Atoms Lecture 4: Electron Configuration

Learning Objective	Openstax 2e Chapter
Electron Spin: A Fourth Quantum Number	6.3
Multielectron Atoms	6.4
The Aufbau Principle	6.4
Electron configurations	6.4

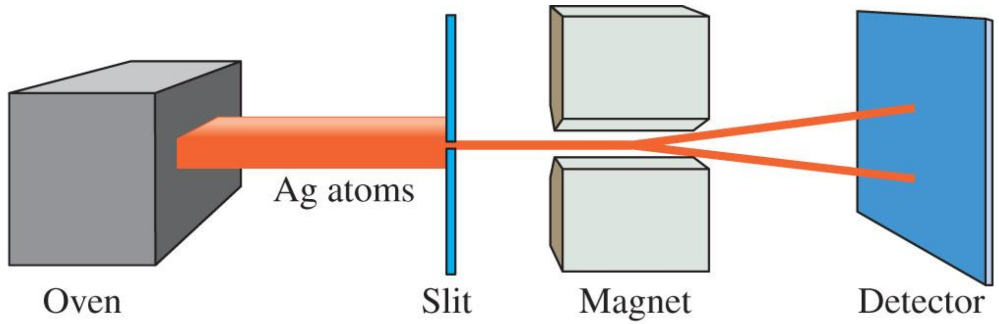
Suggested Practice Problems

Chapter 6 Exercises – Questions: 49, 53, 55, 57, 59, 63

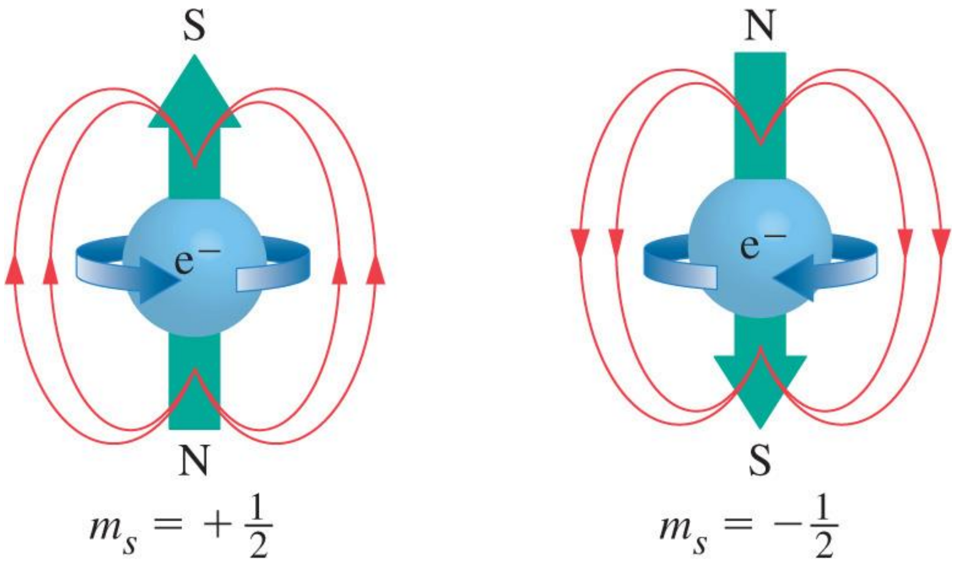
Answers can be found in the Chapter 6 Answer Key

Electron Spin: A Fourth Quantum Number (m_s)

Some unexplained features of the Hydrogen atom spectrum could be explained assuming that electron spins.



The Stern-Gerlach Experiment (1920) is an evidence that the phenomenon of electron spin exists.



In addition to the (n, ℓ, m_ℓ) quantum numbers, there is a 4th quantum number:

