Announcements for Monday, 23SEP2024

- Exam I is Tuesday, 01OCT2024, 7:45-9:05 **PM** (EDT)
  - Coverage: Chapters E-3.5; exam consists of 19 multiple-choice questions and open-ended questions; see "Other Resources" on Canvas for periodic table and formula sheet to be used on the exam
  - Exam Locations will be announced on Canvas this week
- Exam I Calculator Policy
  - Scientific calculators and ***most*** graphing calculators are allowed
  - **TI-Nspire CX series & other calculators with *QWERTY* keyboards are NOT allowed**

- Week 3 Homework Assignments available on eLearning
  - Graded and Timed Quiz 3 – "Atoms" due **tonight at 6:00 PM (EDT)**
- Any **TECHNICAL ISSUES** associated with eLearning (quizzes, practice assignments, etc.) must be reported to **eLearning Tech Support** **(https://techsupport.elearning.rutgers.edu)**

ANY GENERAL QUESTIONS? Feel free to see me after class!

For Next Lecture: Write down the all the possible n, ℓ, and m_ℓ designations for the orbitals composing the **fourth principal energy level**. Answer given next lecture.

n = **4**

$\ell = 0$ $m_\ell = 0$
$\ell = 1$ $m_\ell = +1, 0, -1$
$\ell = 2$ $m_\ell = +2, +1, 0, -1, -2$
$\ell = 3$ $m_\ell = +3, +2, +1, 0, -1, -2, -3$

s-subshell

$n = 4, \ell = 0, m_\ell = 0$

p-subshell

$n = 4, \ell = 1, m_\ell = +1$
$n = 4, \ell = 1, m_\ell = 0$
$n = 4, \ell = 1, m_\ell = -1$

d-subshell

$n = 4, \ell = 2, m_\ell = +2$
$n = 4, \ell = 2, m_\ell = +1$
$n = 4, \ell = 2, m_\ell = 0$
$n = 4, \ell = 2, m_\ell = -1$
$n = 4, \ell = 2, m_\ell = -2$

f-subshell

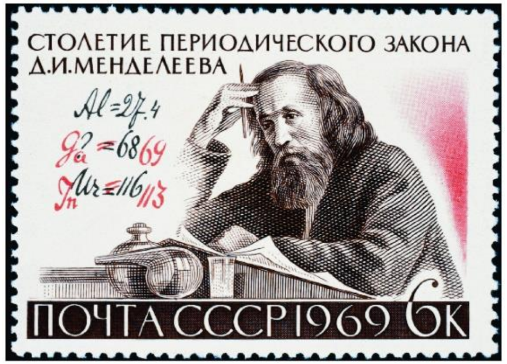
$n = 4, \ell = 3, m_\ell = +3$
$n = 4, \ell = 3, m_\ell = +2$
$n = 4, \ell = 3, m_\ell = +1$
$n = 4, \ell = 3, m_\ell = 0$
$n = 4, \ell = 3, m_\ell = -1$
$n = 4, \ell = 3, m_\ell = -2$
$n = 4, \ell = 3, m_\ell = -3$

Chapter 3: Periodic Properties of the Elements

Some questions we'll try to answer

- How is the modern periodic table arranged and what information does it give us?
- How do electrons occupy orbitals in multi-electron atoms?
- How do we establish the electron configurations of atoms and ions?
- How does an atom's electron configuration impact such properties of an atom such as size, ionization energy, etc.?
- How are electrons specifically arranged in atom?
- How does the size of an ion relate to the size of its parent atom?
- What are the different periodic trends and how can they be explained?

