 and 10 in Moh's scale
- Note the range in Vicker's hardness.

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- Cleavage: planes of weaknesses along which a mineral preferentially breaks.
- Identified with Miller indices. Typically described in terms of crystal form which is a collection of identical crystal faces. For example a {001} cleavage in isometric minerals are all cleavages parallel to (001), (010) and (100) faces.
- Cleavage surface need not be parallel to the crystal faces e.g., Fluorite grows as {001} cube but has {111} octahedral cleavage.
- Theoretically a mineral can be cleaved as this as the thickness of a unit cell
- A cleavage may be:
    - Perfect
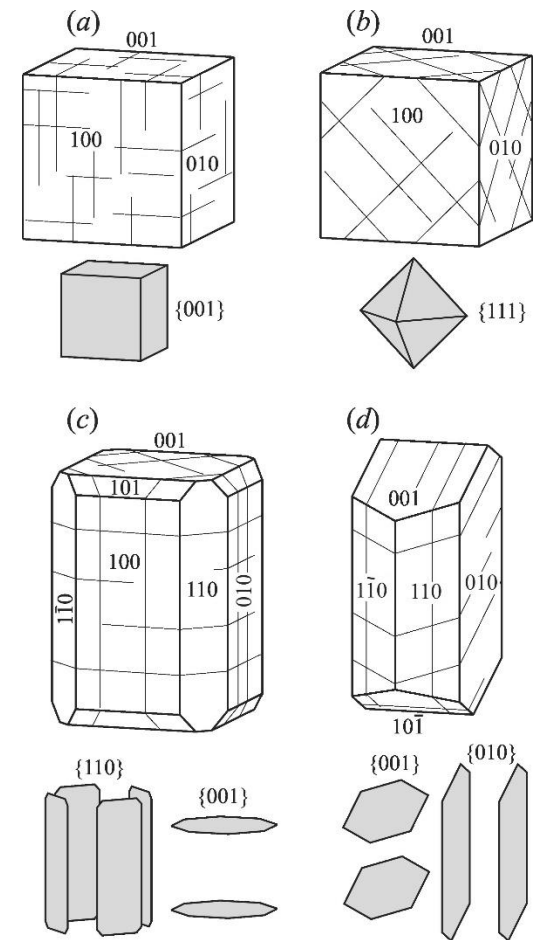   - Good
    - Distinct
    - Indistinct
    - poor

Figure 6.5 Cleavage.

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- Fracture: break without obvious crystallographic control
  - Conchoidal: smooth, curved surface
  - Irregular: as the name suggests
  - Hackly: sharp edged irregularity
  - Splintery: like the end of a broken piece of wood
- Parting: smooth, crystallographic control but mm apart not of unit cell dimension
  - Seen in polysynthetic twinning
  - Seen along exsolution lamellae
  - Described same way as the cleavage : specified by miller indices

Color and Luster

- Light striking any object is reflected, transmitted or absorbed
- Our perception of color and luster is controlled by the balance of these three
- Light is a tiny part of the broad electromagnetic spectrum
- Visible light has wavelength between 400 nm (violet) and 700 nm (red).
  (nm = nanometer = 10^{-9} meter = 10 Å)
- Speed of light in vacuum (V_v) = 10^{17} nm/sec
- Light is slowed down when it enters any material. Velocity (Vm) decreases as mineral density increases