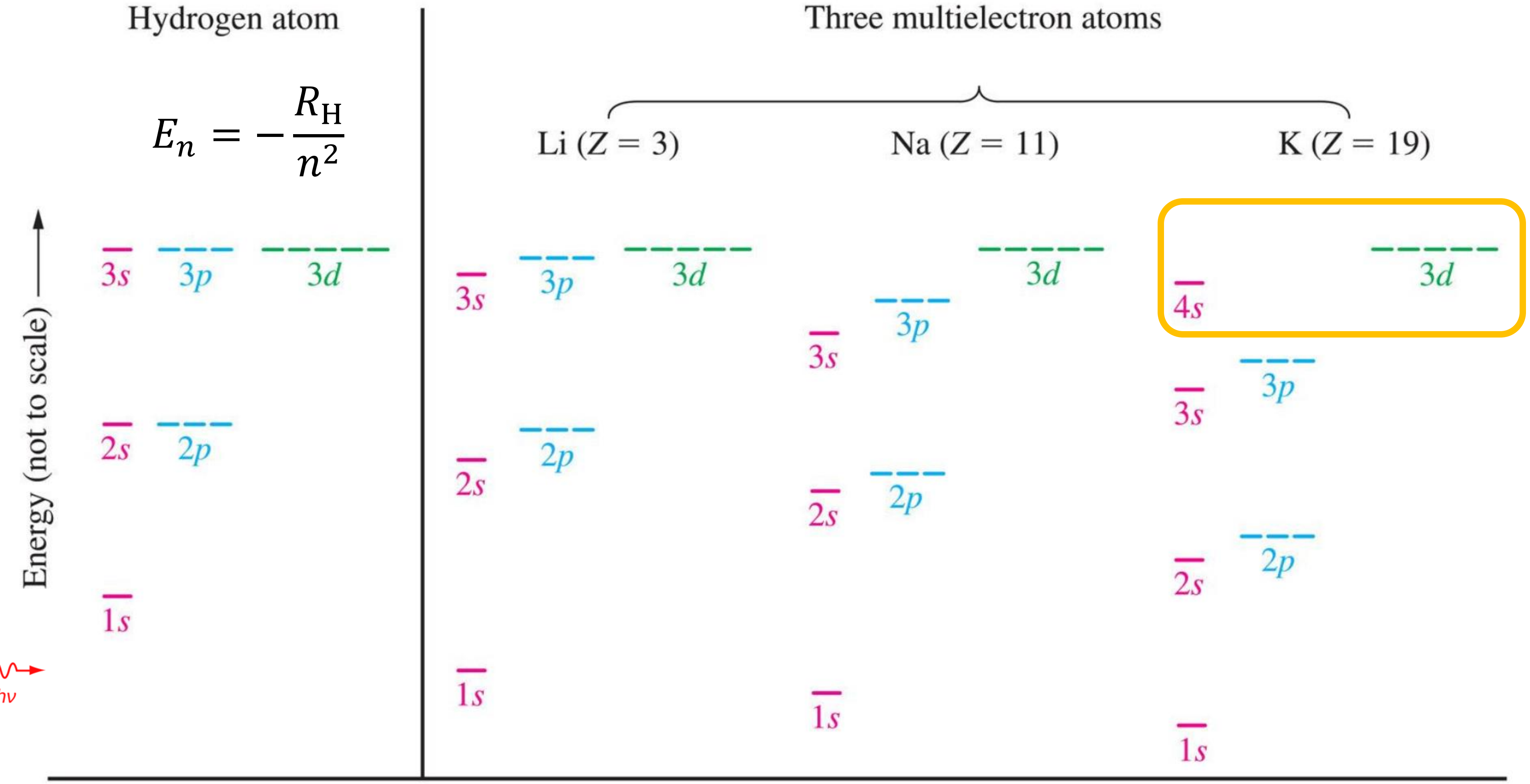
m_s → <u>Electron Spin Quantum Number</u> → Electron Spin

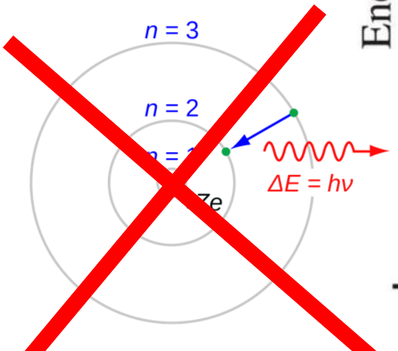
- Describes the orientation of the electron spin
- $m_s = +{}^1/_2 \text{ or } -{}^1/_2$

Pauli Exclusion Principle says that no 2 electrons can have the same set of 4 quantum numbers in an atom.

Multielectron Atoms

The repulsion between electrons means that they stay away from one another in a multielectron atom.
- electrons in orbitals closer to nucleus affect energy of higher orbital electrons
  (related to quantum entanglement – see 2022 Nobel Prize)





Bohr Model (wikipedia)

Penetration and Shielding

Electrons in orbitals closer to the nucleus screen or shield the nucleus from electrons farther away.

- Penetration: ability of electrons in *s*-orbitals that allows them to get close to the nucleus.
  - The *s*-orbitals have a high probability density close to the nucleus (*p*- and *d*-orbitals have zero probability)
  - So, electrons in *s*-orbitals are less screened and (on average) feel greater nuclear attraction.

