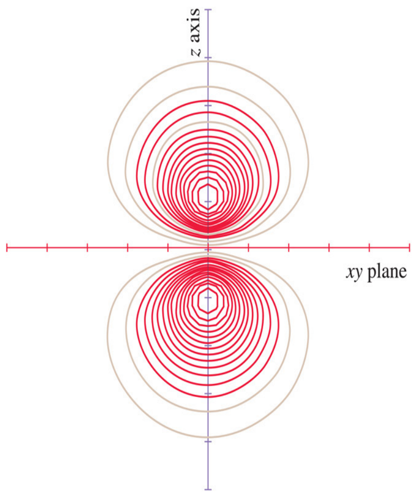
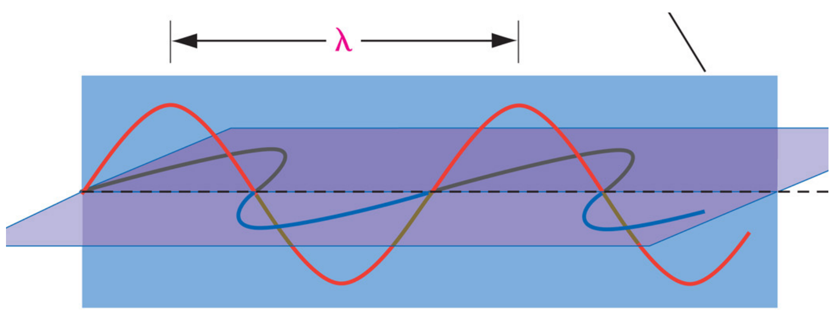
Chapter 7: Electron Configurations

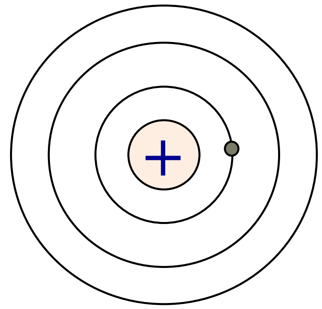




Quick Review of Chapter 6…

Bohr Model:

- treat e^- as a particle
- orbits are quantized → n



$$\Delta E = -R_H \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$

Schrodinger:

- treat e^- as a wave
- quantization arises naturally → $\Psi = f(n, \ell, m_\ell)$
- results in 3D orbitals

Arrangement of Electrons in Atoms

- Electrons in atoms are arranged as:

SHELLS (n)

↓

SUBSHELLS (ℓ)

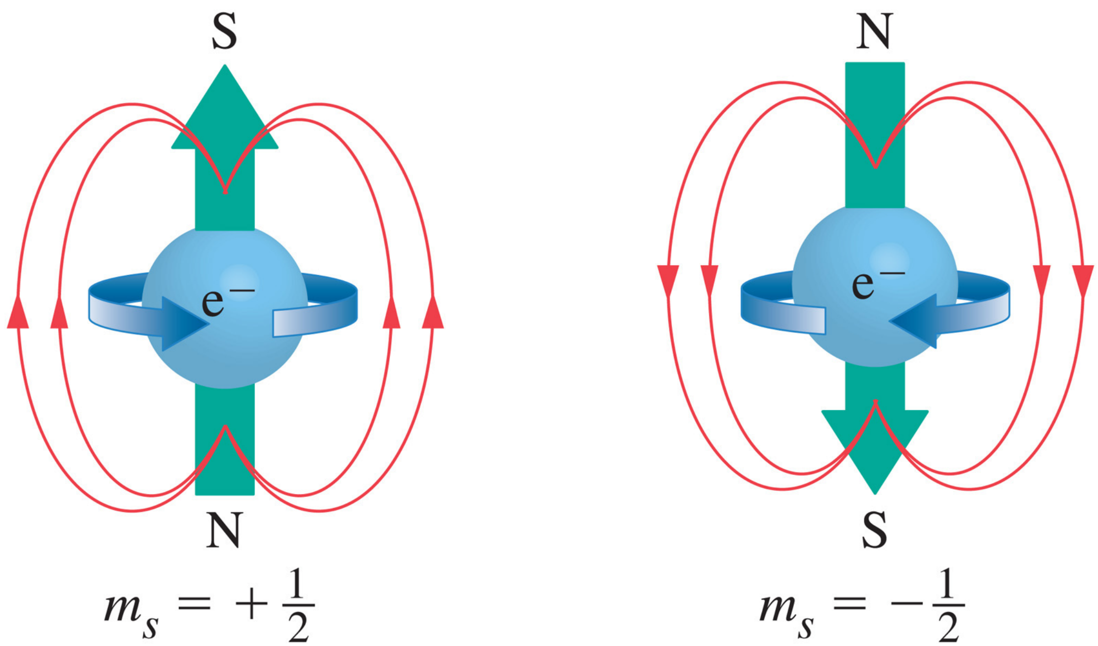
↓

ORBITALS (m_ℓ)

Arrangement of Electrons in Atoms

- Each orbital can be assigned no more than 2 electrons!
- This is tied to the existence of a 4th quantum number, the electron spin quantum number, m_s.

Electron Spin Quantum Number, m_s



It can be proven experimentally that electron have a magnetic moment ("micromagnets") This is correlated with spin of the electron. Two spin directions are given by m_s where m_s = +1/2 and -1/2.

Quantum Numbers Summary

- → shell 1, 2, 3, 4, ...
- → subshell 0, 1, 2, ... n – 1
- → orbital -ℓ ... 0 ... +ℓ
- → electron spin +1/2 and -1/2

Example: Orbital labels

Give the appropriate orbital label (if any) to the following sets of quantum numbers.

a) $n = 2, \ell = 1, m_\ell = 0, \; m_2 = +½$

b) $n = 5, \ell = 3, m_\ell = -3, \; m_2 = -½$

c) $n = 6, \ell = 0, m_\ell = 0, \; m_2 = -½$

d) $n = 5, \ell = 4, m_\ell = 5, \; m_2 = +½$

Your Turn…

How many electrons in an atom can have the quantum number set n = 4, ℓ = 2?

A) 2

B) 3

C) 6

D) 10

E) 14

Pauli Exclusion Principle

- No two electrons in the same atom can have the same set of 4 quantum numbers.
- That is, each electron has a unique address.

$$3,\ 2,\ -1,\ +\tfrac{1}{2}$$

$n = 3$ shell

$\ell = 2$ subshell *d* orbitals

Electrons in Atoms

- When n = 1, then ℓ = 0
  - this shell has a single orbital (1s) to which $2e^-$ can be assigned.