  Index of refraction (n) = V_v/V_m
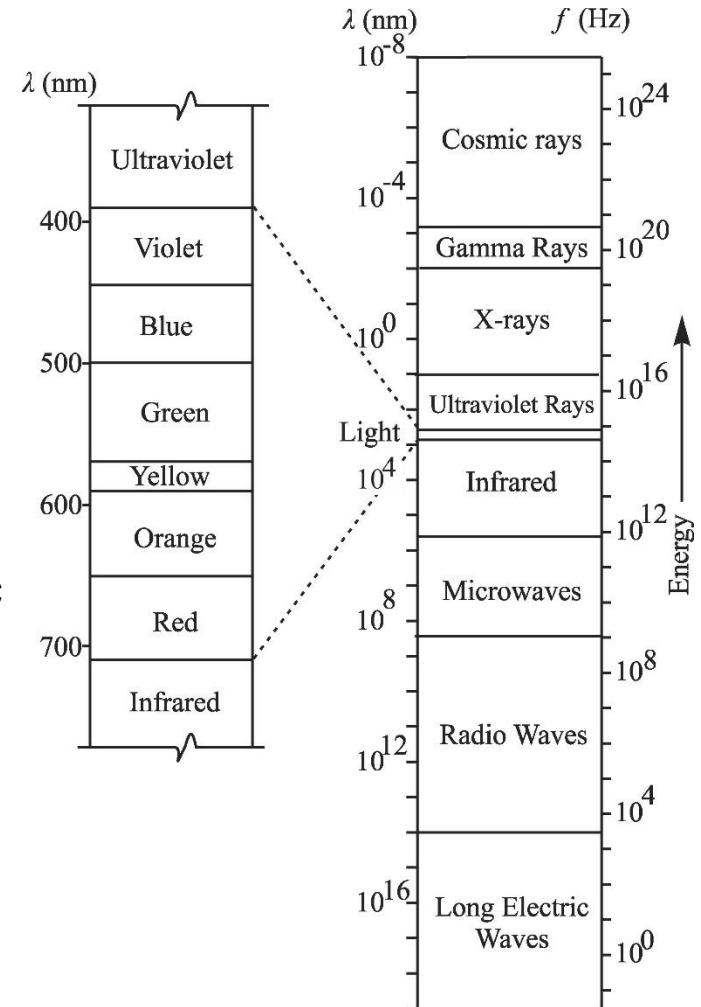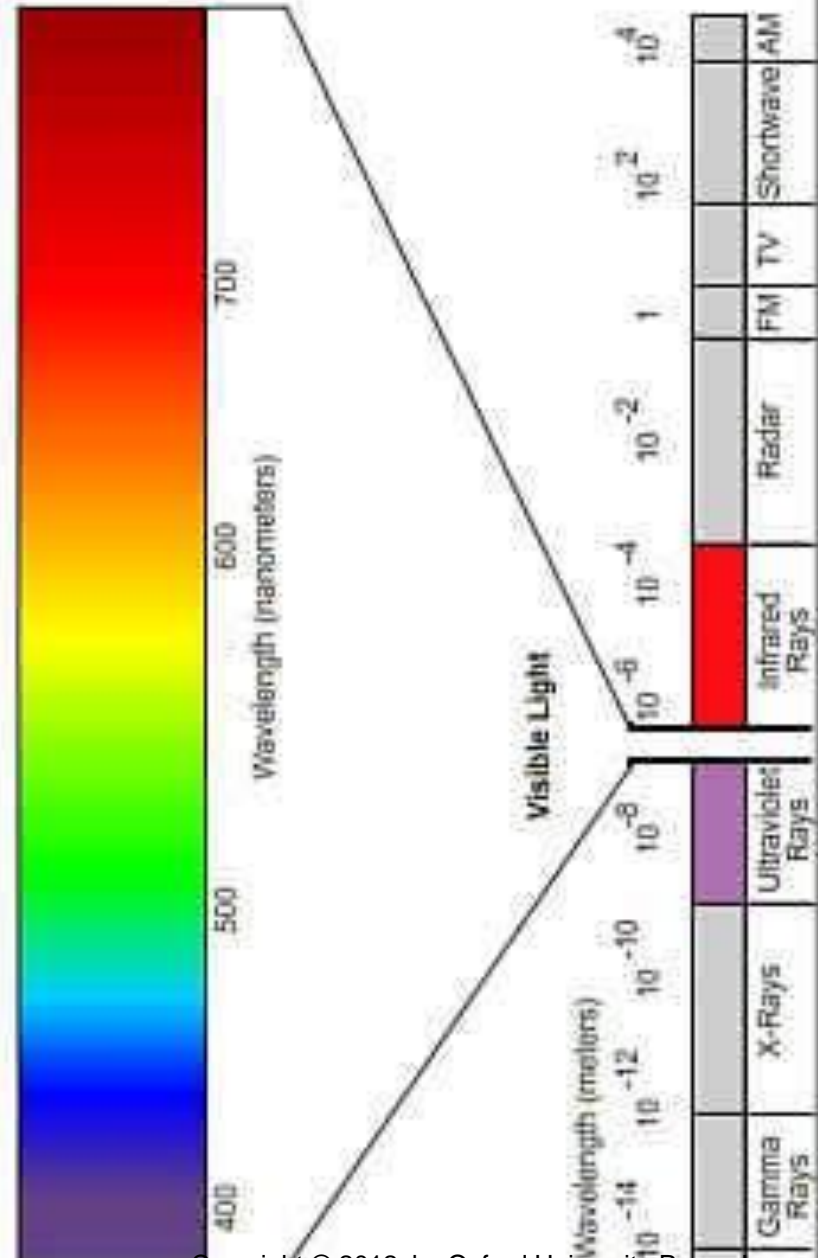- In most minerals n is between 1.5 to 2

Figure 6.6 The electromagnetic spectrum. Visible light, with wavelengths between about 400 and 700 nm, is a small portion of this spectrum (1 nm = 10^{-9}m = 10Å).

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- Human eye has three different color receptors:
  - 660 nm (red)
  - 500 nm (green)
  - 420 nm (blue-violet)
- Our eye interpret monochromatic light (light of a single wavelength) as one of the spectral color (ROYGBIV)
- When yellow monochromatic light (570nm) reaches our eye, it stimulates both red and green receptors almost equally and blue-violet very little. Our brain interprets the color to be halfway between red and green.

Electromagnetic Spectrum: Visible Light

Visible Light

Wavelength (nanometers)

700

600

500

400

Wavelength (meters)

10^4
10^2
1
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}

Shortwave AM
TV
FM
Radar
Infrared Rays
Ultraviolet Rays
X-Rays
Gamma Rays

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- Polychromatic light consists of more than one wavelength
- Still produces sensation of a single color