- The nuclear charge that an electron actually experiences is reduced by intervening electrons to a value of Z_{eff}, called the effective nuclear charge.

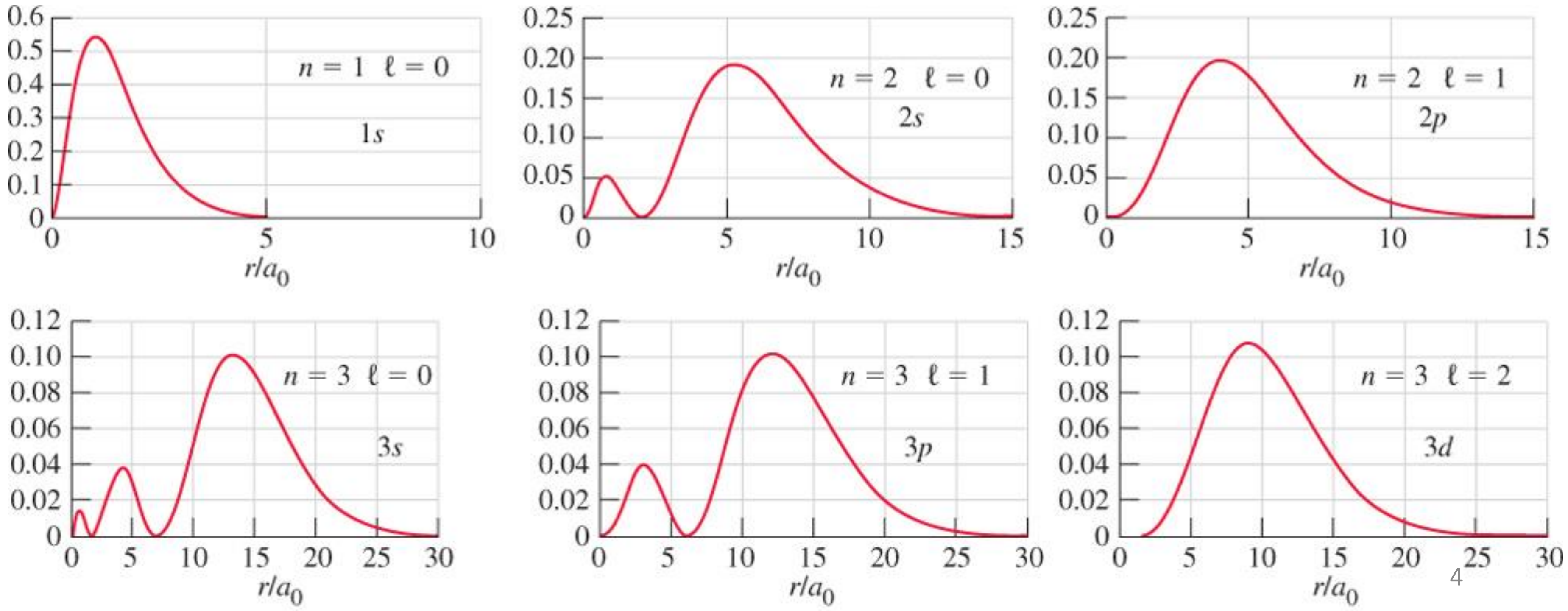


Figure 9: Radial distribution functions: $r^2R^2\ (r)$

Electron Configuration

It designates how electrons are distributed among various orbitals in principle shells and subshells.

1. Electrons occupy orbitals in a way that minimizes the energy of the atom.

1s, 2s, 2p, 3s, 3p, **4s**, 3d, 4p, **5s**, 4d, 5p, 6s, **4f**, **5d**, 6p, 7s, **5f**, **6d**, 7p