- When n = 2, then ℓ = 0, 1
  - 2s orbital $2e^-$
  - three 2p orbitals $6e^-$
  - TOTAL = $8e^-$

Electrons in Atoms

- When n = 3, then ℓ = 0, 1, 2
  - 3s orbital — $2e^-$
  - three 3p orbitals — $6e^-$
  - five 3d orbitals — $10e^-$
  - TOTAL = $18e^-$

Assigning Electrons to Atoms

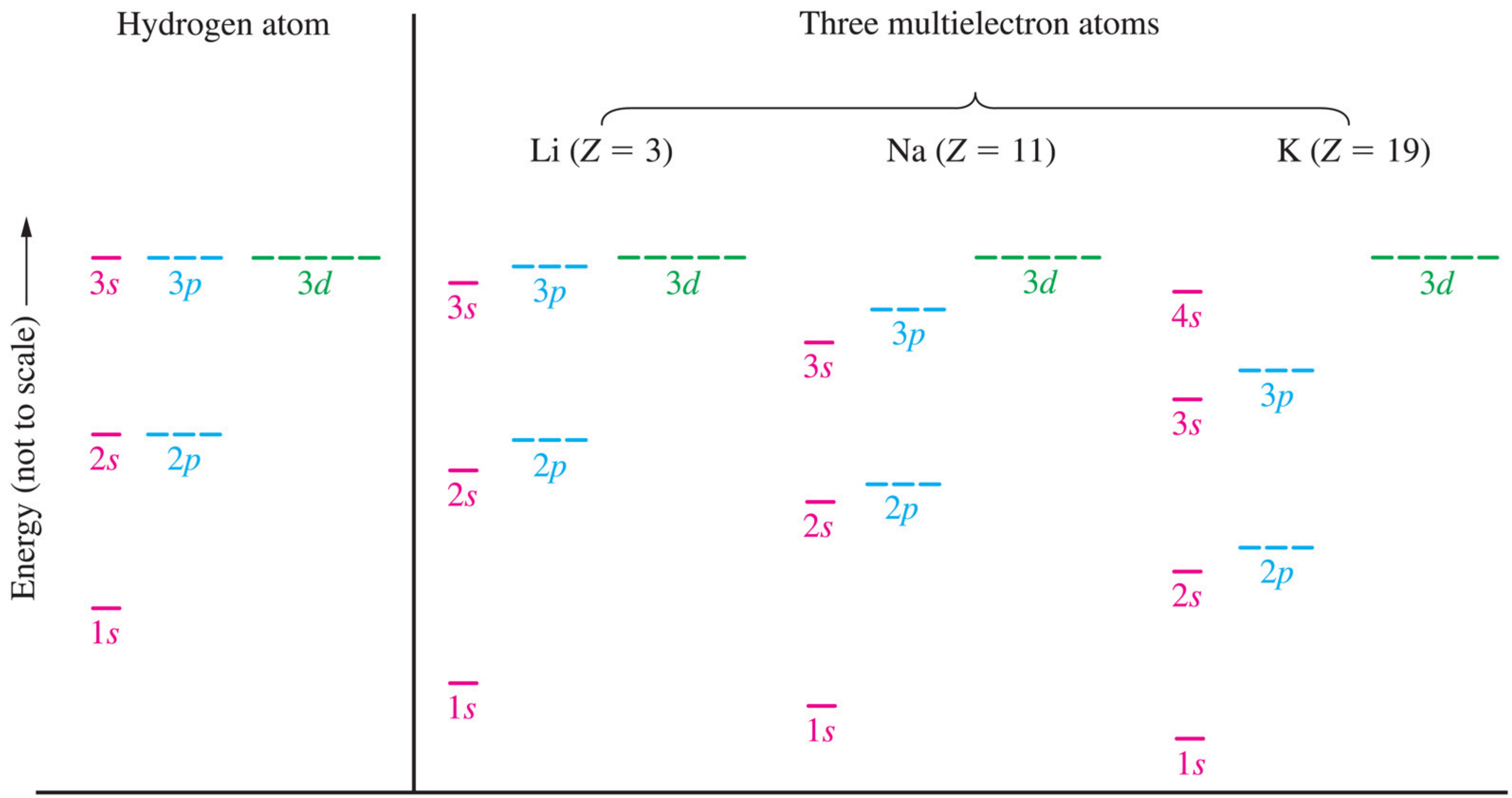
- **Aufbau Principle:** electrons are generally assigned to orbitals of successively higher energy.
- For the ____________________, $E = -(R_H/n^2)$

Energy depends only on n

- For ____________________________, a new factor arises: mutual repulsion between electrons

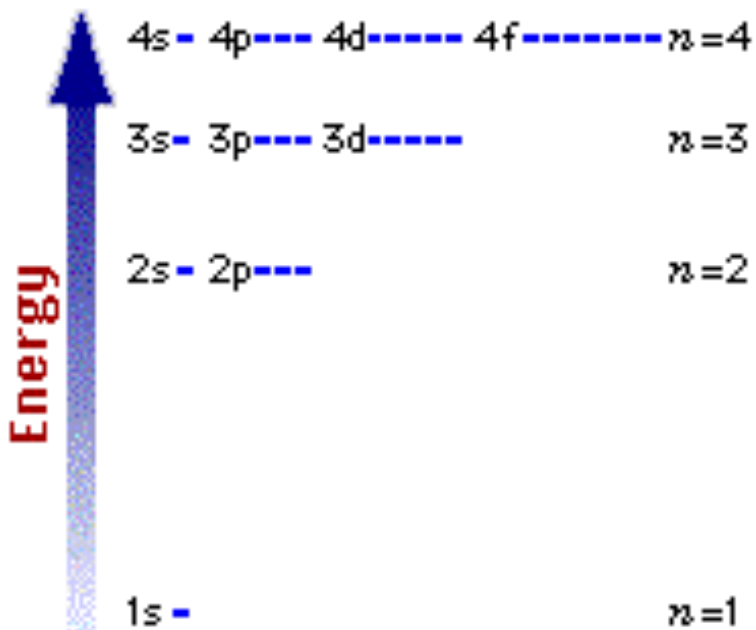
Energy depends on n and ℓ

Mono- vs. Multi-electron Atoms



When a set of orbitals are of the same energy, the orbitals are said to be "________________"

Assigning Electrons to Subshells



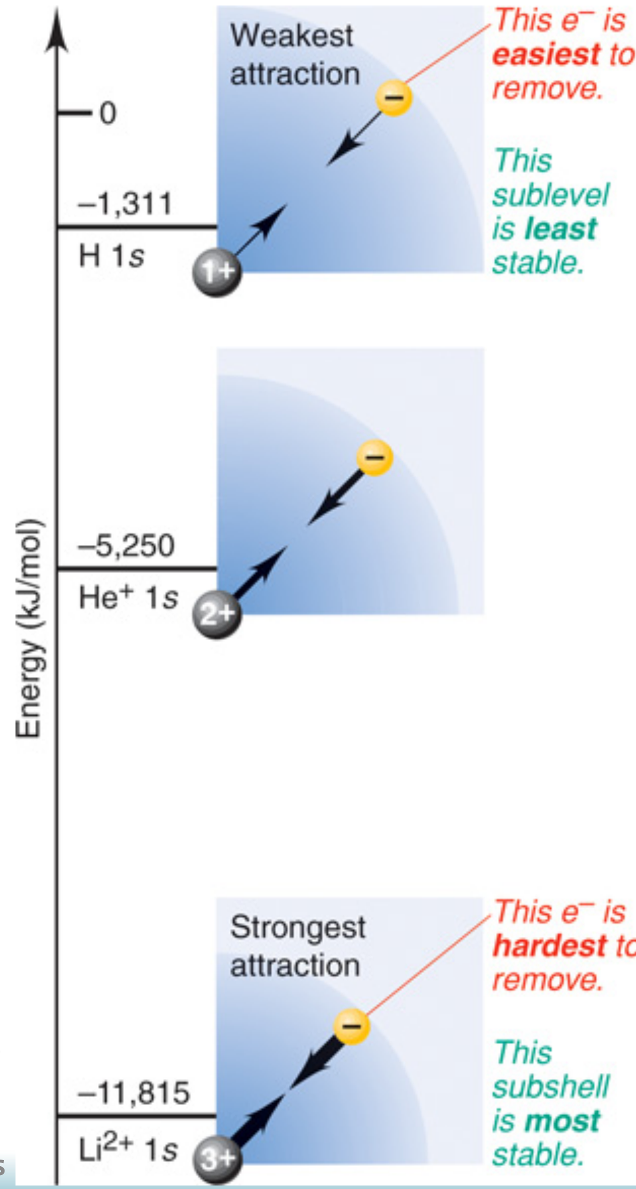
- In H atom, all subshells of same n have <u>same energy</u>.
- In multi-electron atom:

  a) subshells increase in energy as value of n+ℓ increases.

  b) for subshells of same n+ℓ, subshell with lower n is lower in energy.

Why do we lose degeneracy?

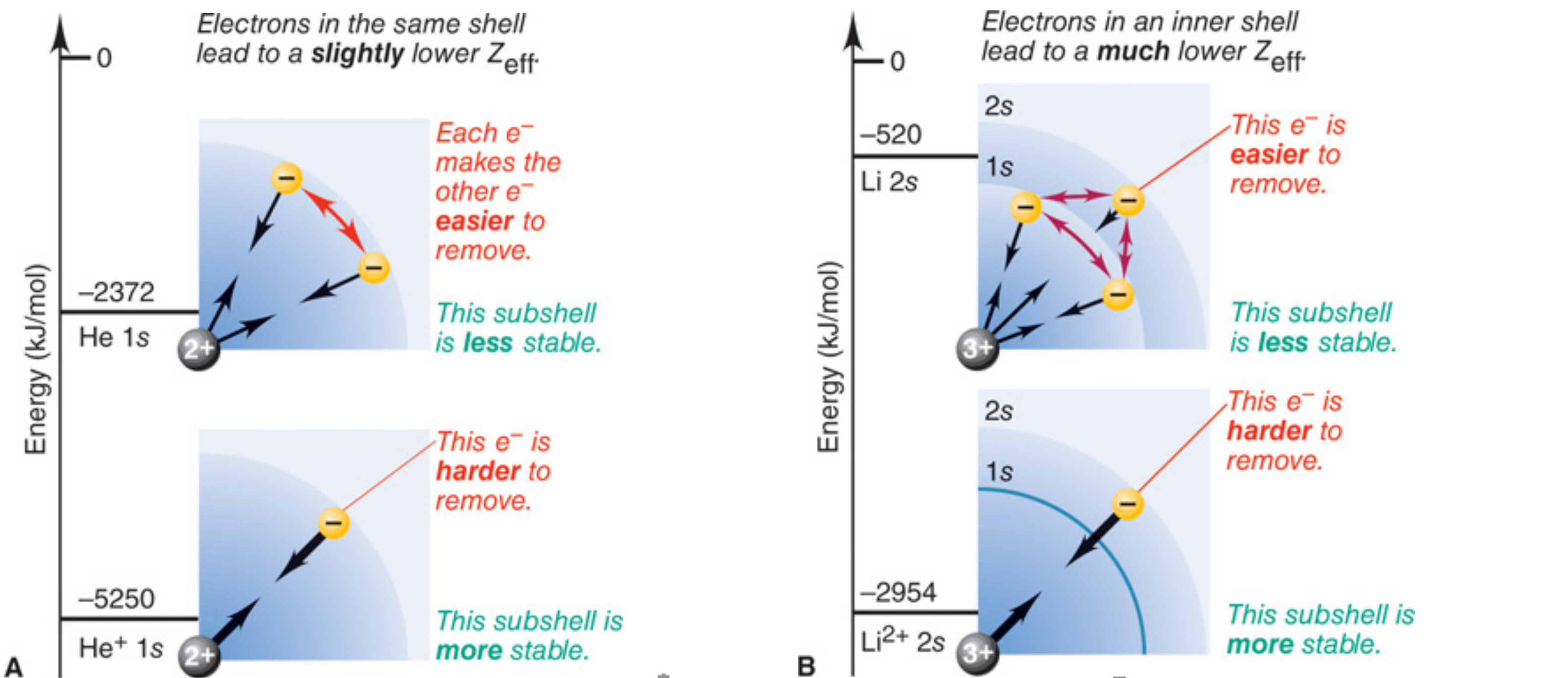
1. **Effect of Nuclear Charge**
   – a larger number of protons in the nucleus increases nucleus-electron attractions



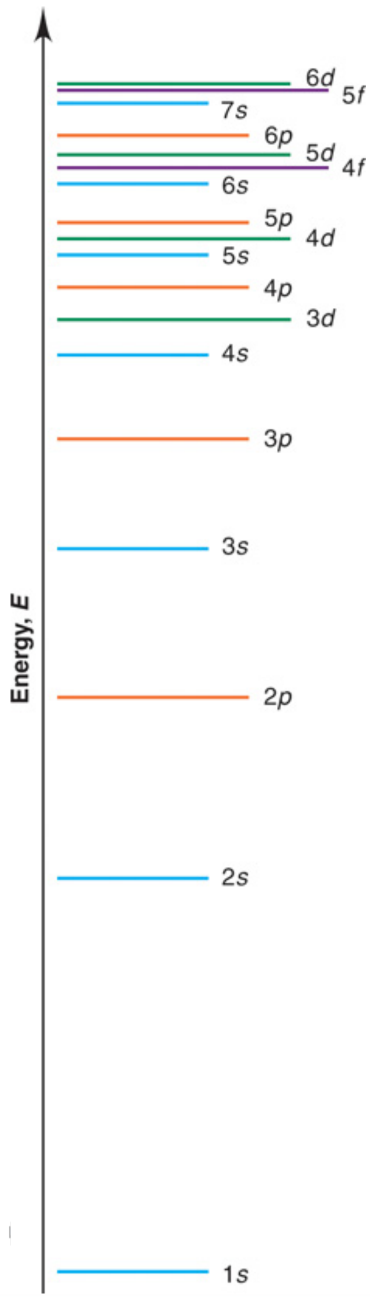
Why do we lose degeneracy?

