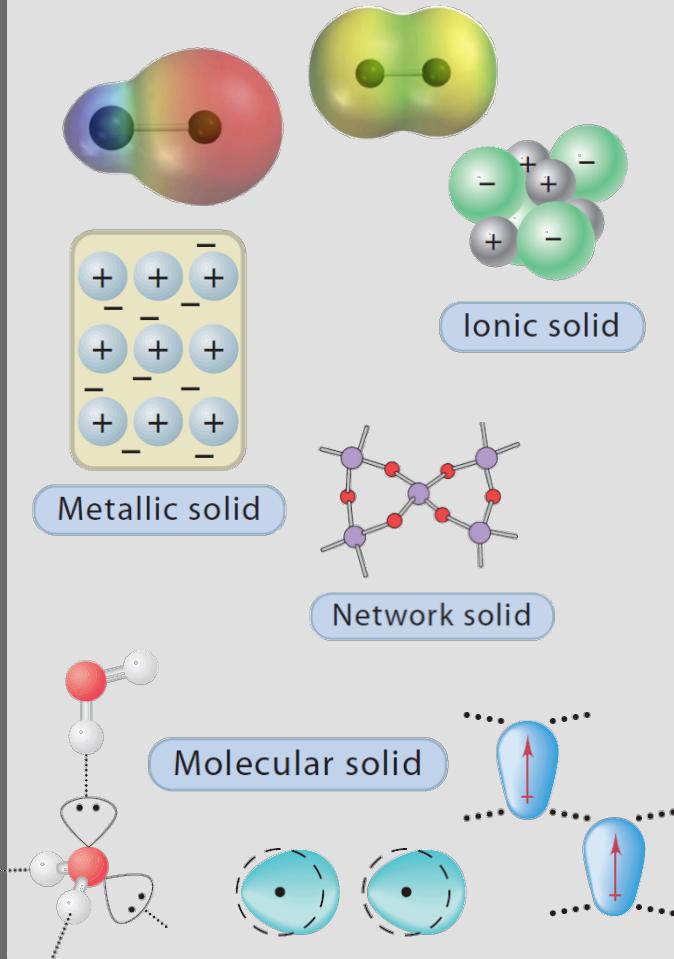


Welcome to
APS104S – Introduction to Materials &
Chemistry

Lecture 2
January 6, 2016

Atomic Structure & Bonding

CHAPTER 2_C



topics:

atomic models

electronic structure & quantum mechanics

quantum numbers

bonding forces and energies

primary interatomic bonds

secondary bonding

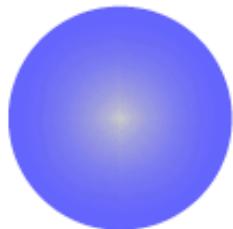
Subjects we will study today

- Atomic models (Bohr model; wave mechanical model)
- Quantum numbers
- Orbitals
- Aufbau principle
- Electronic structure

Atomic models

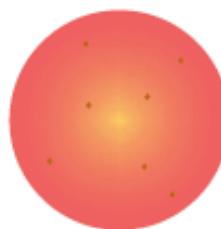
Evolution of atomic models

1803



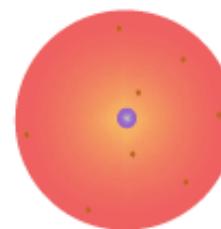
Dalton proposes the indivisible unit of an element is the atom.

1904



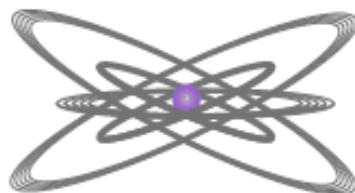
Thomson discovers electrons, believed to reside within a sphere of uniform positive charge (the "plum pudding" model).

1911



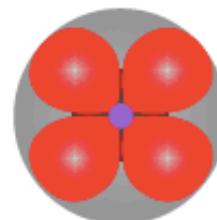
Rutherford demonstrates the existence of a positively charged nucleus that contains nearly all the mass of an atom.

1913



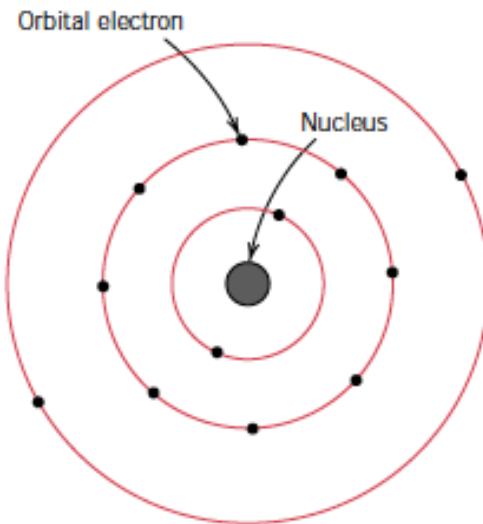
Bohr proposes fixed circular orbits around the nucleus for electrons.

1926



In the current model of the atom, electrons occupy regions of space (orbitals) around the nucleus determined by their energies.

Bohr's model (1913)