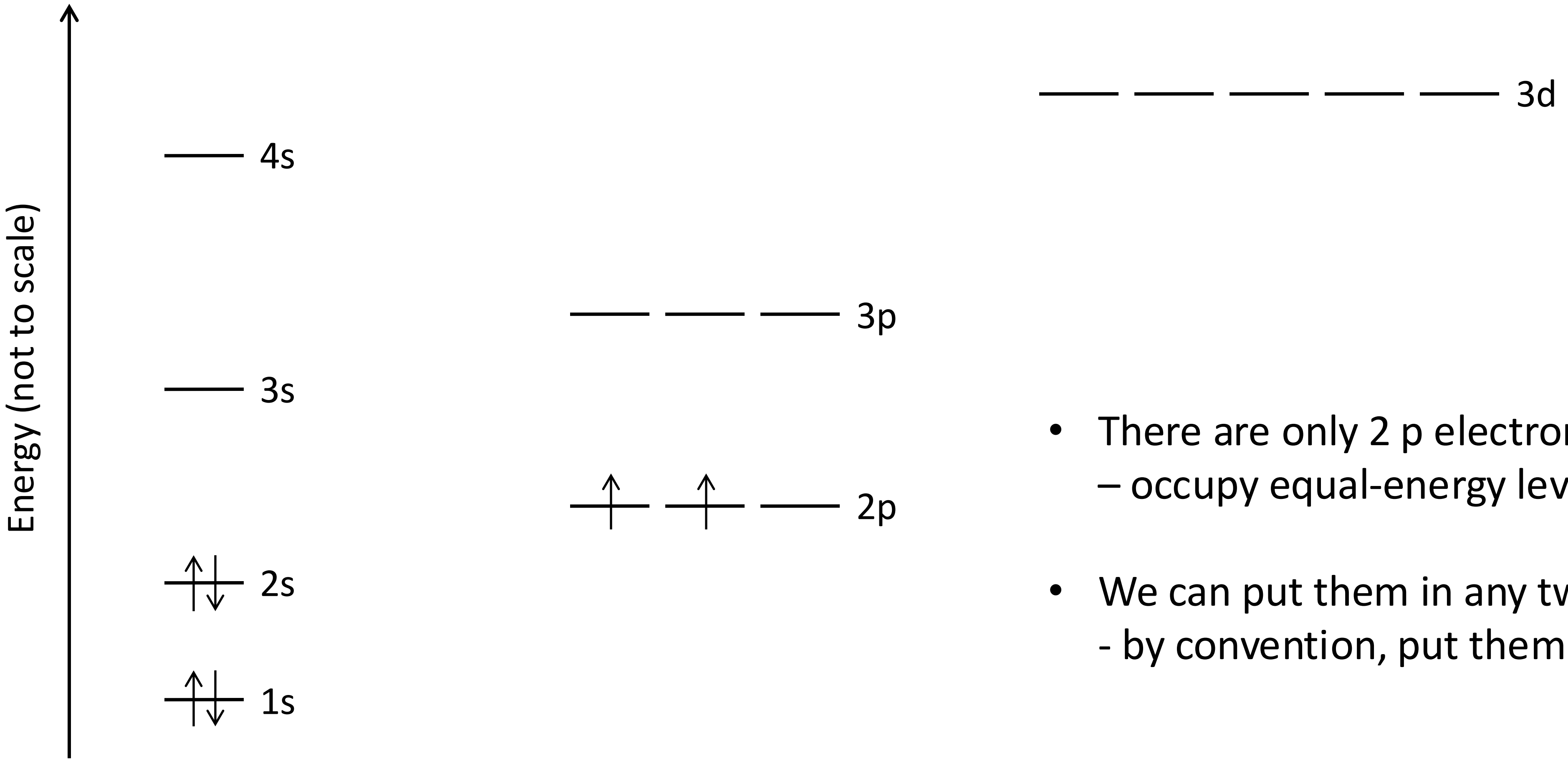
2. Only two electrons may occupy the same orbital, and these electrons must have opposite spin: **Pauli Exclusion Principle.**

$n = 1$	1 s orbital			2 electrons
$n = 2$	1 s orbital	3 p orbitals		8 electrons
$n = 3$	1 s orbital	3 p orbitals	5 d orbitals	18 electrons

3. When orbitals of identical energy (degenerate orbitals) are available, electrons initially occupy these orbitals singly with parallel spins: **Hund's Rule.**