    - that color might not be present in the light
    - Sensation of yellow can be produced by stimulating reg, green and blue-violet receptors in proper proportion.
    - Might not be a color of the spectrum – e.g., brown or purple light
    - If entire visible spectrum is present in the light, the eye perceives it as white light.
- 4% of mostly male population are color blind. Problem in optical mineralogy
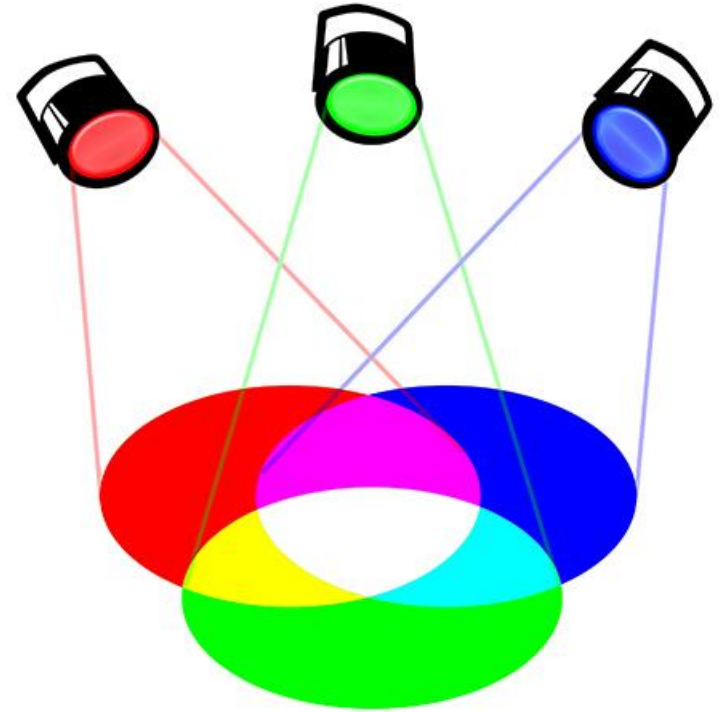
RGB
Transmitted light, additive

Luster

- Minerals: Opaque (mostly metallic minerals) and Transparent (ionic and covalent)
- Metallic and nonmetallic
- Thus: metallic lusters:
  – If >50% of the light is reflected: Shiny like Gold
  – 20-50% light reflected: normal metallic luster
  – <20% light reflected: submetallic
- and non-metallic lusters:
  – most of the light is transmitted and as little as 5% is reflected.
  – Depends on the index of refraction and texture
  – High index of refraction → brilliant luster
  – Check Table 6.2 for varieties of non-metallic luster
- **Color of a mineral** is the wavelength of light that the mineral reflects or transmits → the wavelength that reaches our eyes.
- A red minerals looks red because it reflects or transmits red light and absorbs most of the blue end of the spectrum.