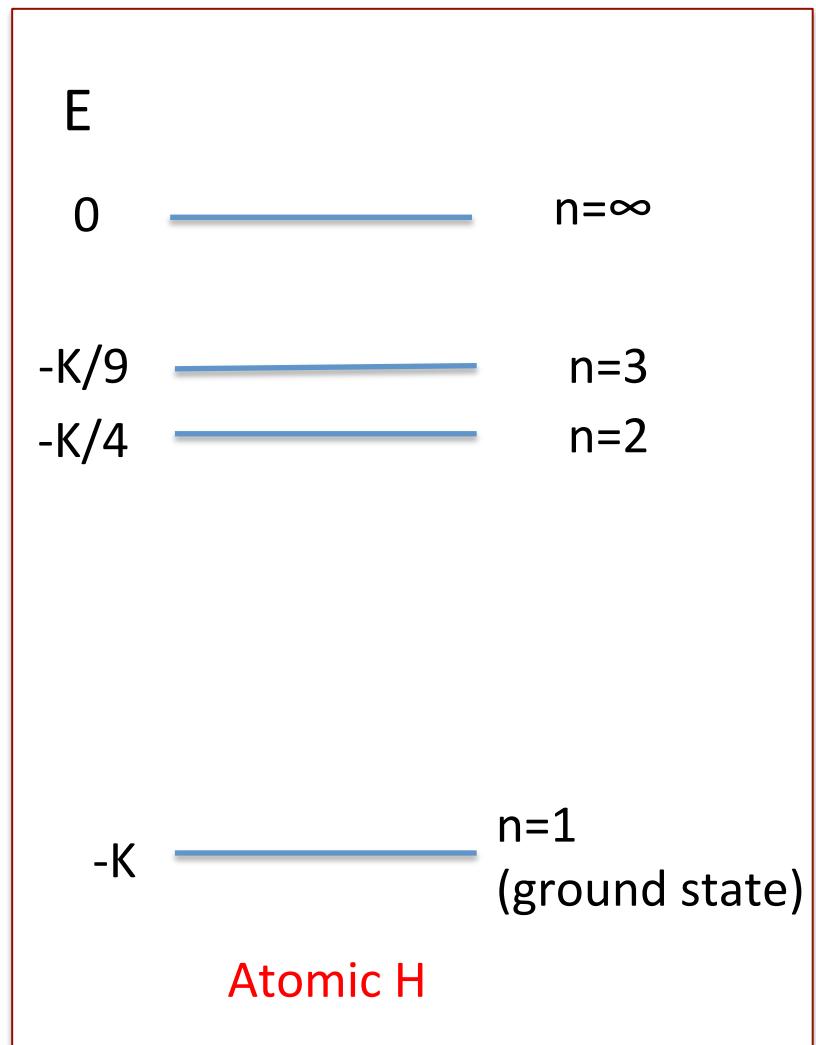
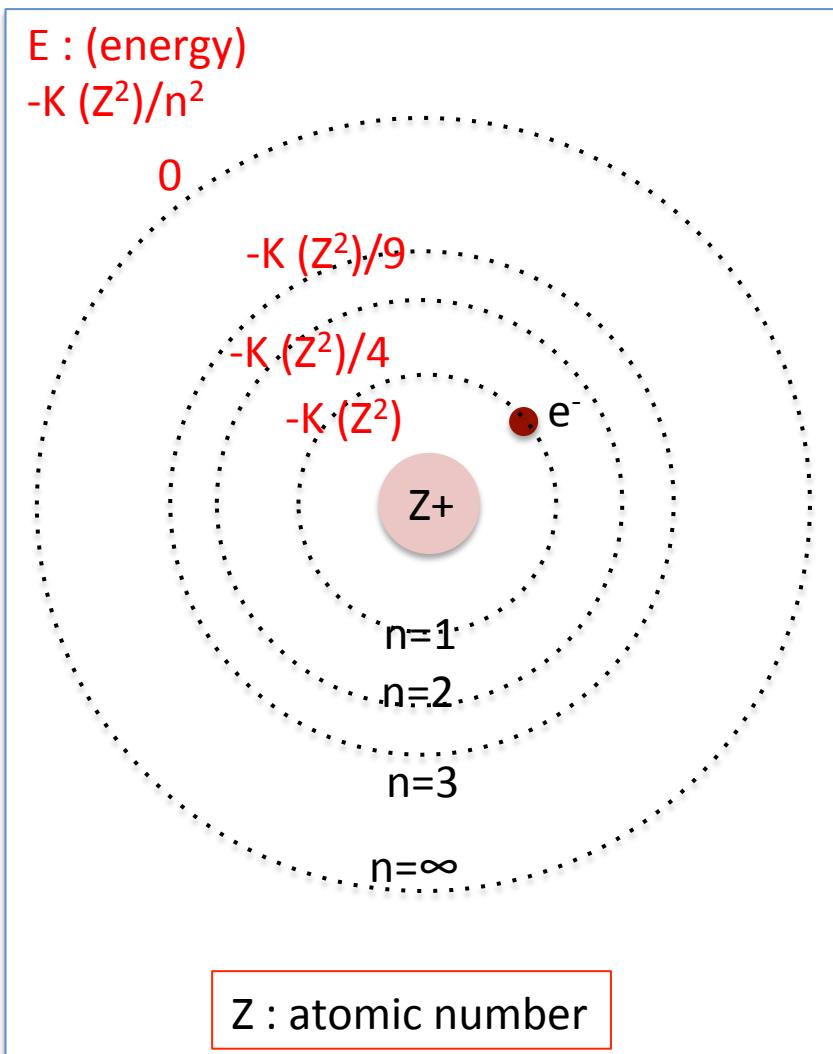


He developed a quantitative model for the atom – called **Planetary Model**. (e^- orbiting the positive nucleus in a circular orbit)

Central ideas:

- Nucleus is dense & electrons that are only allowed in certain circular **orbits**.
- Electrons undergo changes in energy only by moving between energy levels.
- Energy of electrons and the radii of orbitals are **quantized** (function of n).