Example: Carbon Atom

C: 6 electrons

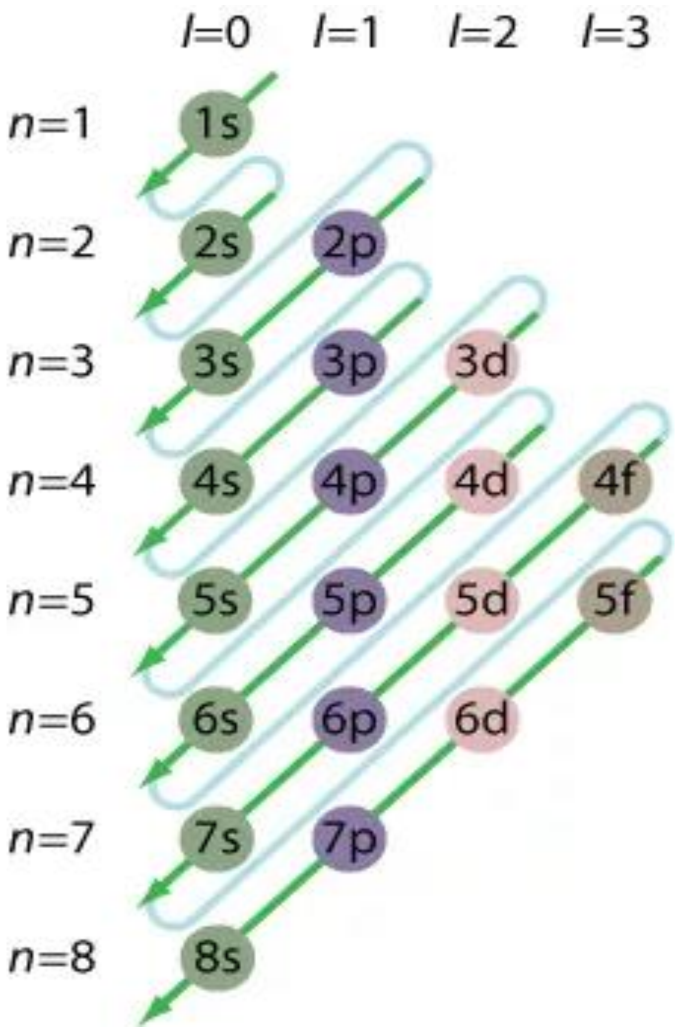


- There are only 2 p electrons
  – occupy equal-energy levels singly (Hund's Rule)

- We can put them in any two 2p orbitals
  - by convention, put them in p_x and p_y first

The Aufbau Process

It designates how electrons are distributed among various orbitals in principle shells and subshells.