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Mineral Color

- Electrons occur in different shells
- Outer shells are in higher energy levels compared to the inner shells
- If the energy of the incident electromagnetic radiation (like light) passing through a material is equal to the difference in energy between an electron and a vacant higher energy orbital, the incident energy is absorbed and the electron is bumped to the vacant higher energy level leaving a lower energy vacancy.
- When the bumped electron falls back to it's original energy level, it emits electromagnetic radiation some of which might be in visible light range (photoluminescence)

- Theories that explain bumping of electrons to reemit visible light in minerals:
  - **Crystal field theory**
  - **Band theory**
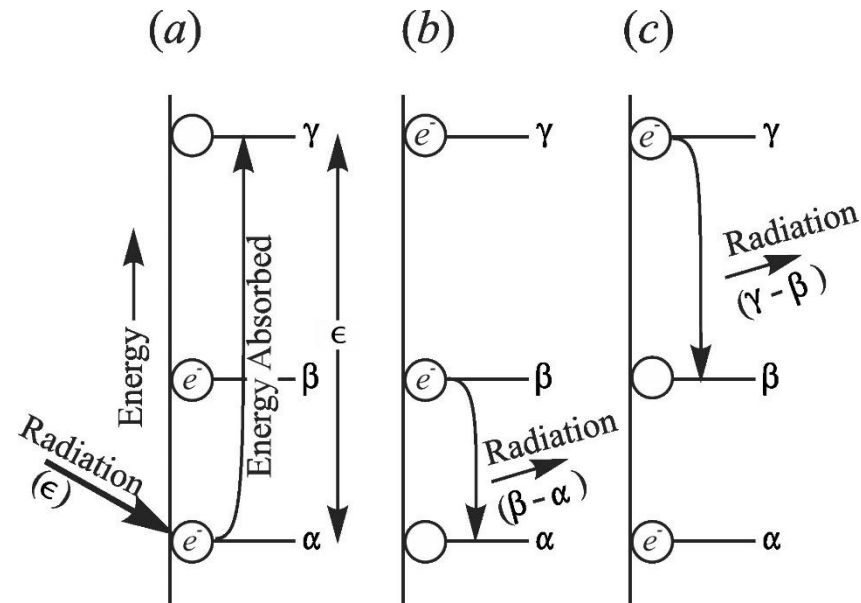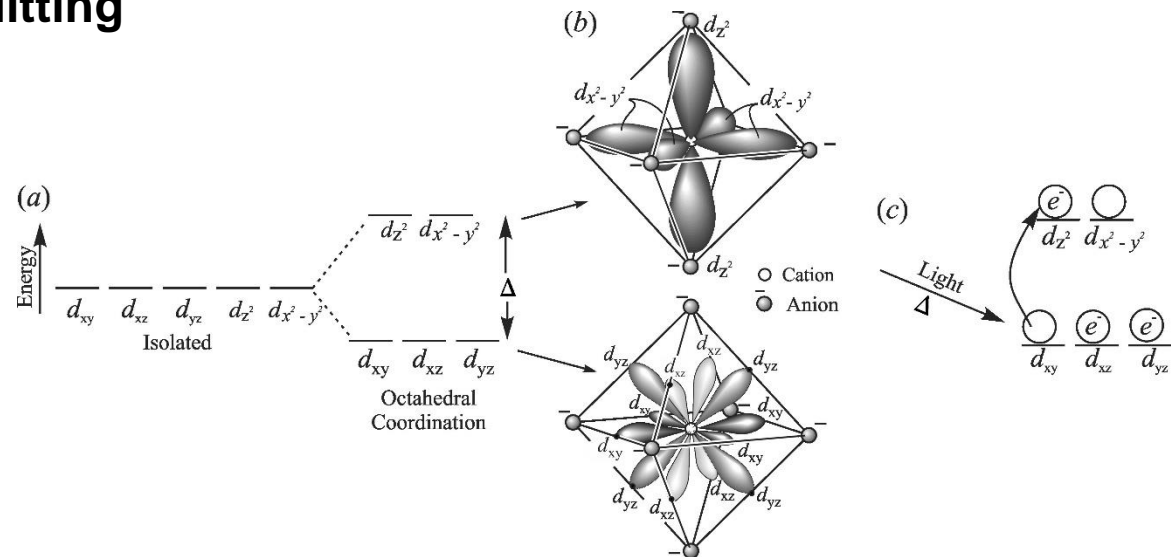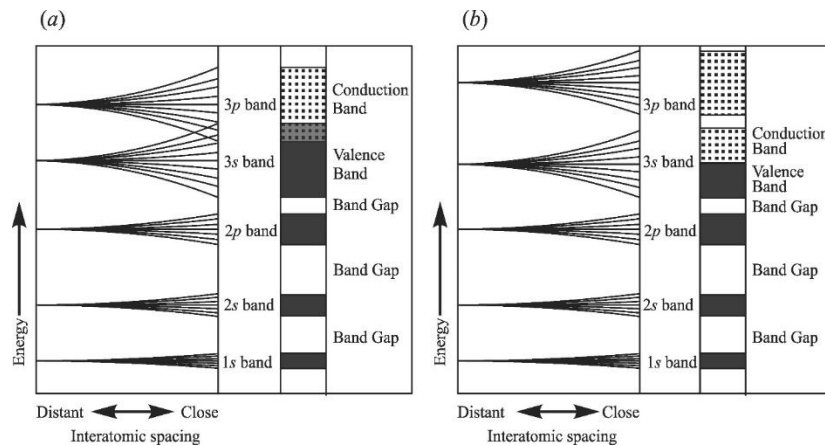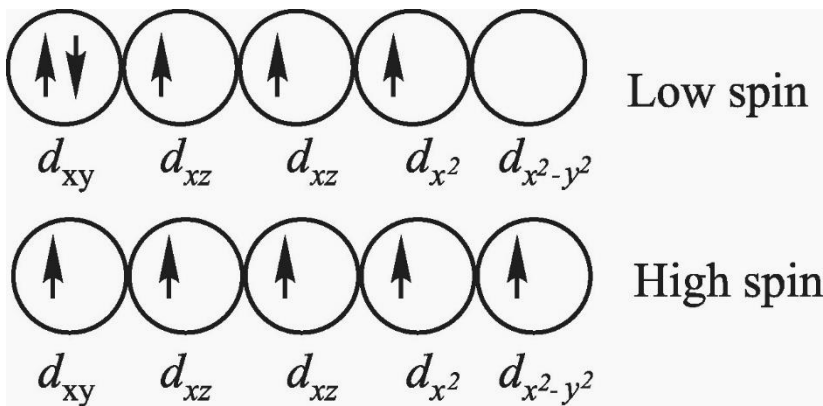 - **Charge transfer transitions**
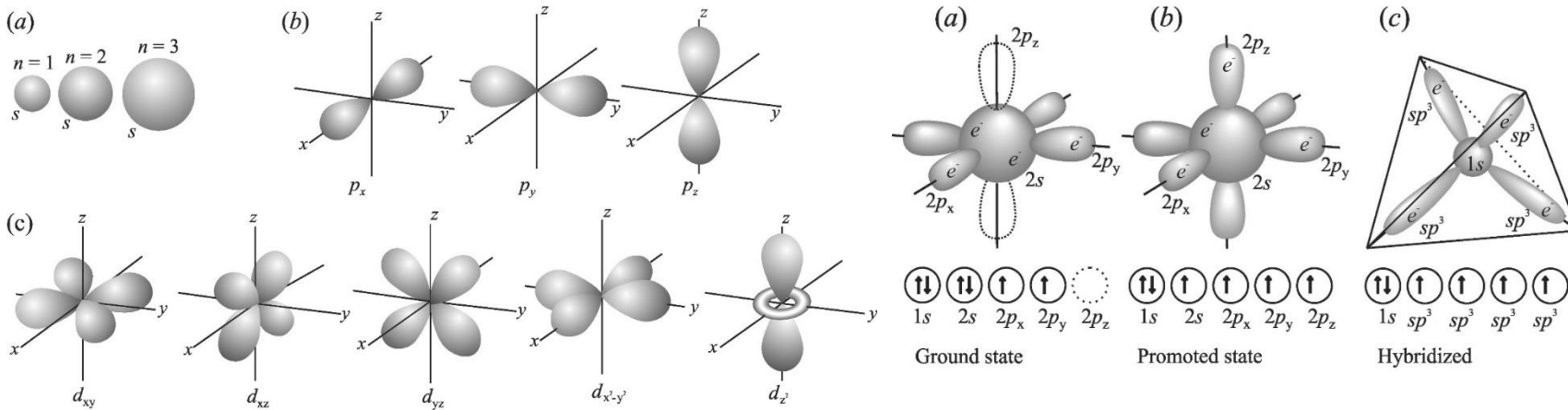 - **Color centers**