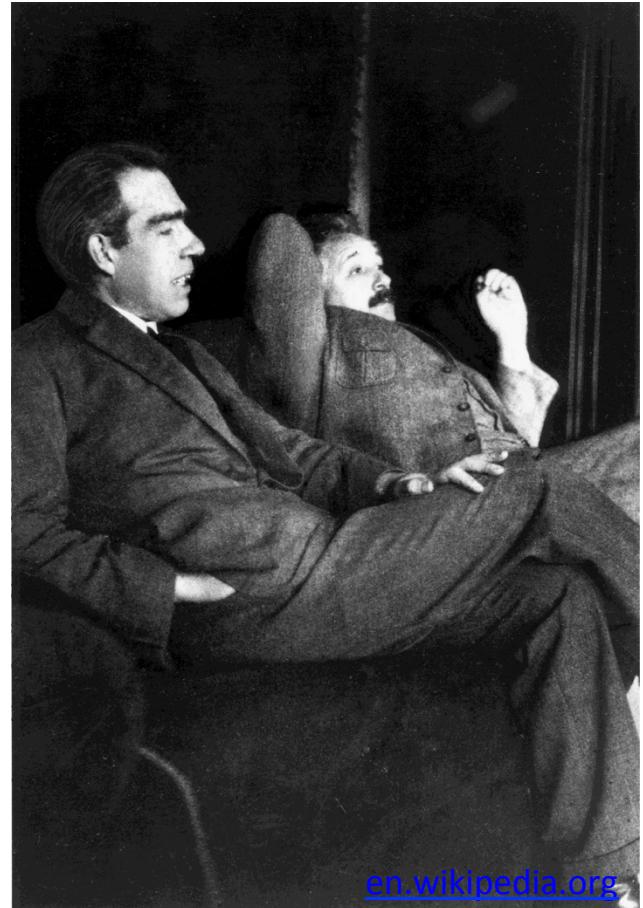
Bohr's model (1913)



About Niels Bohr



Plate 31 Royal visit to Carlsberg on May 22, 1957. From left to right, Queen Elizabeth, the Duke of Edinburgh, Niels Bohr, Crown Princess (later Queen) Margrethe, Mrs Bohr, King Fredrik IX. (Niels Bohr Archive.)



en.wikipedia.org

[Niels Bohr with Albert Einstein \(December 1925\)](#)

More advanced model

Wave-mechanical model

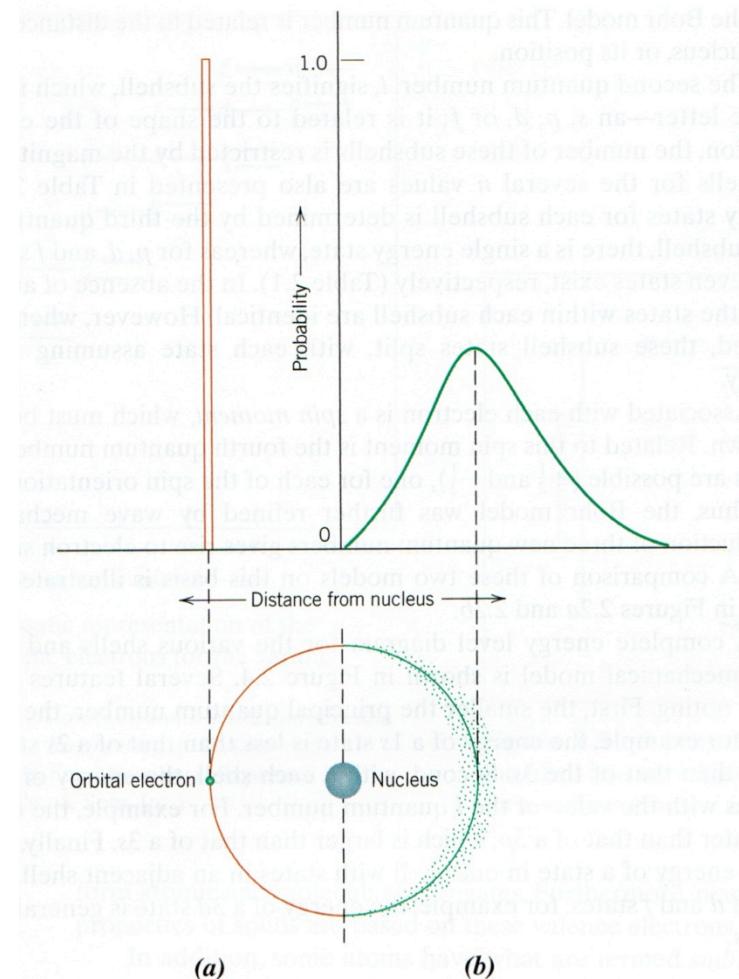
Wave-mechanical model

There are some limitations with the Bohr model

The model to address this:
wave-mechanical model

- electron exhibit both wavelike and particle-like properties

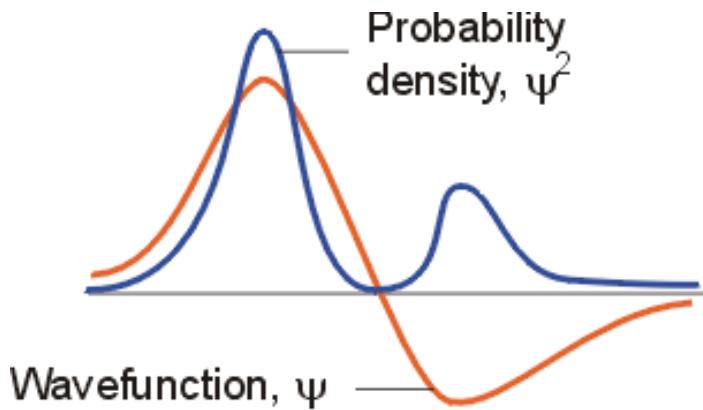
- Its position is not a discrete orbit, but the probability of an electron being at various locations around the nucleus



Some clarifications about orbitals

- **Question:** could you locate the precise position of the electron? A German physicist, **Werner Heisenberg**, answered “**no**” in what he called the **uncertainty principle**.
- We can never know both the **momentum and position** of an electron in an atom. Therefore, Heisenberg said that we shouldn't view electrons as moving in well-defined orbits about the nucleus!
- With Heisenberg's uncertainty principle in mind, an Austrian physicist named **Erwin Schrodinger** derived a set of equations or **wave functions** (Ψ) in 1926 for electrons.
- According to Schrodinger, electrons confined in their orbits would set up standing waves and **you could describe only the probability** (Ψ^2) **of where an electron could be**.
- The distributions of these probabilities formed regions of space about the nucleus were called **orbitals**. Orbitals could be described as **electron density cloud**.
- The densest area of the cloud is where you have the greatest probability of finding the electron and the least dense area is where you have the lowest probability of finding the electron.