https://www.thoughtco.com/

Ground state "Electron Configuration" of first 18 elements in "*spdf*" notation

H: $1s^1$

He: $1s^2$

Li: $1s^2 2s^1$

Be: $1s^2 2s^2$

B: $1s^2 2s^2 2p^1$

C: $1s^2 2s^2 2p^2$

N: $1s^2 2s^2 2p^3$

O: $1s^2 2s^2 2p^4$

F: $1s^2 2s^2 2p^5$

Ne: $1s^2 2s^2 2p^6$

Na: $1s^2 2s^2 2p^6 3s^1$

Mg: $1s^2 2s^2 2p^6 3s^2$

Al: $1s^2 2s^2 2p^6 3s^2 3p^1$

Si: $1s^2 2s^2 2p^6 3s^2 3p^2$

P: $1s^2 2s^2 2p^6 3s^2 3p^3$

S: $1s^2 2s^2 2p^6 3s^2 3p^4$

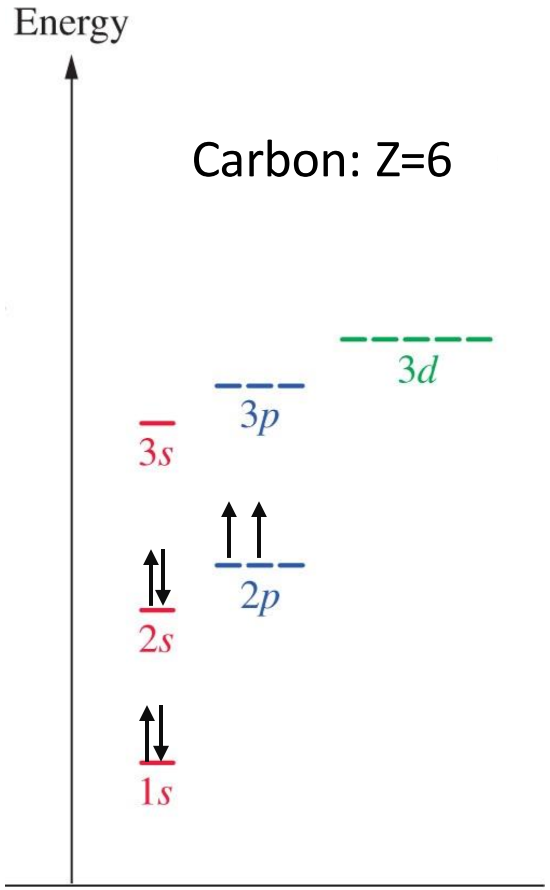
Cl: $1s^2 2s^2 2p^6 3s^2 3p^5$

Ar: $1s^2 2s^2 2p^6 3s^2 3p^6$

Notations for Electron Configuration

Schemes for writing out electron configurations with different level of detail

Ground State Electron Configuration of Carbon



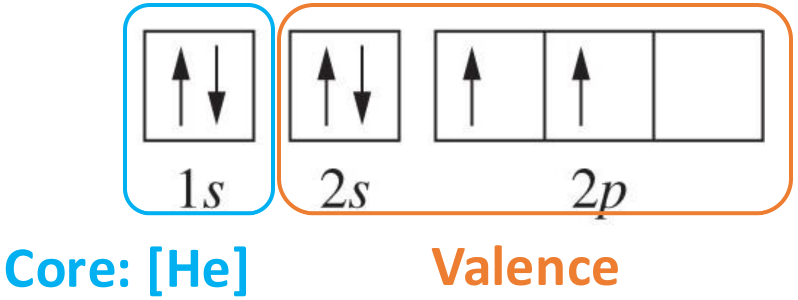
- *spdf* notation (expanded):

$$1s^2\ 2s^2\ 2p_x^1\ 2p_y^1$$

- *spdf* notation (condensed):

$$1s^2 2s^2 2p^2$$

- Orbital Diagram:

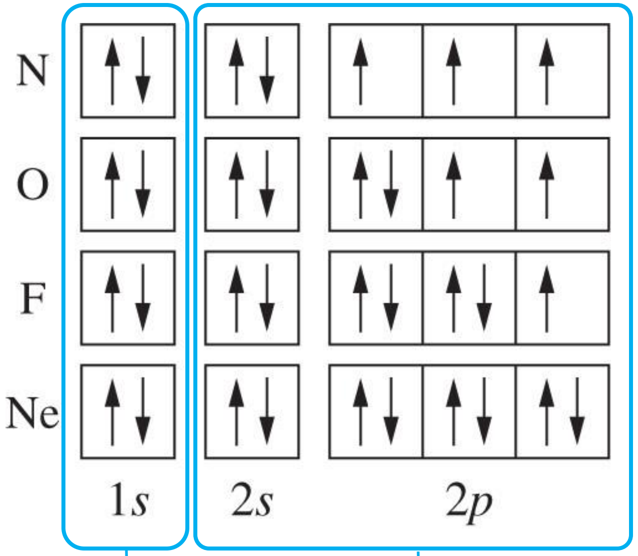


- *spdf* Nobel-gas-core abbreviated notation (condensed):

$$[\mathrm{He}]\ 2s^2 2p^2$$

The Aufbau Process cont.

Filling orbital diagrams through Row 3 and the nobel gas abbreviated electron configuration notations