Figure 6.7 Absorption of electromagnetic radiation.

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Crystal Field Theory:

- Color produced by crystal field transition is common in ionic bonded minerals that contain cations with partially filled 3d orbitals (Ti, V, Cr, Mn, **Fe**, Co, Ni, and Ca) whose outer orbitals contain unpaired electrons
- These elements are known as **Chromophore elements** because they are effective in absorbing visible light and producing mineral colors**.**
- In isolated cations all electrons in the five subshells of 3d orbital has the same energy (but different magnetic and spin quantum numbers)
- In a coordinated polyhedral with say, Oxygen, the negative charges of the anion produces an electric field (crystal field) which interacts with the electrons of the cation
- **Some of the electrons end up with higher energy and some with lower energy → Crystal field splitting**

- Orbitals directed towards anions end up with higher energy, those directed between the anions end up with lower energy
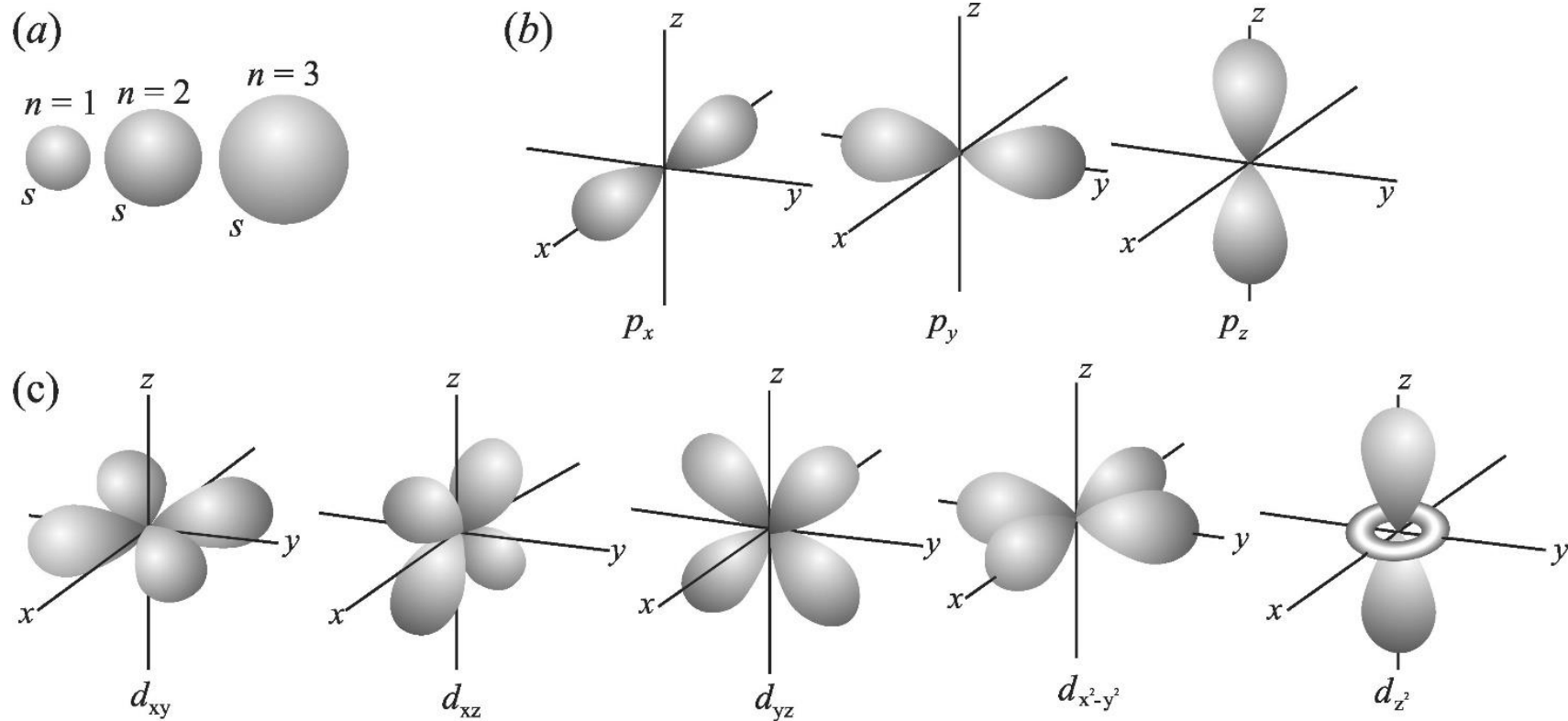
(a)

$n = 1$ $n = 2$ $n = 3$

s s s

(b)

p_x p_y p_z

(c)

d_{xy} d_{xz} d_{yz} $d_{x^2-y^2}$ d_{z^2}

(a)

$2p_z$ e^- e^- e^- e^- $2s$ $2p_y$ $2p_x$

$1s$ $2s$ $2p_x$ $2p_y$ $2p_z$

Ground state

(b)

$2p_z$ e^- e^- e^- $2s$ $2p_y$ $2p_x$

$1s$ $2s$ $2p_x$ $2p_y$ $2p_z$

Promoted state

(c)

e^- sp^3 e^- sp^3 $1s$ e^- sp^3 sp^3 e^-

$1s$ sp^3 sp^3 sp^3 sp^3

Hybridized

Low spin

d_{xy} d_{xz} d_{xz} d_{x^2} $d_{x^2-y^2}$

High spin

d_{xy} d_{xz} d_{xz} d_{x^2} $d_{x^2-y^2}$

(a)

Energy

$3p$ band Conduction Band
$3s$ band Valence Band
  Band Gap
$2p$ band Band Gap
$2s$ band Band Gap
$1s$ band

Distant ⟷ Close
Interatomic spacing

(b)

Energy

$3p$ band Conduction Band
$3s$ band Conduction Band
  Valence Band
  Band Gap
$2p$ band Band Gap
$2s$ band Band Gap
$1s$ band

Distant ⟷ Close
Interatomic spacing

Figure 3.1 Geometry of orbitals in the *s, p,* and *d* subshells. Orbitals represent the volume of space around a nucleus in which an electron is most probably located.

- When the coordination polyhedral are combined to construct a mineral – energy levels produced by crystal field splitting are spread into energy bands (Pauli's exclusion principle)

- The difference in energy between the low energy and high energy levels matches that of visible light

- In ruby small amount of Cr substitute for Al in pure corundum (Al_2O_3)

- Crystal field splitting produces excited energy levels B, C and D with energy levels = 1.9 eV, 2.2 eV, and 3.0 eV

- Yellow green (550 nm) and violet light (400 nm) has the exact energy levels that can bump up ground state electron to C and D levels and are hence absorbed. That leaves red (and small amount blue) as the transmitted light which makes ruby appear to be of rich red color.
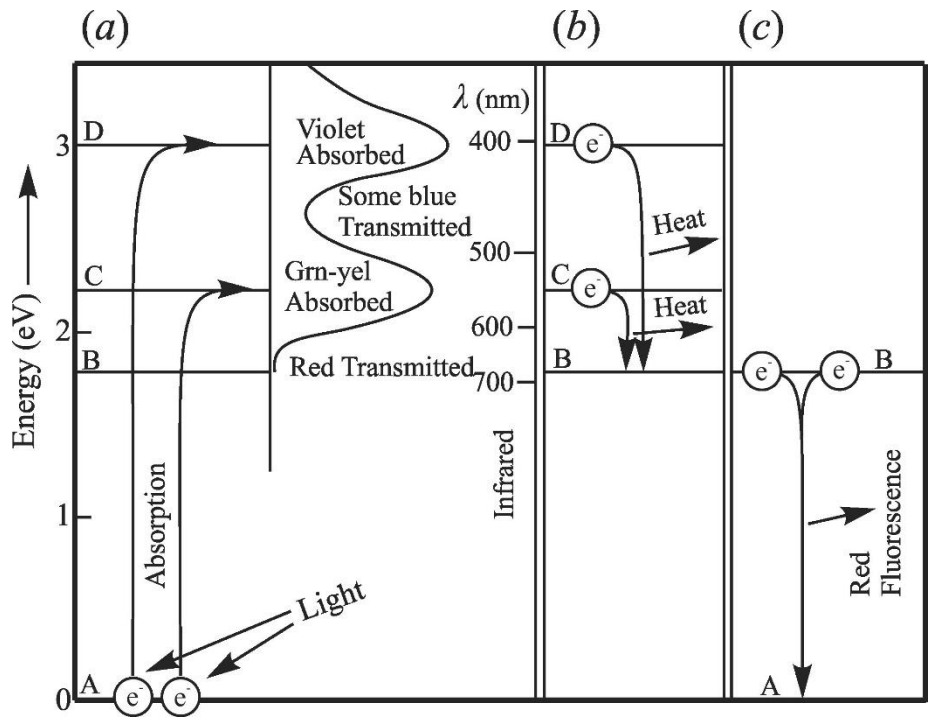
Figure 6.9 Light absorption in ruby.