Schrödinger's quantum mechanical model of the atom



- ORBITAL** : the region of space within which an electron is found.
- Ψ (wave function) does NOT describe the exact location of the electron.
 - Ψ^2 is proportional to the probability of finding an e^- at a given point.

3 **Quantum Numbers** are needed to describe an **orbital**.

4 **Quantum Numbers** are needed to define the state of an **electron**.

Quantum numbers & Orbital shapes

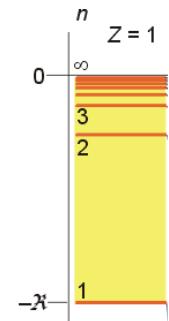
Quantum numbers

- In wave mechanics, four quantum numbers are needed to characterize each e^- in an atom
- **Shells** → principle quantum number ($n=1,2,3,4,5$) indicated as (K,L,M,N,O)
- **Sub-shells** “angular quantum number” → l (0, ..., $n-1$) (orbital shape)
- **Magnetic quantum number:** m_l (- l , ..., l) (the number of energy states for each sub-shell) ($p_x, p_y, p_z \rightarrow -1, 0, +1$)
- **Spin quantum number** (m_s) (+ $1/2$, - $1/2$)

$$E = E(n, l, m_l, m_s)$$

Principle quantum number, n

Principle quantum number (n) determines the size (distance of the electron from the nucleus) and the energy of the atomic orbital.



Allowed Values: $n = 1, 2, 3, \dots$

- As n increases, the **number of allowed orbitals** and **their size increases**.
- The increased size allows the **electrons to reside further from the nucleus**.
- As the electron moves away from the nucleus, **its energy increases**, therefore n also indicates the **energy of electrons**.

Angular momentum quantum number - l

- The orbitals belonging to each **shell** are classified into **sub-shells** distinguished by a quantum number l .
- The **angular momentum quantum number** defines the three dimensional **shape** of the orbitals found within a particular shell.

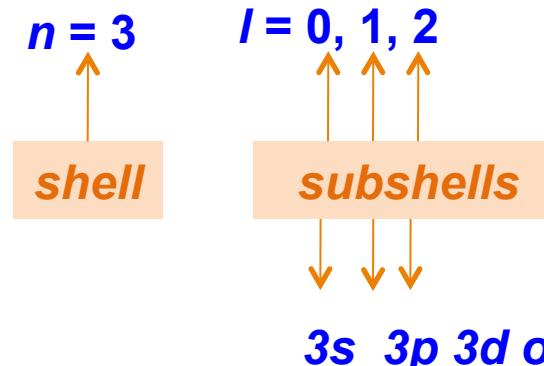
Allowed Values: $l = 0, 1, 2, 3, \dots n-1$

Quantum Number l 0 1 2 3 4

Sub-shell Notation s p d f g

Increasing Energy 

Example:



Magnetic quantum number - m_l

A **subshell** with quantum number l consists of $2l + 1$ individual orbitals.

The **magnetic quantum number**, m_l , distinguishes orbitals of a given n and l by their **orientation in space**.

Allowed Values: $m_l = -l, \dots, +l$

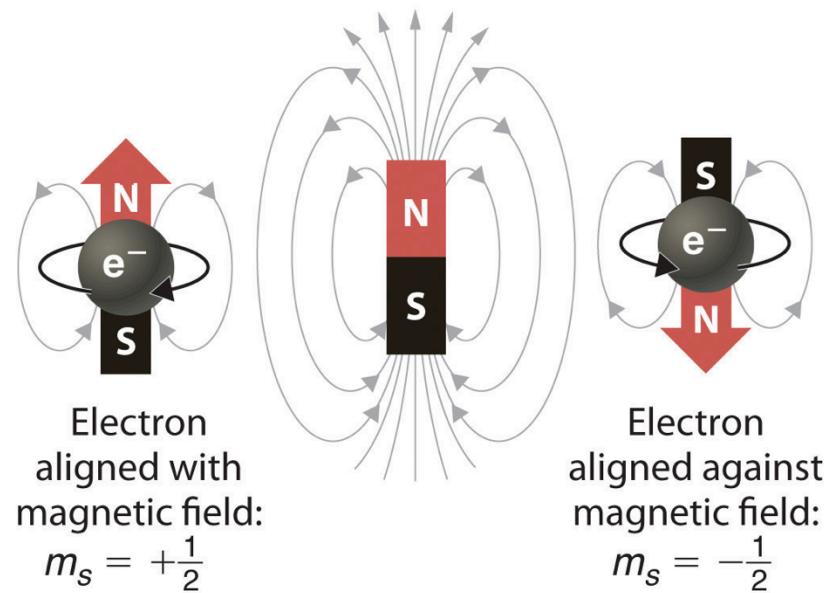
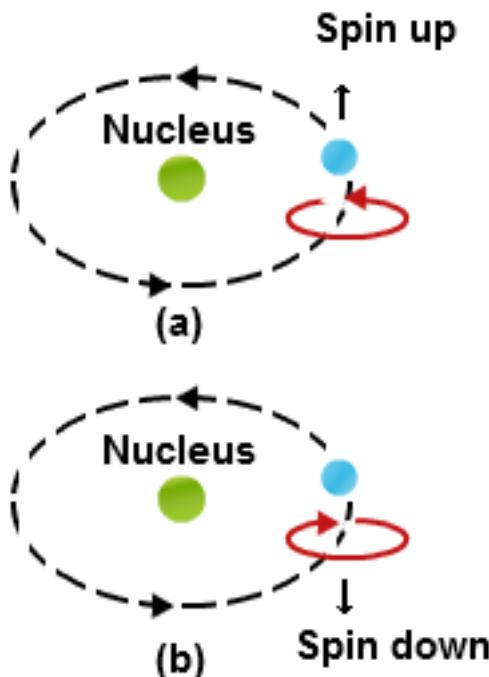
Example: for a 3 p orbital ($n = 3, l=1$)