$[He]\ 2s^2 2p^3$

$[He]\ 2s^2 2p^4$

$[He]\ 2s^2 2p^5$

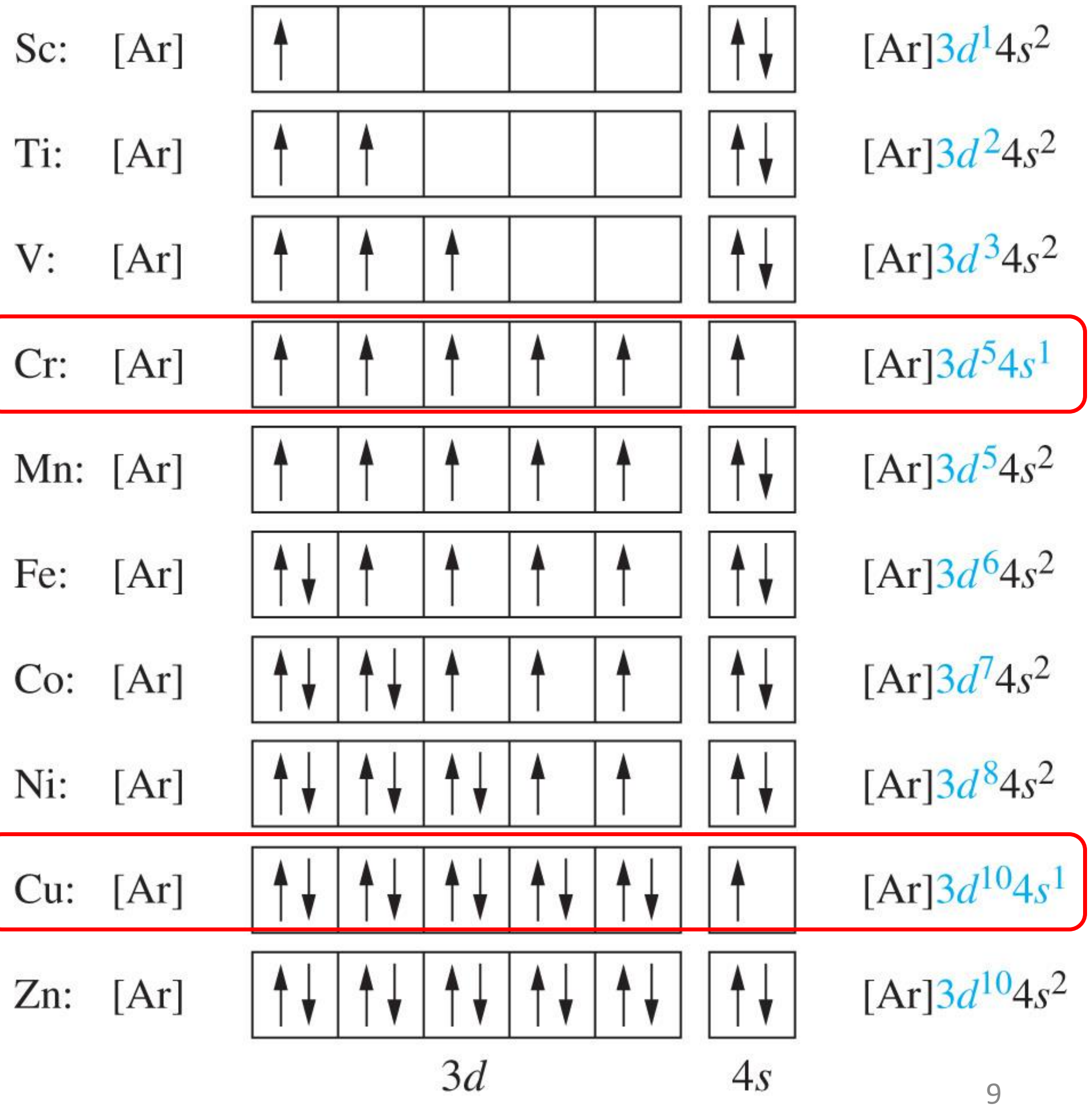
$[He]\ 2s^2 2p^6$

Core **Valence**

[He]: $1s^2$

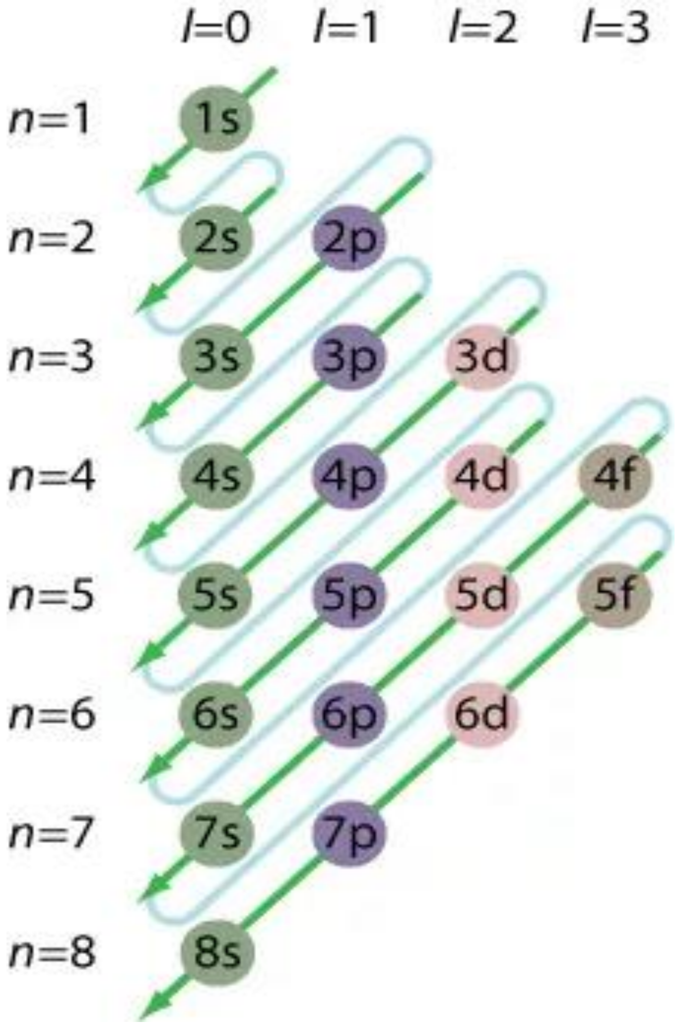
[Ar]: $1s^2 2s^2 2p^6 3s^2 3p^6$

Half-filled subshells and filled subshells have "special stability".