Band Theory:

- In metallic bonds, the energy level of valence band overlaps with that of conduction band
- Conduction band contains a continuum of available vacant energy levels
- So entire visible spectrum can be absorbed to move electrons from valence bands to conduction band – so no light passes through the mineral
- Some light is radiated when the excited electrons fall back to lower energy positions – which gives the metal it's color.
    - Minerals with a substantial amount of covalent bnds have a band gap between the valence and conduction bands.
    - If the band gap is smaller than the energy level of visible light all the light is absorbed→black or gray
    - If the band gap is intermediate, high energy, short wavelength light from the violet end will be absorbed → the mineral will appear red (as in Cinnabar)
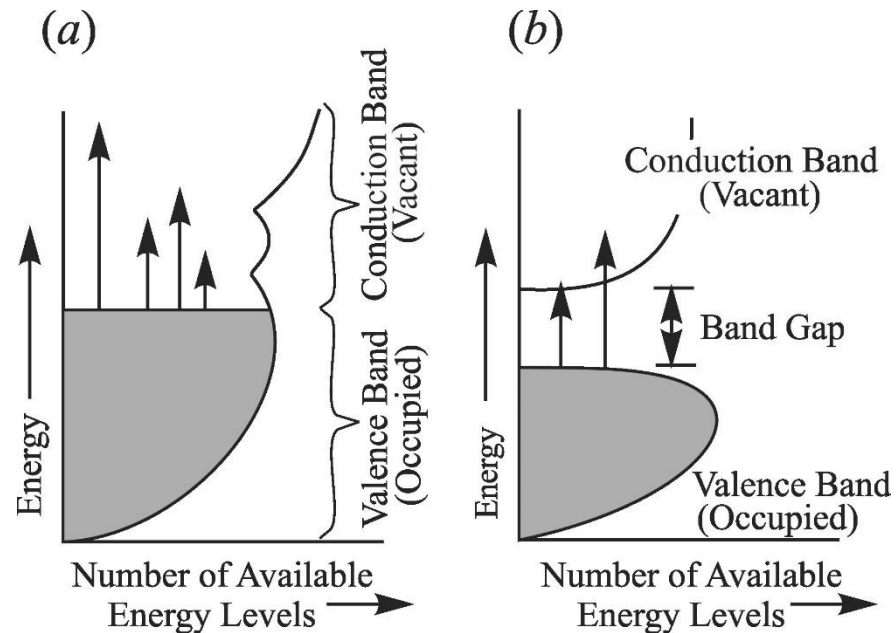   - If the band gap is large no light is absorbed, as in Diamond and the mineral appear as white or colorless

(a) *(b)*

Figure 6.10 Band theory.

# Charge Transfer Transitions or (molecular orbital transitions)

- When valence electrons are bumped into higher energy level in adjacent cation

- Differently charged cations occupy sites A and B

- Lowered charge cation at A absorbs electromagnetic radiation and bumps an electron to the higher charge cation in B.

- Fe^{2+} bumps electron to Fe^{3+} or Ti^{4+} cations

- Usually the energy difference = red end of the spectrum $\rightarrow$ which is thus absorbed – making the mineral appear blue e.g., in Sapphire

- Sapphire is a gem variety of corundum where a small amount of Fe or Ti substitute for Al

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Electron Color Center
- In structures with Frenkel defect (missing ions) an electron might be present in the vacant spot to maintain charge neutrality.
- This electron is held in place by the crystal field of the adjacent anions and cations.
- This electron can be bumped to higher energy level of the adjacent ions
- If the energy of visible light matches any of the steps to which the electron can be bumped. That light will be absorbed. Ex: **Fluorite**

Hole Color Center
- When Fe^{3+} replaces Si^{4+} in quartz
  Charge balance is maintained by introducing a monovalent cation like H+ elsewhere in the structure
  - When a high-energy radiation ejects an electron from Oxygen anion – that electron stays trapped somewhere in the structure leaving the oxygen with a hole or missing electron
  - The hole has energy level to which other electrons in Oxygen can be bumped when red light is absorbed making the mineral violet in color. Ex: **Amethyst**

Figure 6.11 Color centers.
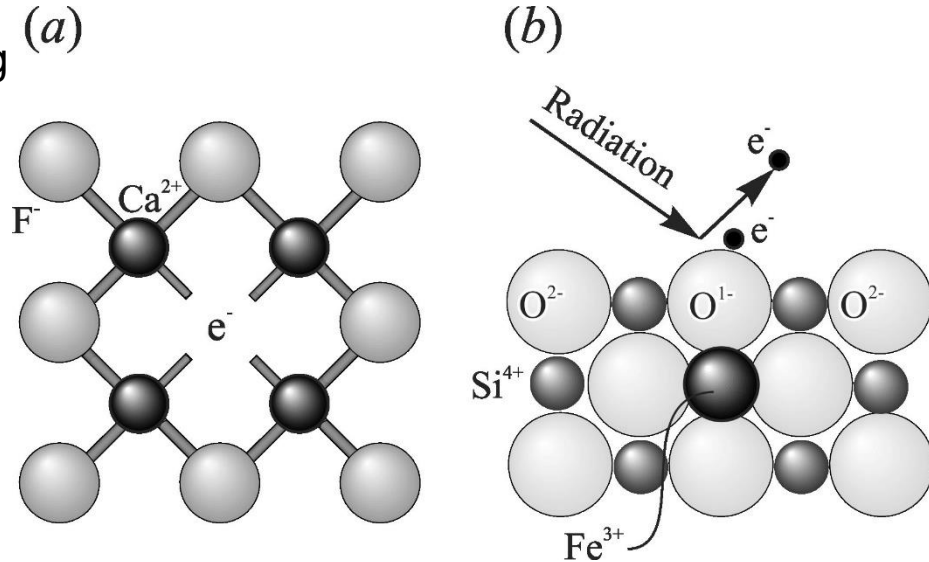
Color centers are defects and this can be produced by radiation (used to enhance colors of gemstones) and can be removed by heating (Fluorite becomes colorless by heating)