$m_l = -1, 0, 1$

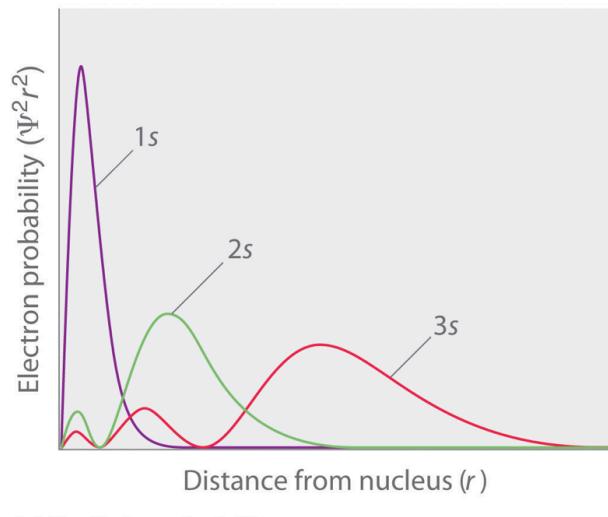
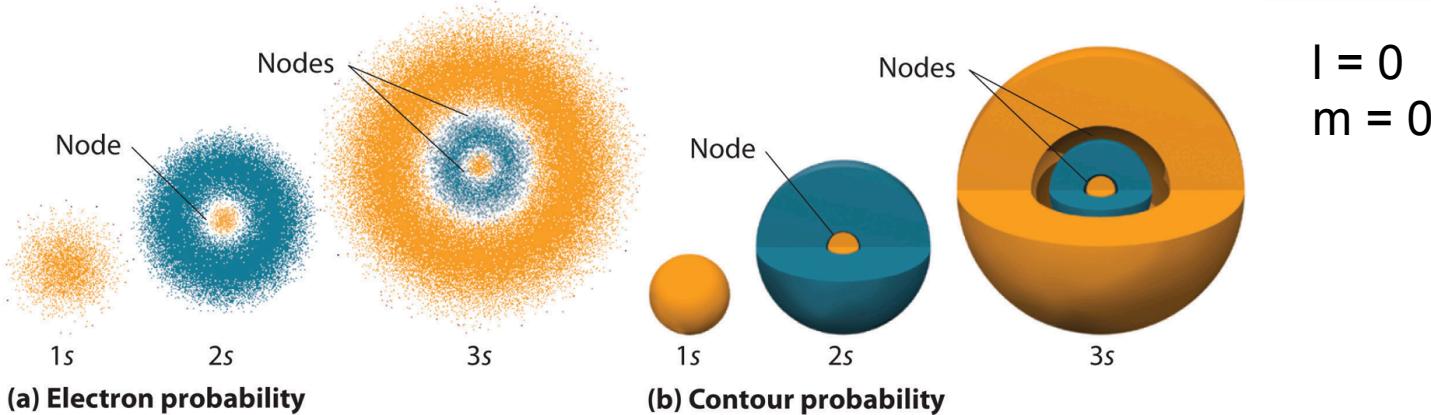
p_x, p_y, p_z

Spin quantum number - m_s

- While revolving in an orbit, electron spins too.
- Proposed that electron spins either up or down – (4th quantum number (s) = electron spin)