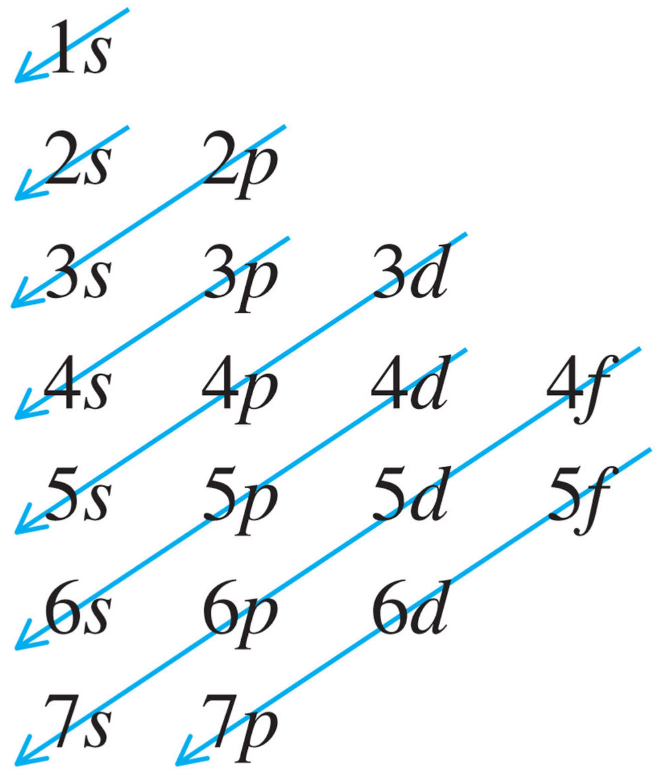
2. Effect of Electron Repulsions

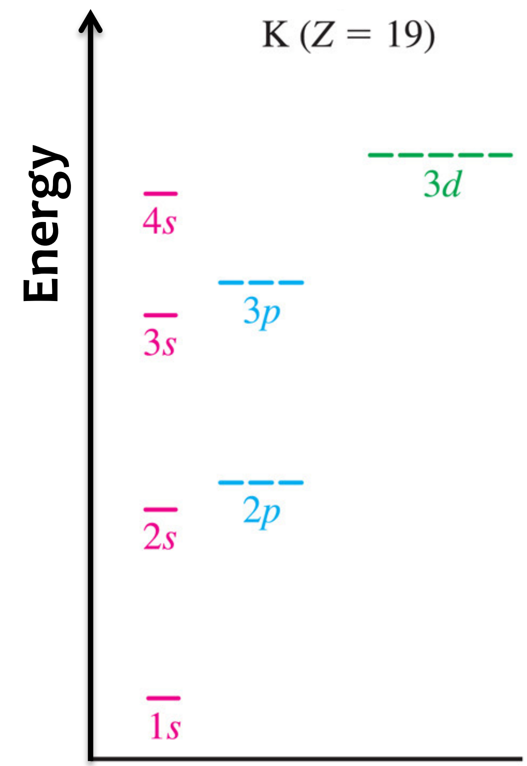
– electrons “shield” other electrons from the nuclear charge



Electron Filling Order







Electron Configurations

There are three ways to represent atomic electron configurations

1. spdf notation

For helium: $1s^2$

indicates the shell

indicates the subshell

indicates the number of e⁻ in the subshell

Electron Configurations

2. noble gas notation

- This is a useful short cut for writing long configurations
- Use the noble gas which precedes the element of interest in the periodic table to abbreviate its electronic configuration

Lithium: $1s^2 2s^1$ Helium: $1s^2$

$\therefore$ We can represent lithium as: $[He]2s^1$

Chlorine: $1s^2 2s^2 2p^6 3s^2 3p^5$ Neon: $1s^2 2s^2 2p^6$

$\therefore$ We can represent chlorine as: $[Ne]3s^2 3p^5$

Electron Configurations of Some Elements

Group	Element	Configuration
1	H	$1s^1$
	Li	$[He]2s^1$
	Na	$[Ne]3s^1$
	K	$[Ar]4s^1$
	Rb	$[Kr]5s^1$
	Cs	$[Xe]6s^1$
	Fr	$[Rn]7s^1$
17	F	$[He]2s^2 2p^5$
	Cl	$[Ne]3s^2 3p^5$
	Br	$[Ar]3d^{10} 4s^2 4p^5$
	I	$[Kr]4d^{10} 5s^2 5p^5$
	At	$[Xe]4f^{14} 5d^{10} 6s^2 6p^5$
18	He	$1s^2$
	Ne	$[He]2s^2 2p^6$
	Ar	$[Ne]3s^2 3p^6$
	Kr	$[Ar]3d^{10} 4s^2 4p^6$
	Xe	$[Kr]4d^{10} 5s^2 5p^6$
	Rn	$[Xe]4f^{14} 5d^{10} 6s^2 6p^6$

Electron Configurations

3. orbital box notation

- this method breaks down each subshell into individual orbitals, shown as boxes
- electrons are shown as arrows: ↑ is spin +½, ↓ is spin -½

[↑][↓] – electrons are paired

[↑][↑] – electrons are parallel

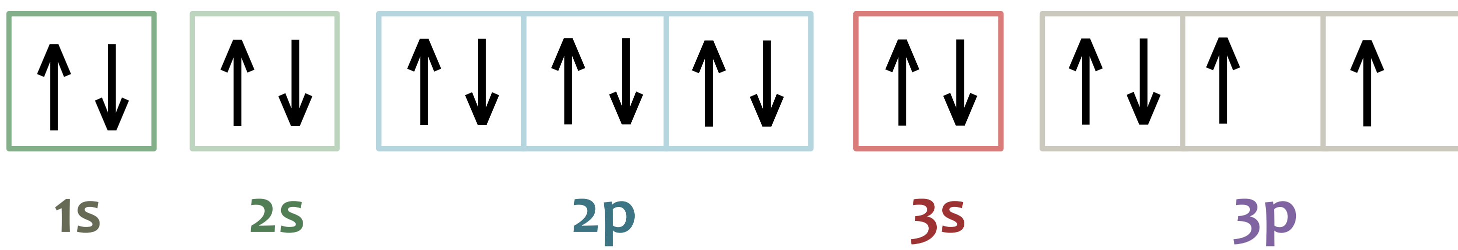
Electron Configurations

Example: sulfur (element #16)

spdf = $1s^2 2s^2 2p^6 3s^2 3p^4$

noble gas = $[Ne]3s^2 3p^4$

orbital box =



Filling Orbitals

- **Aufbau Principle:** work from lowest energy orbitals to highest
- **Pauli Exclusion Principle:** no two electrons may have all four quantum numbers alike (i.e. max 2 e^- per orbital!)
- **Hund's Rule:** fill degenerate orbitals one electron at a time, with parallel spins

	1s	2s	2p			3s	3p		
H	↑								
He	↑↓								
Li	↑↓	↑							
Be	↑↓	↑↓							
B	↑↓	↑↓	↑						
C	↑↓	↑↓	↑	↑					