Color from Mechanical Causes

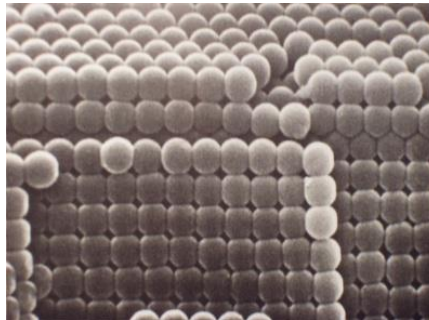- Jasper gets red color from finely dispersed inclusion of Hematite. Graphite inclusions can make calcite black.

- **Chatoyancy:** silky appearance because of parallel fine fibres -- satin spar variety of Gypsum ($CaSO_4$, $2H_2O$)
- **Asterism**: Star produced by finely fibrous rutile aligned aligned with 2 fold symmetry axis normal to c axis

Play of Color: Opal structure acting as diffraction grating

Iridescence is produced by thin film of oxide on a mineral surface the way oil on water produces color

Idiochromatic: Minerals that contain chromophone elements in their mineral formula or are opaque have consistent color – can exhibit a range of color as composition changes

**Allochromatic:** color due to chromophore impurities, light colored when pure

Luminescence

- Material absorbs one form of energy and then reemit the energy as visible light. The energy source may be mechanical, therma or electromagnetic
  - **Triboluminiscence**: seen in some materials when these are struck or crushed, or rubbed or scratched. Very faint, need darkness to see
  - **Thermoluminescence**: emits visible light when heated. Best between 50 – 100 C , lost above 475 C. At >550 C materials become incandescent and begin to glow.
  - **Photoluminescence**: materials emit light in response to being exposed to visible or ultraviolet light
    - **Fluoroscent:** disappears when light source is turned off
    - **Phosphorescent:** continues emitting light even after exciting radiation is turned off

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- Electron spin creates magnetic field
- Paired electrons cancel out each other's magnetic field, unpaired electrons produces magnetic behavior
- Diamagnetic: no element in mineral with unpaired spin.
- Minerals with elements with unpaired spins in one or more orbitals:
  - Paramagntic
  - Ferromagnetic ⎤ Displayes
  - Ferrimagnetic ⎦ attraction to magnet
  - Antiferromagnetic

- Transition metals (Fe, Mn, Ti, Cr) whose 3d orbitals are only partially filled have unpaired electrons
- Strength of magnetism depends on the number of unpaired electrons
- Fe^{3+} and Mn^{3+} have maximum 5 unpaired
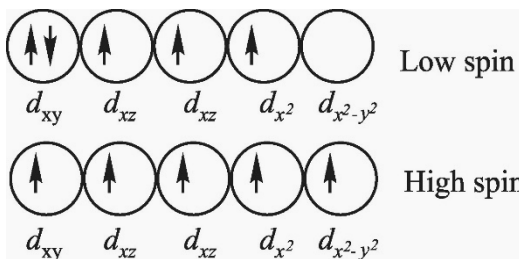
	Spin Configuration	μ_B	No External Field	In External Field	External Field Removed
(a) Diamagnetic	Quartz (SiO_2) Si^{4} (↑↓)(↑↓)(↑↓) 3p	0			
	$2O^{2}$(↑↓)(↑↓)(↑↓) 3p	0	Net = 0	Weak Repulsion	Net = 0
		0			
(b) Paramagnetic	Olivine (Fe_2SiO_4) $2Fe^{2+}$(↑↓)(↑)(↑)(↑)(↑) 3d	+8			
	Si^{4+} (↑↓)(↑↓)(↑↓) 3p	0			
	$4O^{2}$ (↑↓)(↑↓)(↑↓) 2p	0	Net = 0	Weak Attraction	Net = 0
		8			
(c) Ferromagnetic	Iron (Fe) Fe (↑↓)(↑↓)(↑↓)(↑)(↑) 3d	+2			
		2	Net = 0	Strong Attraction	Net Magnetization
(d) Ferrimagnetic	Magnetite $^{IV}Fe^{2+}$(↑↓)(↑)(↑)(↑)(↑)	+4			
	$^{VI}Fe^{3+}$(↑)(↑)(↑)(↑)(↑) } 3d	+5			
	$^{IV}Fe^{3+}$(↓)(↓)(↓)(↓)(↓)	-5			
	$4O^{2}$(↑↓)(↑↓)(↑↓) 2p	0	Net = 0	Moderate Attraction	Net Magnetization
		4			
(e) Anti-ferromagnetic	Ilmenite (<-183C) $^{VI}Fe^{2+}$(↑↓)(↑)(↑)(↑)(↑) 3d	+4			
	$^{VI}Fe^{2+}$(↑↓)(↓)(↓)(↓)(↓)	-4			
	$^{VI}2Ti^{4+}$(↑↓)(↑↓)(↑↓) 3p	0	Net = 0	Repelled	Net = 0
		0			

Low spin / High spin
d_{xy} d_{xz} d_{xz} d_{x^2} $d_{x^2-y^2}$

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- Paramagnetism: Magnetic moment of atoms are not mutually aligned
- Olivine contains Fe2+ which has four unpaired electrons in 3d orbitals
- All have spins in the same direction: **Hund's Rule**
- In a strong magnetic field these magnetic moments tend to align and the olivine is attracted to a magnet
- Magnetic attraction is weak.
- Amount of attraction depends on magnetic susceptibility
- Magnetism is lost when the external field is removed
- Franz Isodynamic Separator

- **Ferromagnetic** materials like Iron are capable of retaining magnetic polarity because **exchange coupling** allows atoms with unpaired electrons to be systematically aligned.