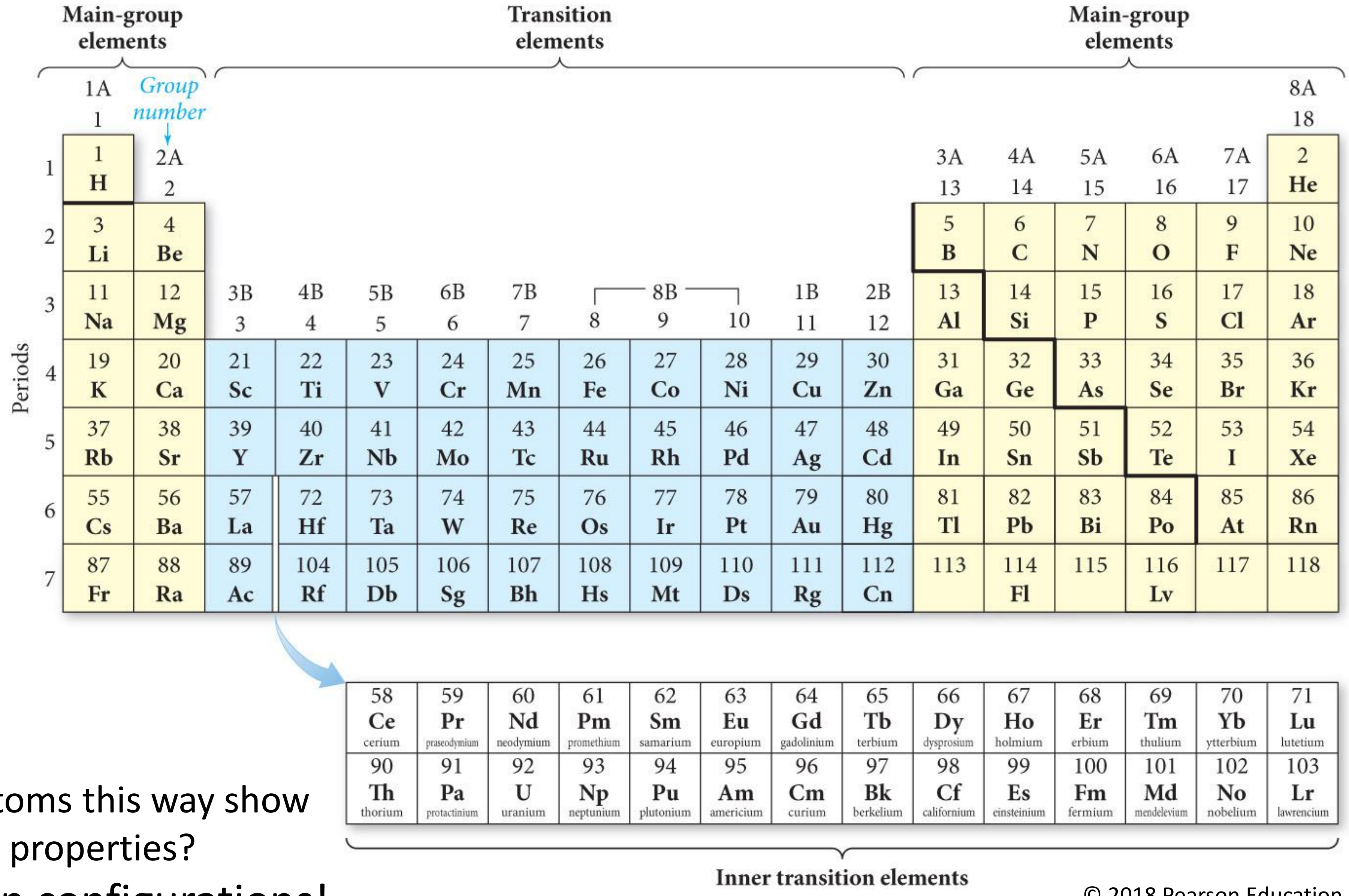
The Periodic Table of Elements



- Compact way to summarize a large number of observations about the elements
  - information not only given by the explicit numbers
  - information based on an atom’s position within the table (row and column)
  - **periodic properties of the elements =** predictable properties based on an element’s position
- historically there were several attempts to systematically group the elements
- (1869) Dmitri Mendeleev
  - the first successful version grouped the atoms horizontally by increasing atomic mass
  - rows were arranged so that elements with similar properties fell in the same vertical columns
  - predicted the existence and properties of elements not yet discovered
  - eventually changed to list the elements by increasing atomic number which led to even better correlation of properties

The Modern Periodic Table

- periods vs. groups (or families)
    - chemical similarities in groups
- metals vs. nonmetals vs. metalloids
- main group vs. transition vs. inner-transition
    - main group most predictable
    - A/B numbering
- A-numbering of main-group elements will
    - give # valence e^-s
    - allow determination of ionic charges



Why does grouping the atoms this way show similarities in their properties?

Because of the electron configurations!

Electron Configurations: How Electrons Occupy Orbitals

- Electrons occupy atomic orbitals in a specific order
  - generally the lowest energy orbitals available are occupied first
  - when an orbital gets filled with the maximum number of electrons, the next higher energy orbitals begin to fill until all the electrons in an atom find a home