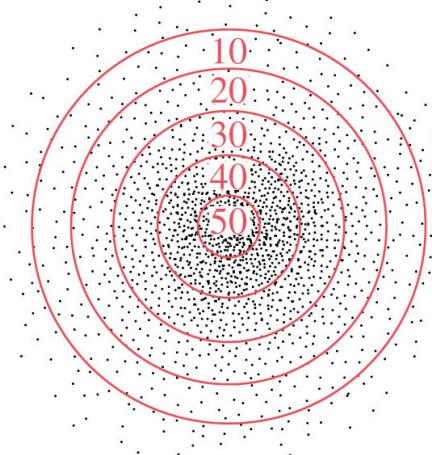


Orbital shapes – s orbital



(c) Radial probability

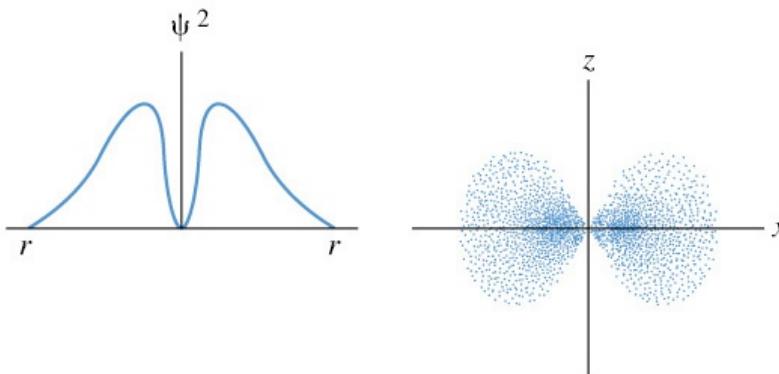
Dartboard: 1s Orbital Analogy



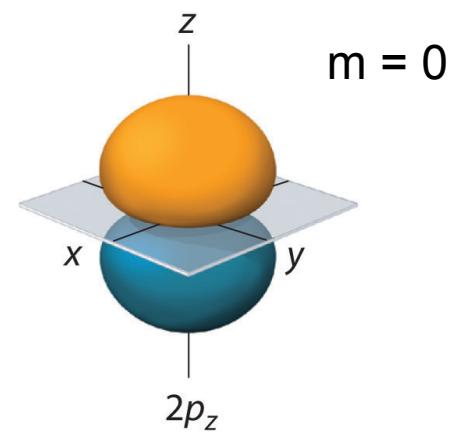
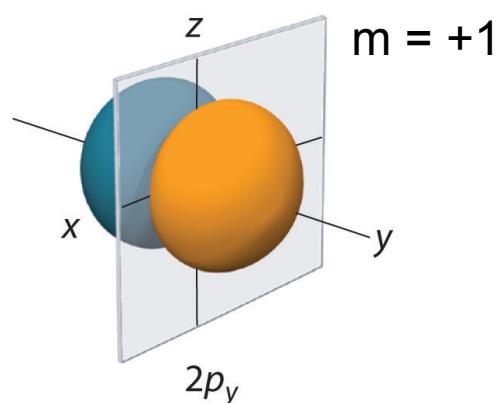
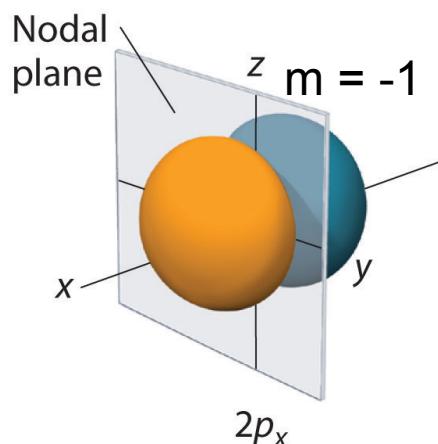
Orbital: For illustration, it is taken to be a **boundary surface** enclosing the **volume** where an electron spends most of the time (95%).

Orbital shapes – p orbital

$l = 1$



The Three Equivalent 2p Orbitals of the Hydrogen Atom



The **p orbitals** are **dumbbell shaped** with their electron density concentrated in **identical lobes** residing on opposite sides of a **nodal plane**.

Quantum numbers

shell	Sub-shell	Number of orbitals			
<i>n</i>	<i>l</i>	<i>Subshell Designation</i>	<i>m_l</i>	<i>Number of Orbitals in Subshell</i>	<i>Number of Orbitals in Shell</i>
1	0	1s	0	1	1
2	0	2s	0	1	4
	1	2p	-1, 0, 1	3	
3	0	3s	0	1	9
	1	3p	-1, 0, 1	3	
	2	3d	-2, -1, 0, 1, 2	5	
4	0	4s	0	1	16
	1	4p	-1, 0, 1	3	
	2	4d	-2, -1, 0, 1, 2	5	
	3	4f	-3, -2, -1, 0, 1, 2, 3	7	

Values of n, l, and m, through n = 4

Let's go to the periodic table and see if this reconciles

Electron filling in the periodic table

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18			
1 H Hydrogen 1.008	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	He			
1 Li Lithium 6.94	2 Be Beryllium 9.0121...	3 Na Sodium 22.989...	4 Mg Magnesium 24.305	5 Ca Calcium 40.078	6 Sc Scandium 44.955...	7 Ti Titanium 47.867	8 V Vanadium 50.9415	9 Cr Chromium 51.9961	10 Mn Manganese 54.938...	11 Fe Iron 55.845	12 Co Cobalt 58.933...	13 Ni Nickel 63.546	14 Cu Copper 65.38	15 Zn Zinc 65.38	16 Ga Gallium 69.723	17 Ge Germanium 72.63	18 As Arsenic 74.921...	19 Se Selenium 78.971	20 Br Bromine 79.904	21 Kr Krypton 83.798
1 Rb Rubidium 85.4678	2 Sr Strontium 87.62	3 Y Yttrium 88.90584	4 Zr Zirconium 91.224	5 Nb Niobium 92.90637	6 Mo Molybdenum 95.95	7 Tc Technetium (98)	8 Ru Ruthenium 101.07	9 Rh Rhodium 102.90...	10 Pd Palladium 106.42	11 Ag Silver 107.8682	12 Cd Cadmium 112.414	13 In Indium 114.818	14 Sn Tin 118.710	15 Sb Antimony 121.760	16 Te Tellurium 127.60	17 I Iodine 126.90...	18 Xe Xenon 131.293	19 Rn Radon (222)		
1 Cs Caesium 132.90...	2 Ba Barium 137.327	3 Hf Hafnium 178.49	4 Ta Tantalum 180.94...	5 W Tungsten 183.84	6 Re Rhenium 186.207	7 Os Osmium 190.23	8 Ir Iridium 192.217	9 Platinum 195.084	10 Gold 196.96...	11 Mercury 200.59	12 Thallium 204.38	13 Pb Lead 207.2	14 Bi Bismuth 208.98...	15 Po Polonium (209)	16 Astatine (210)	17 Rn Radon (222)	18 Uuo Ununoctium (294)			
1 Fr Francium (223)	2 Ra Radium (226)	3 Rf Rutherfordium (267)	4 Db Dubnium (268)	5 Sg Seaborgium (271)	6 Bh Bohrium (272)	7 Hs Hassium (270)	8 Mt Meitnerium (276)	9 Ds Darmstadtium (281)	10 Rg Roentgenium (280)	11 Cn Copernicium (285)	12 Uut Ununtrium (284)	13 Fm Flerovium (289)	14 Uup Ununpentium (288)	15 Lv Livermorium (293)	16 Unnoctium Ununoctium (294)	17 Uuo Ununoctium (294)	18 He Helium 4.002602			

For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.