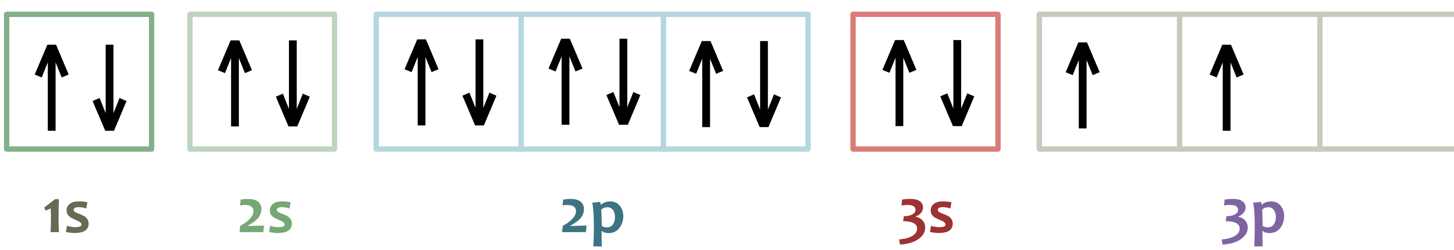
	1s	2s	2p			3s	3p		
N	↑↓	↑↓	↑	↑	↑				
O	↑↓	↑↓	↑↓	↑	↑				
F	↑↓	↑↓	↑↓	↑↓	↑				
Ne	↑↓	↑↓	↑↓	↑↓	↑↓				
Na	↑↓	↑↓	↑↓	↑↓	↑↓	↑			
Mg	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓			

Example: Electron Configurations

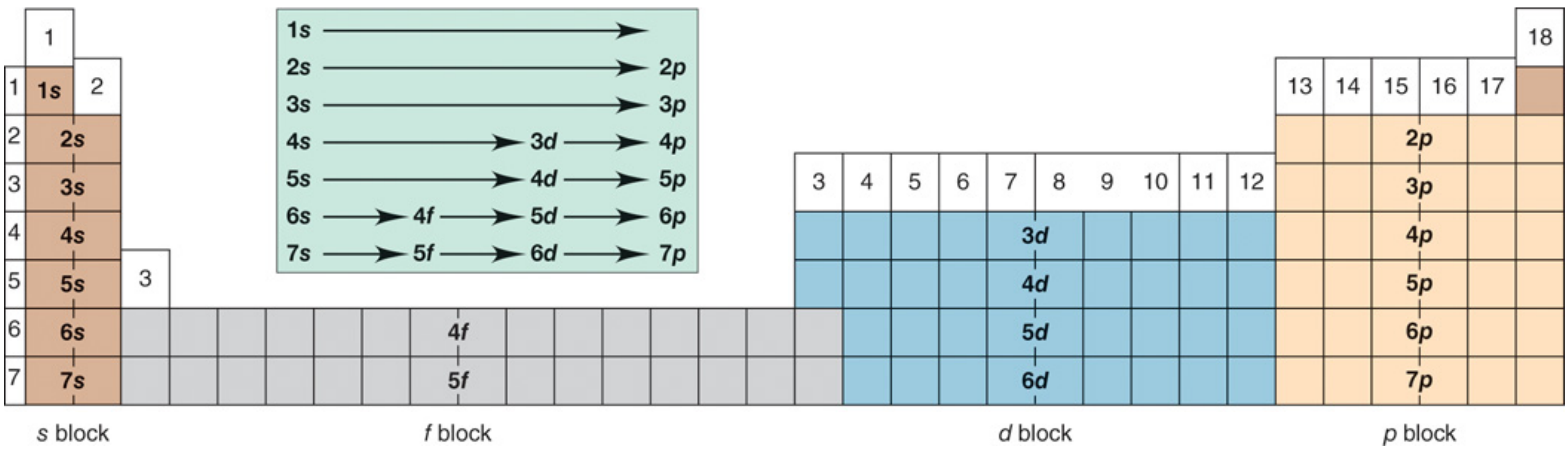
What are the spdf, noble gas, and orbital gas configurations of silicon?

Silicon: 14th element in the table – 14 electrons

- spdf notation: $1s^2 2s^2 2p^6 3s^2 3p^2$
- noble gas notation: $[Ne]3s^2 3p^2$
- orbital box notation:



Extended Periodic Table



Examples: electron configurations

Which element has the electronic configuration $[Kr]5s^2 4d^5$?

What is the value of *n* for the valence shell of an iodine atom and how many valence electrons does it have?

Your Turn…

Which of the following COULD be a full set of quantum numbers for the electron gained when an S^{-} ion becomes an S^{2-} ion?

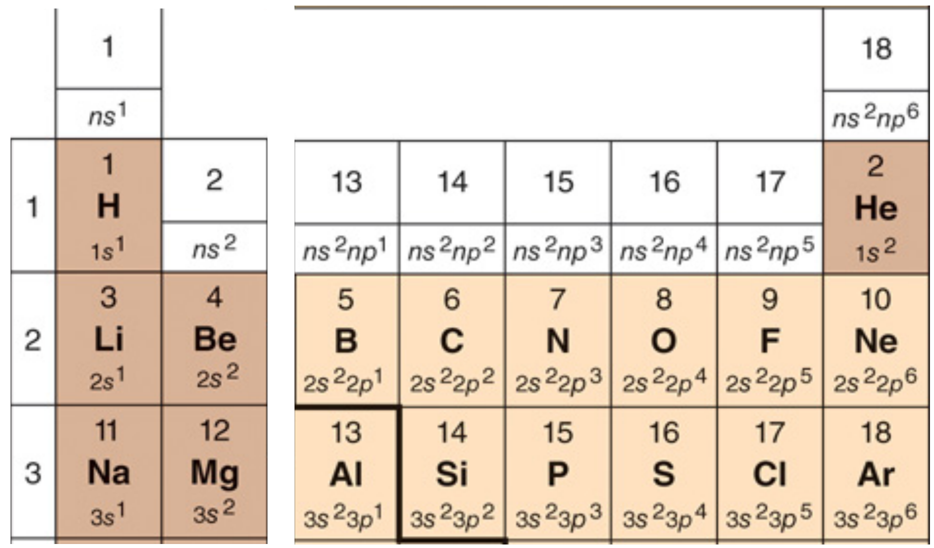
A) $n = 3, \ell = 2, m_\ell = -1, m_s = +1/2$