- magnetic moments of adjacent ions are in parallel alignment within individual domains (microscopic volumes) but adjacent domains need not be so.

- With the application of strong external magnetic field domains with moments parallel to the external field expands and other less favorably aligned shrink – thus making the crystal permanently magnetized.

- The material remains magnetized even after the external field is removed

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- **Ferrimagnetism:**
  - Magnetic moments of atoms/ions in adjacent structural sites have antiparallel magnetic moments because of exchange coupling
  - The magnetic moments of these atoms cancel each other
  - As long as some additional atoms have unpaired electrons they can produce a magnetic moment and if they do not have antiparallel partner then the mineral will display magnetic property
  - In **Magnetite**, written as $^{IV}Fe^{3+}\uparrow{}^{VI}(Fe^{3+}\downarrow Fe^{2+}\uparrow) O_4$ – the tetrahedral and octahedral Fe3+ have opposite spins and their magnetic moment cancel each other but Fe2+ in octahedral sites have spins aligned and thus magnetite has a net magnetic moment
- **Antiferromagnetism:**
  - antiparallel spins cancel each other so zero magnetic moment.
  - Ilmenite (FeTiO3) is antiferromagnetic below -183C (Nèel Temperature) and antiparallel arrangement is destroyed and it becomes paramagnetic
- **Curie temperature**: above this temp all exchange coupling are destroyed and ferri/ferromagnetism is destroyed but regained if cooled below Curie temperature

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Electrical Conductivity:

- Minerals with metallic bonding has highest conductivity followed by van der waal's bonding.
- Ionic and covalent bonded minerals have low conductivity – no loose electrons
- Even in electrical insulators some current flows by migration of point defects like Schottky or Frenkel defects.
- Conductivity in insulators increases with increasing temp because ions can migrate more freely.
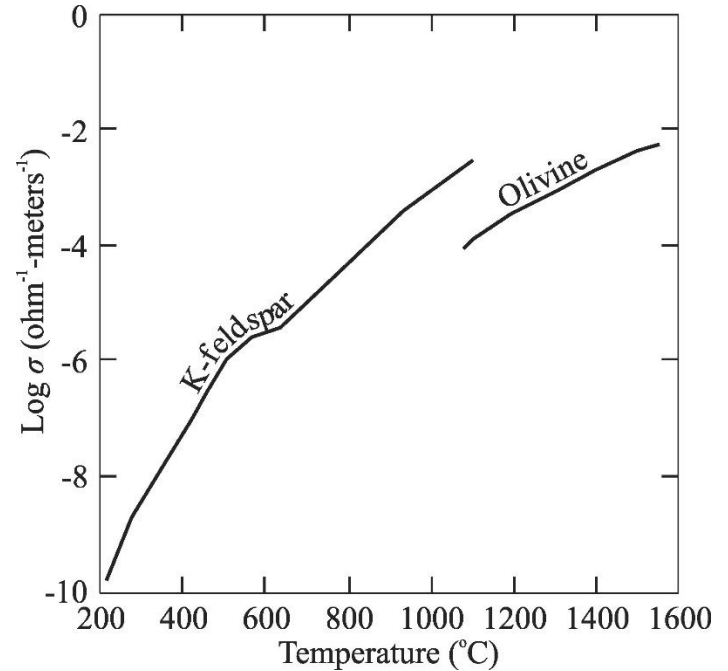

Figure 6.14 Electrical conductivity σ in units of reciprocal ohm-meters (ohm^{-1}-meter^{-1}) of olivine and K-feldspar. Olivine data at 70 kbar pressure from Yousheng and others (1998); K-feldspar data from Guseinov and Gargatsev (2002).

Piezoelectricity
- When deformed, piezoelectric minerals develop electrical polarity
- Ex: Quartz, Topaz, Tourmaline
- The reverse is also true – if a electric charge is applied to quartz – the mineral will deform (**electrorestriction**) --- if alternate current is applied, it will vibrate
- Occurs only in crystals that lack a center of symmetry

Pyroelectricity:
- Change in temperature causes the development of electric polarity and development of a voltage.
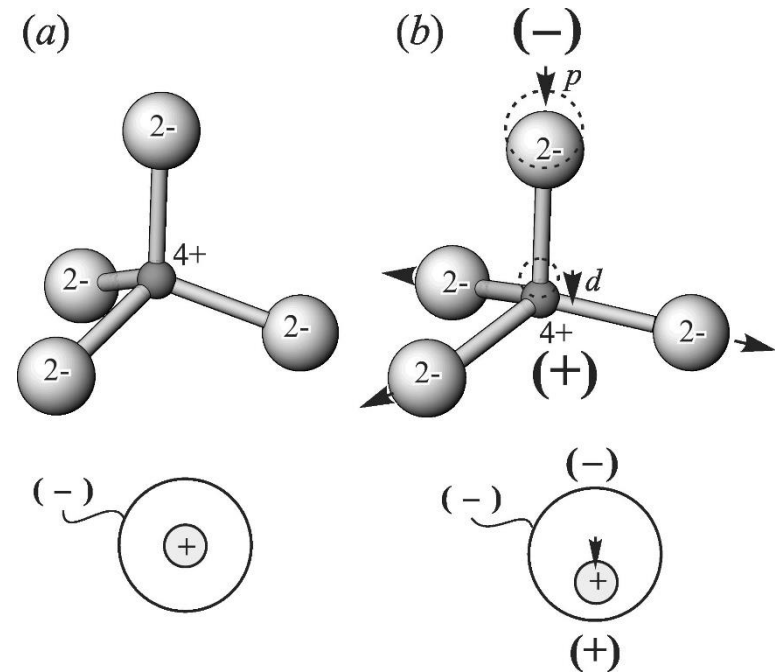- **Other properties:**
  - Taste
  - Smell
  - Reaction with acid

Figure 6.15 Piezoelectricity.

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