Periodic Table Design & Interface Copyright © 1997 Michael Dayah, Ptable.com Last updated May 22, 2015

57	2	58	2	59	2	60	2	61	2	62	2	63	2	64	2	65	2	66	2	67	2	68	2	69	2	70	2	71	2
La	8	Ce	8	Pr	8	Nd	18	Pm	8	Sm	18	Eu	18	Gd	8	Tb	8	Dy	8	Ho	8	Er	8	Tm	8	Yb	8	Lu	8
Lanthanum 138.90...	2	Cerium 140.116	2	Praseodymium 140.90...	2	Neodymium 144.242	2	Promethium (145)	2	Samarium 150.36	2	Europium 151.964	2	Gadolinium 157.25	2	Terbium 159.92...	2	Dysprosium 162.500	2	Holmium 164.93...	2	Erbium 167.259	2	Thulium 168.93...	2	Ytterbium 173.054	2	Lutetium 174.9668	2
89	2	90	2	91	2	92	2	93	2	94	2	95	2	96	2	97	2	98	2	99	2	100	2	101	2	102	2	103	2
Ac	8	Th	8	Pa	18	U	18	Np	18	Pu	18	Am	18	Cm	18	Bk	18	Cf	18	Es	18	Fm	18	Md	18	No	18		
Actinium (227)	2	Thorium 232.0377	10	Protactinium 231.03... 2	2	Uranium 238.02... (237)	2	Neptunium (239)	2	Plutonium (240)	2	Americium (243)	2	Curium (247)	2	Berkelium (247)	2	Californium (251)	2	Einsteinium (252)	2	Mendelevium (257)	2	Fermium (258)	2	Nobelium (259)	2	Lawrencium (262)	3

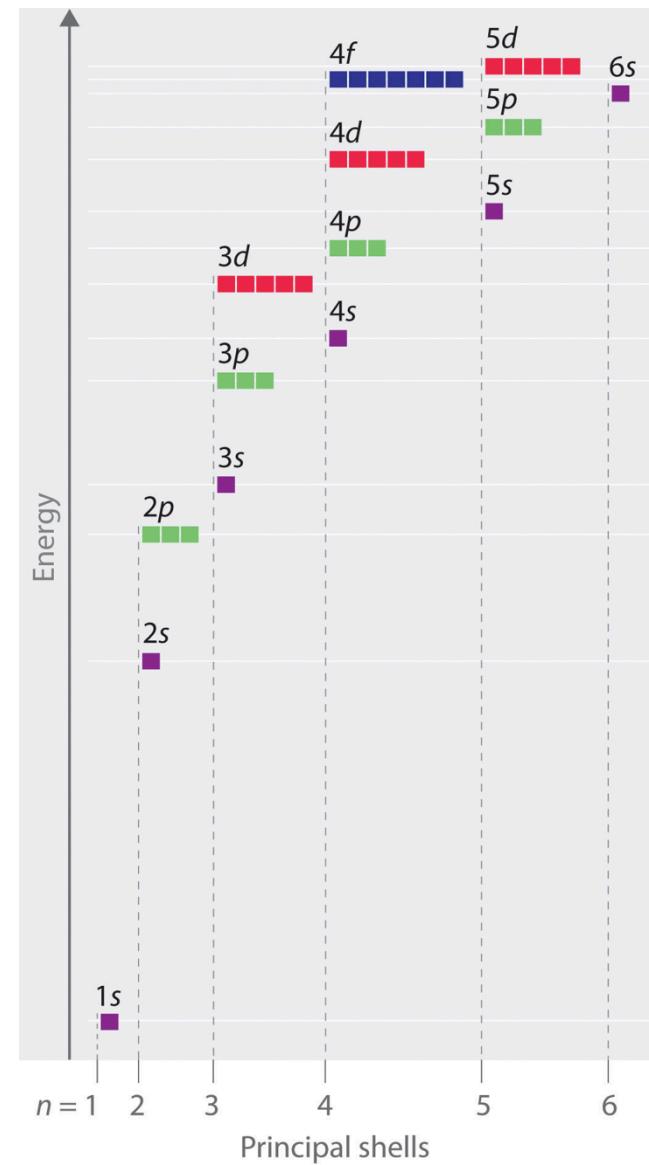
Discrepancy between populating electrons just in ascending quantum numbers

Electronic structure (Aufbau principle)

Modified energy-level diagram

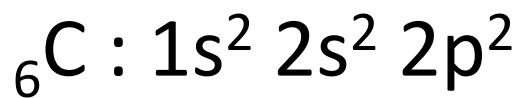
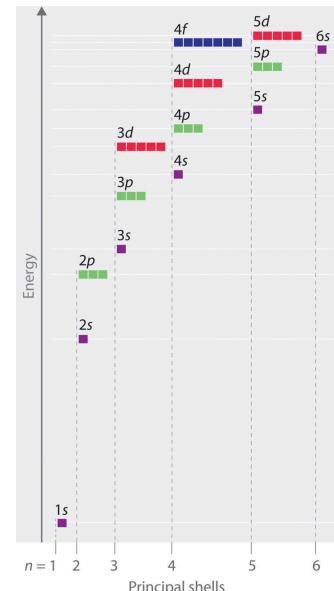
Is drawn based on the **Aufbau principle**
(directs the electron filling sequence)

Aufbau is a German noun that means "construction". The Aufbau principle is sometimes called the **building-up principle**.

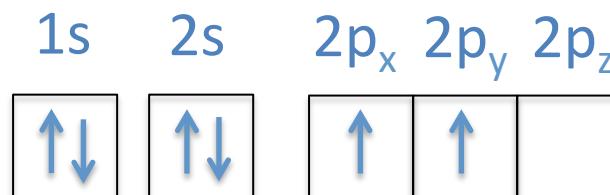


There are 3 parts to the Aufbau (construction) principle

- **Pauli exclusion principle:** in any atom, each e^- has a unique set of 4 quantum numbers (n, l, m_l, m_s) (like SIN for each e^-).
- Electrons fill orbitals from lowest to highest energy.
- **Hund's rule:** degeneracy: orbitals of equivalent energy strive for unpaired electron spins.