B) $n = 2, \ell = 1, m_\ell = 0, m_s = -1/2$

C) $n = 6, \ell = 1, m_\ell = +1, m_s = -1/2$

D) $n = 3, \ell = 1, m_\ell = +1, m_s = -1/2$

E) $n = 4, \ell = 3, m_\ell = -1, m_s = +1/2$

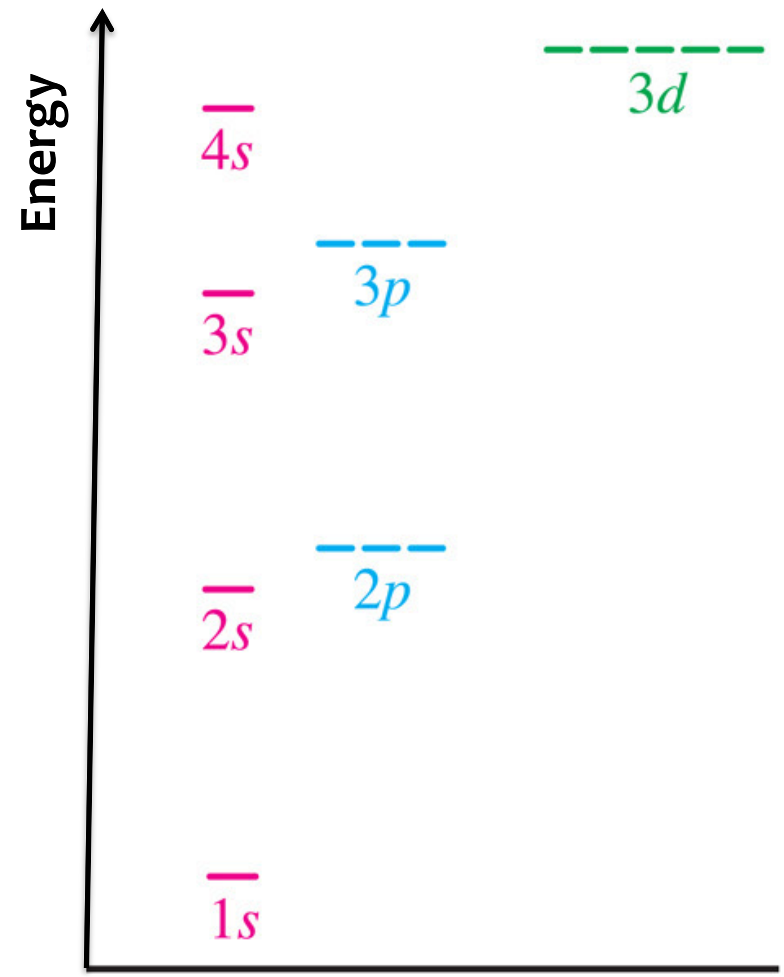


Drawing Orbital Diagrams

Silicon: 14th element in the table – 14 electrons

spdf notation: $1s^2 2s^2 2p^6 3s^2 3p^2$

noble gas notation: $[Ne] 3s^2 3p^2$

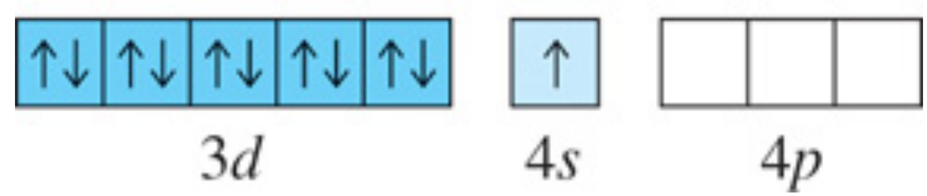


Exceptions… unfortunately

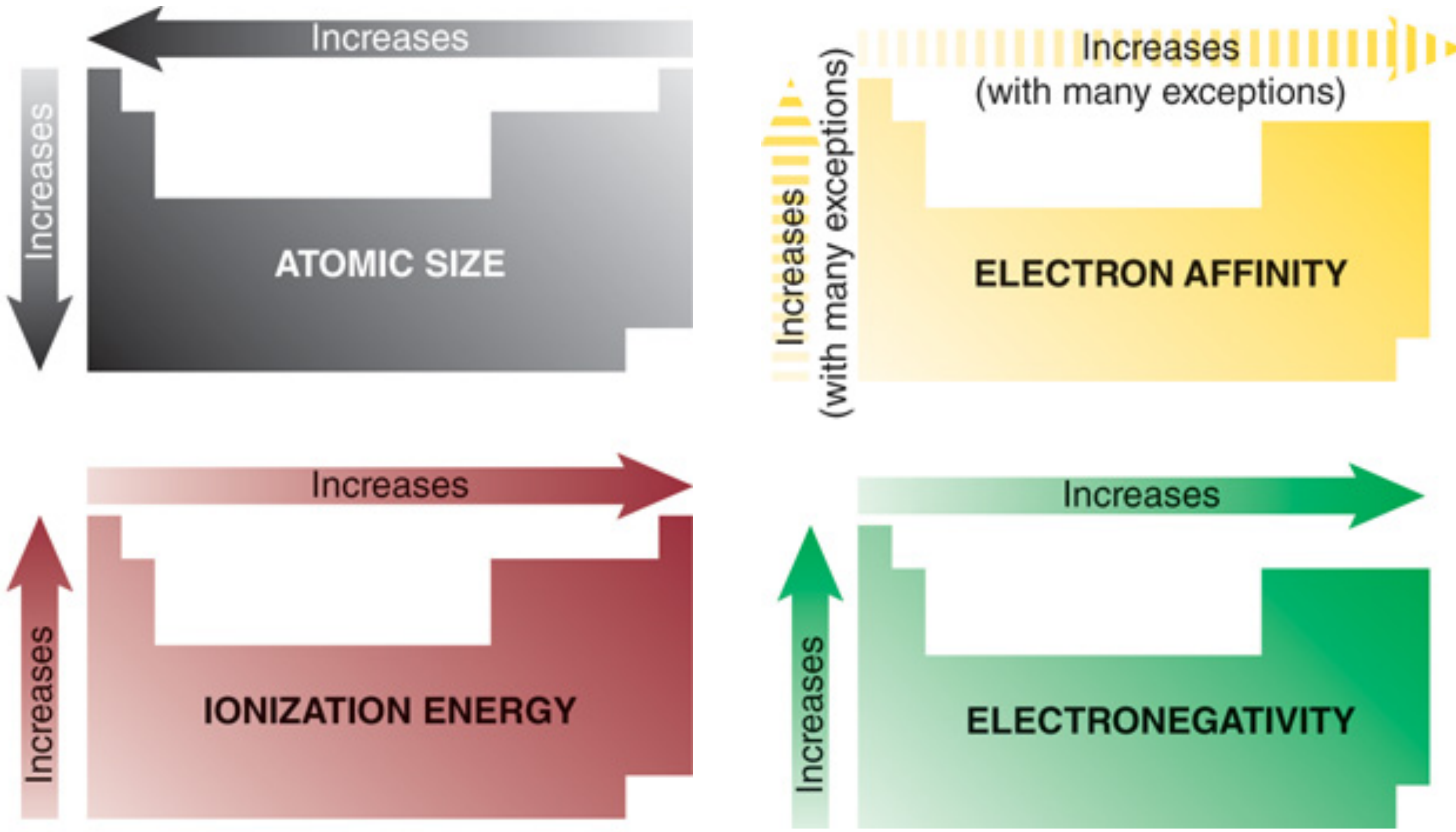
- the orbital energy order becomes less reliable as atomic number increases
- sometimes, certain configurations are "more stable" than others
- two notable exceptions to remember:

Cr (Z = 24) [Ar] $3d^5 4s^1$

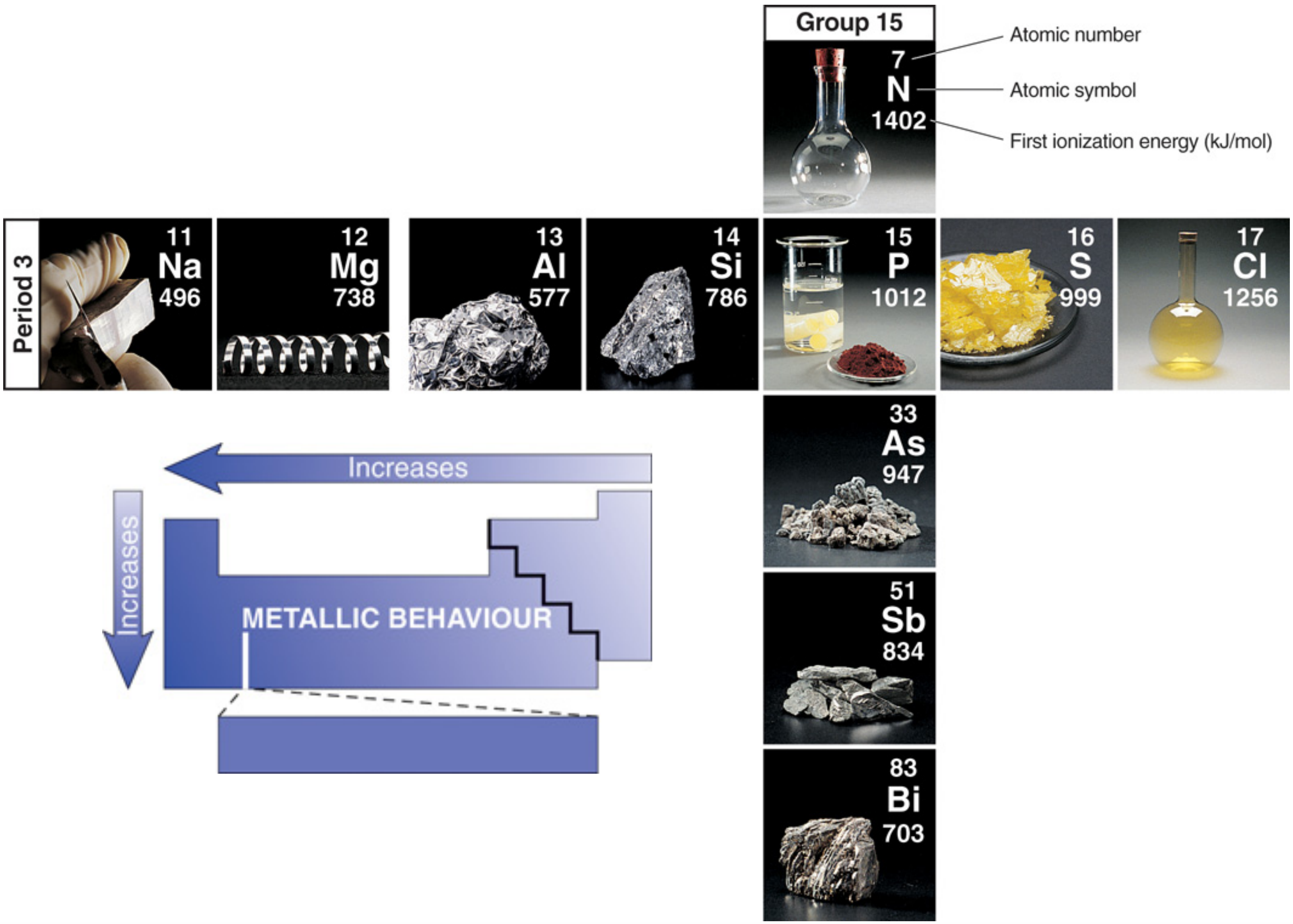
Cu (Z = 29) [Ar] $3d^{10} 4s^1$



7.3: Using Electron Configurations in Periodic Trends



7.4 Atomic Properties and Chemical Reactivity



Your Turn…

Which of the following has the ground state electron configuration $1s^2 2s^2 2p^6$?