Electron Configuration & The Periodic Table

Elements in the same group of the table have similar electron configurations.



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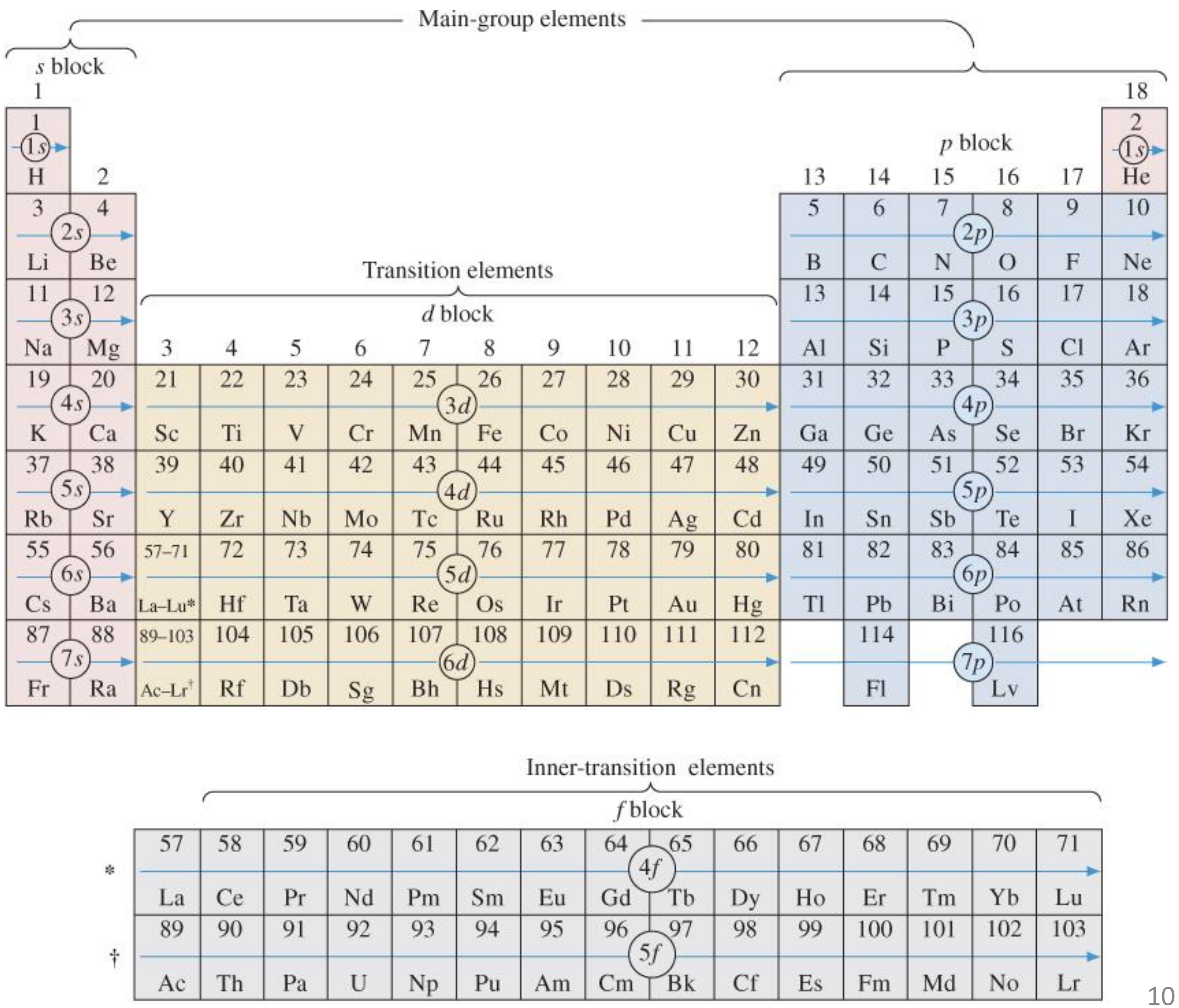

Example

Write the <u>noble-gas-core-abbreviated</u> electron configuration of the following atoms?

- Argon (Z=18)

  [Ne]$3s^2 3p^6$

- Calcium (Z=20)

  [Ar]$4s^2$

- Bismuth (Z=83)

  [Xe]$6s^2 4f^{14} 5d^{10} 6p^3$