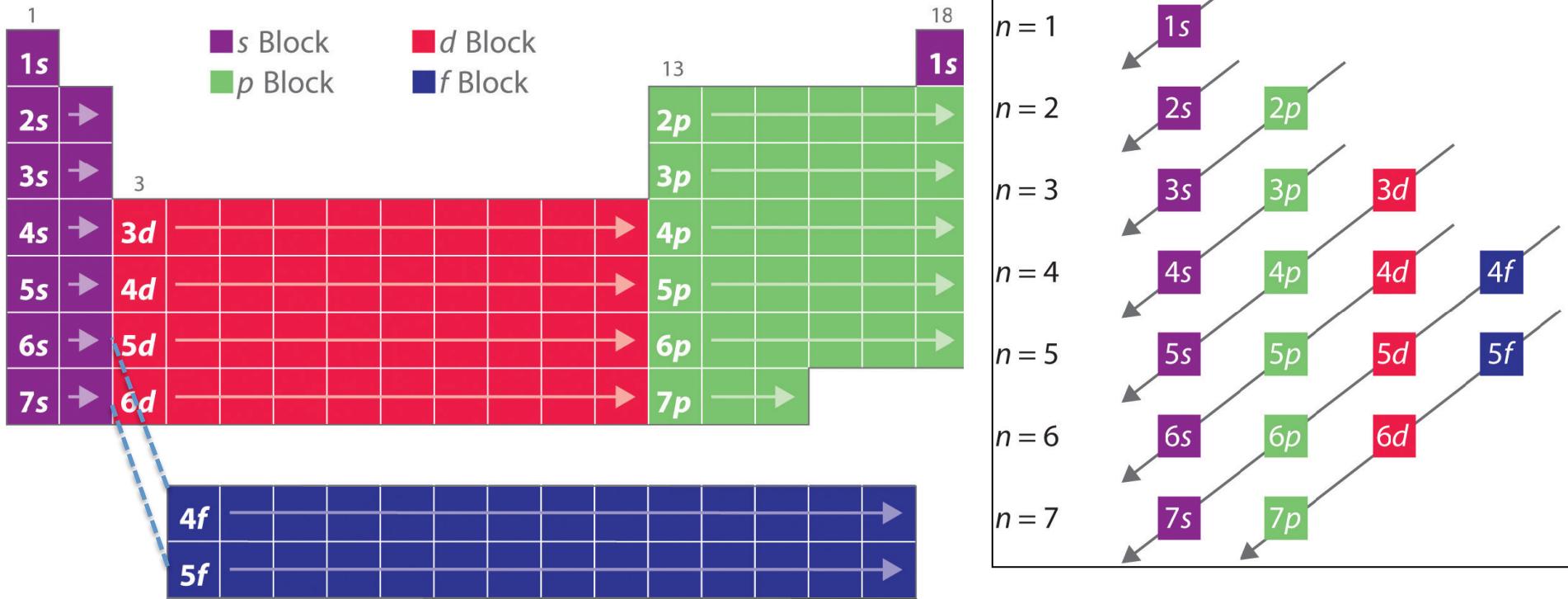


$l = 0 \quad l = 1$



Box representation

Aufbau Principle - Predicting the Order in Which Orbitals are Filled in Multi-electron Atoms



Example 1

Write out the electron configuration for the following elements:

Boron (z=5): [He] 2s²2p¹

Potassium (z=19): [Ar] 4s¹

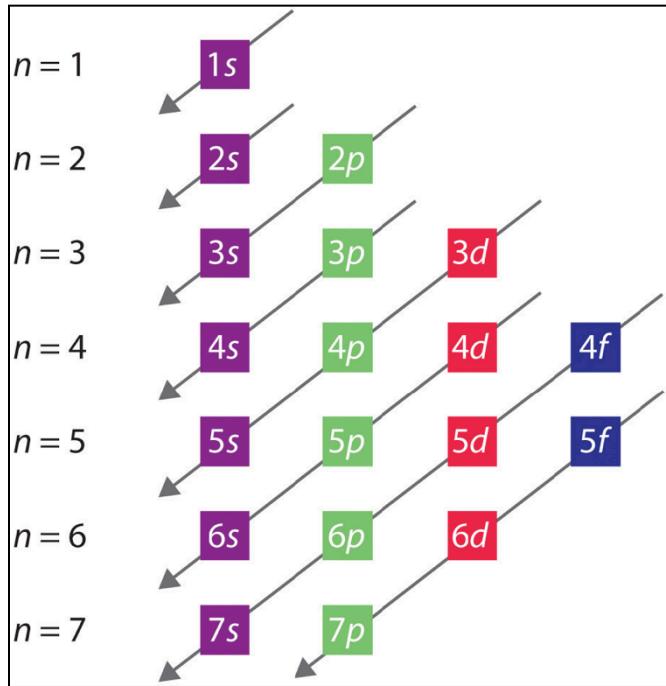
Chromium: [Ar]3d⁵4s¹

Copper: [Ar]3d¹⁰4s¹

Example 2

- We have the electronic structure of two ions ($A^{3+}:3d^{10}$) and ($B^{3+}:3d^5$). Find their position and atomic number in the periodic table:
 - $A: 3d^{10} 4s^2 4p^1 \rightarrow n=4$; group 13 $\rightarrow {}_{31}Ga$
 - $B: 3d^6 4s^2 \rightarrow n=4$; group 8 $\rightarrow {}_{26}Fe$

Note: 4s orbital gets filled before 3d, and it loses electrons before 3d since it's on outer shell.



 Groups 13-18	 Groups 1-12
 Detailed Periodic Table	 Detailed Periodic Table

Example 3

How many orbitals and subshells are found within the principal shell $n = 4$? How do these orbital energies compare?

Shell “4” → subshell: 0, 1, 2, 3 → 4s, 4p, 4d, 4f

Number of orbitals: 1 (s) + 3 (p) + 5 (d) + 7 (f) = 16

Example 4

Identify the element with each ground state electron configuration.

- [He]2s²2p¹

$$Z = 2+2+1 = 5 \rightarrow B$$

- [Kr]5s²4d¹⁰5p⁴

Z =

$$36 + 2 + 10 + 4 =$$

52 → Te