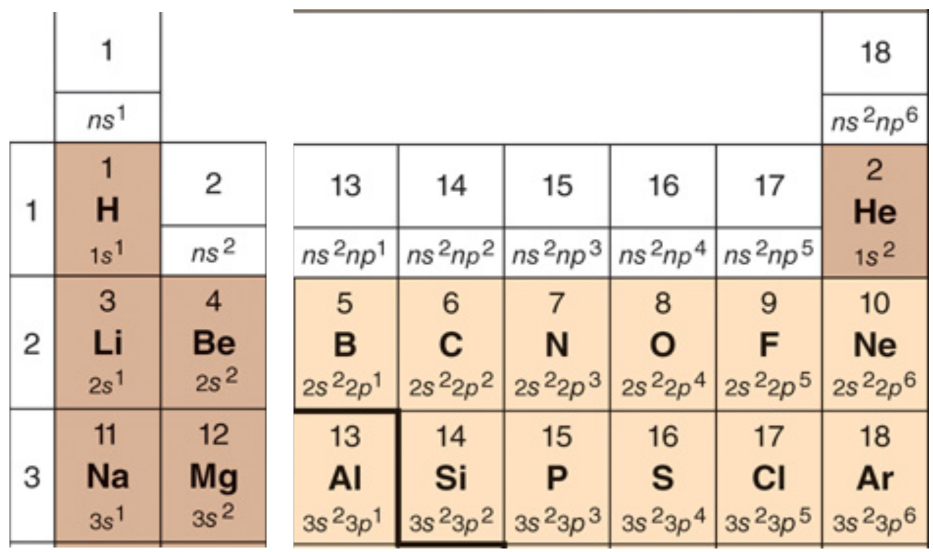
A) Mg^{2+}

B) Ne

C) Na^+

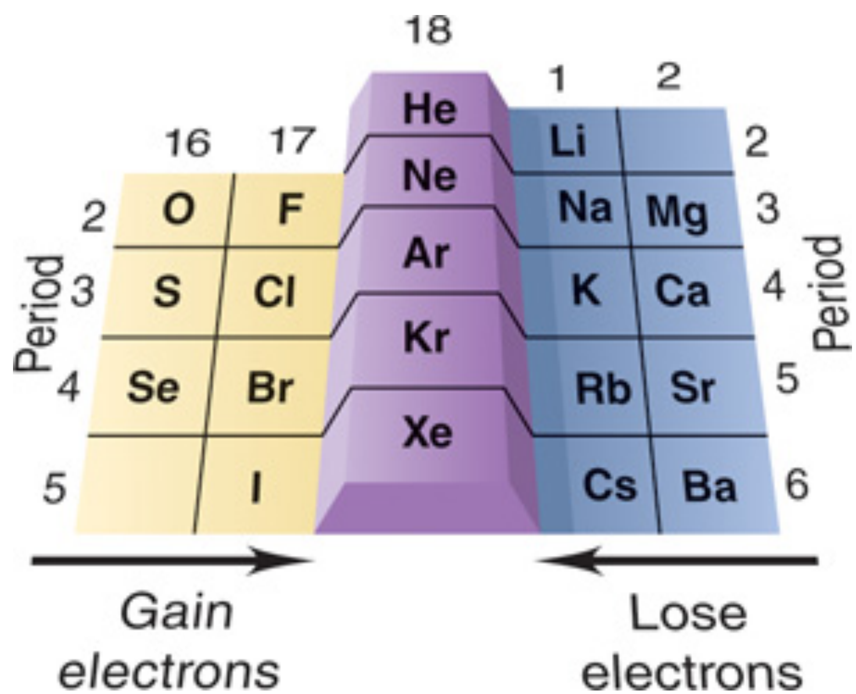
D) O^{2-}

E) all of the above



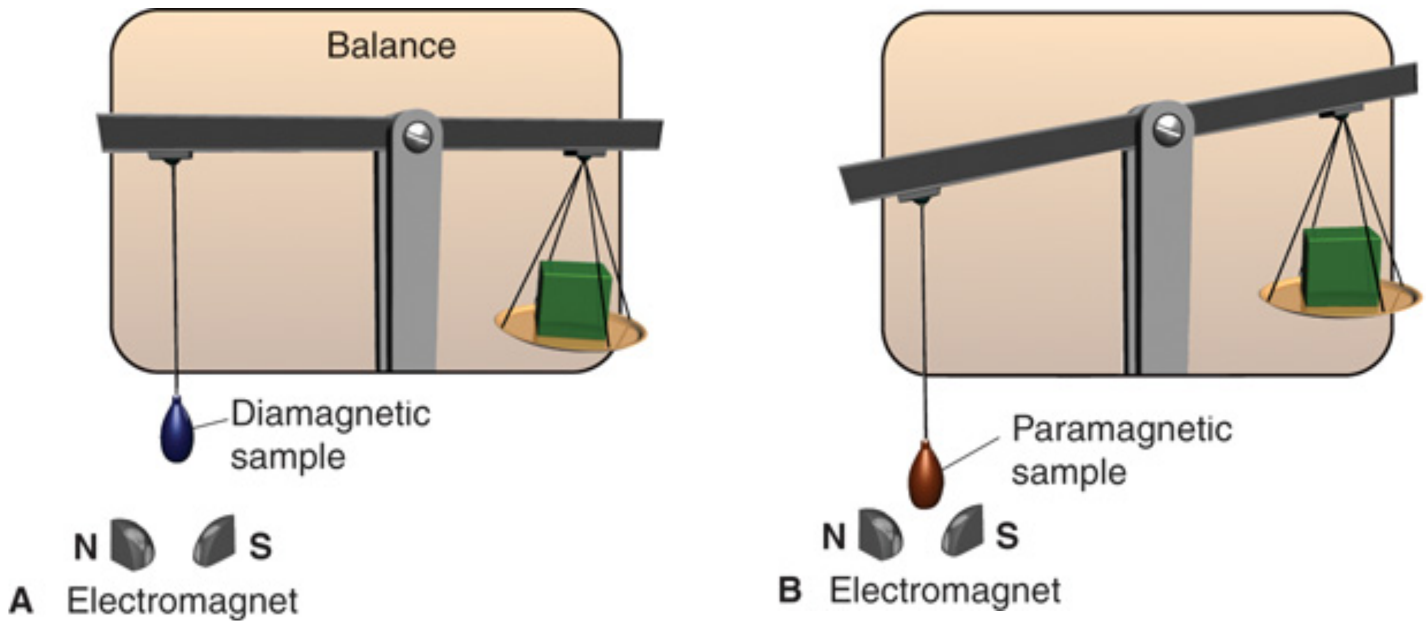
Forming Ions

- **metals** tend to **lose** electrons
- **non-metals** tend to **gain** electrons
- stable configuration = *iso-electronic* with noble gases

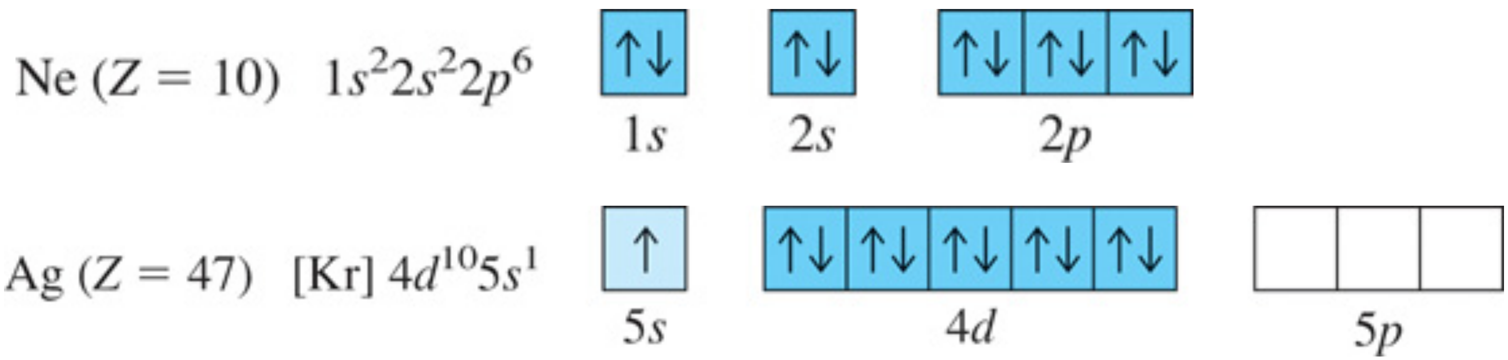


Magnetic Properties

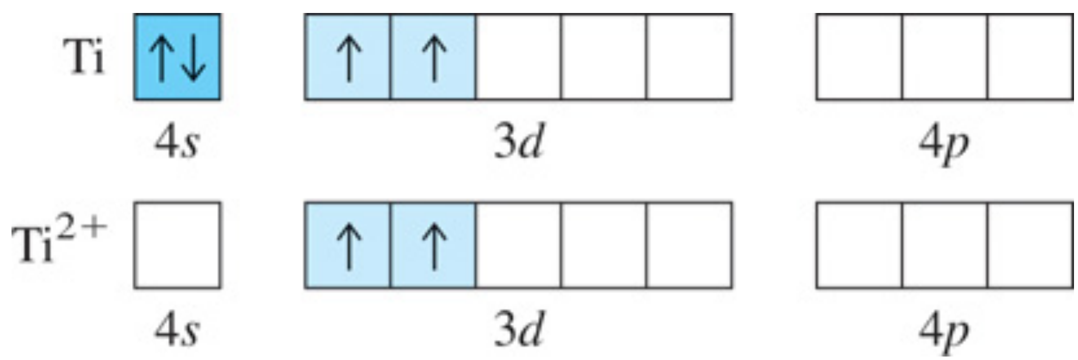
- all electrons are **paired** = **diamagnetic**
- at least 1 **unpaired** electron = **paramagnetic**



Magnetic Properties - Examples



- magnetic studies can be used to determine e⁻ configurations:



Examples: orbital energy diagrams

Draw orbital energy diagrams for the following: Sc, Sc^{3+}, Cr, Cr^{+}, Fe, Fe^{3+}.

Which species are paramagnetic?

Chapter 7: Key Concepts

1. The 4th Quantum Number, m_s
2. Electron Configurations
3. Orbital filling: Aufbau Principle, Pauli Exclusion Principle, Hund's Rule
4. General Atomic Properties
   – diamagnetism vs. paramagentism

Chapter 7 Suggested Problems

7.1, 7.11, 7.13, 7.16,

7.21, 7.23, 7.31, 7.35,

7.39, 7.71, 7.73, 7.75,

7.77, 7.79, 7.89