ground state = all electrons are in the lowest energy orbitals possible

excited state = some electron(s) are in higher energy orbitals

example for hydrogen: $2s^1$ rather than $1s^1$

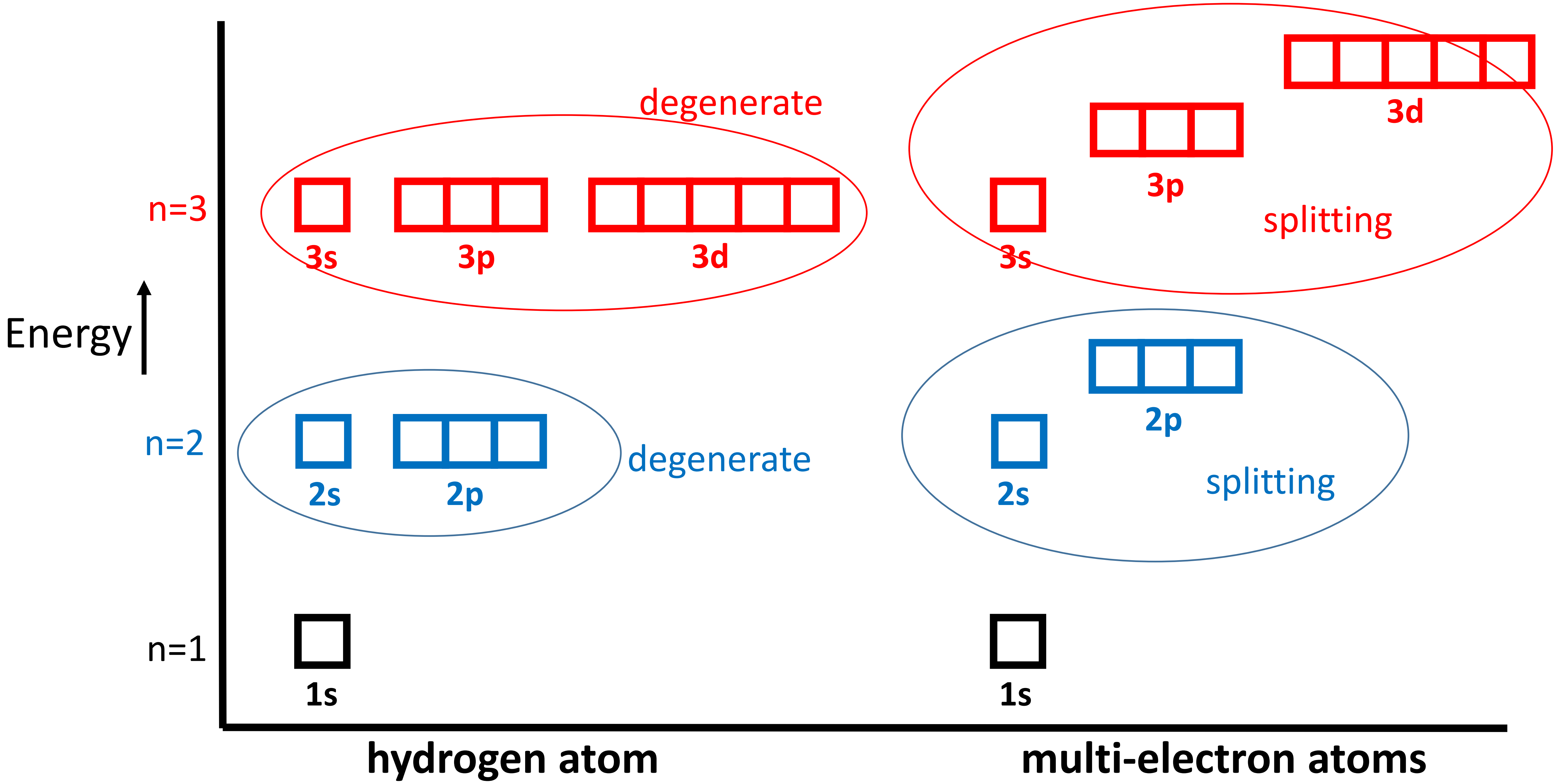
Orbital Energies: Hydrogen vs. Multi-electron Atoms

How do orbitals in a hydrogen atom differ from orbitals in multi-electron atoms?

1. in the hydrogen atom, the energy of an electron is simply given by the value of **n** (i.e., the principal energy level) and **NOT** the sublevel
   - Energy (n=1) **<** Energy (n=2) **<** Energy (n=3)…
   - But Energy (3s) = Energy (3p) = Energy (3d)
     - the sublevels are **degenerate** (i.e., of equal energy)

2. in a multi-electron atom, the energy of an electron depends on both the values of n and **ℓ** (i.e., the principal level and the sublevel)
   - Energy (n=1) **<** Energy (n=2) **<** Energy (n=3)…
   - But ***for given value of n***: Energy (s) **<** Energy (p) **<** Energy (d) **<** Energy (f)

Orbital Energies: Hydrogen vs. Multi-electron Atoms



Energies of s-, p-, d-, and f-orbitals

Why do the orbital energies differ in a multi-electron atom?

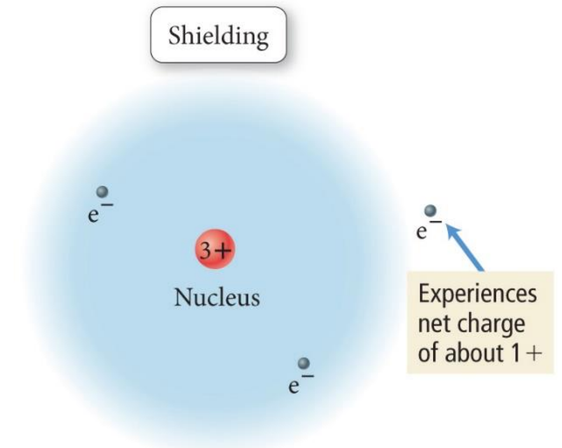
$$E = \frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{r}$$

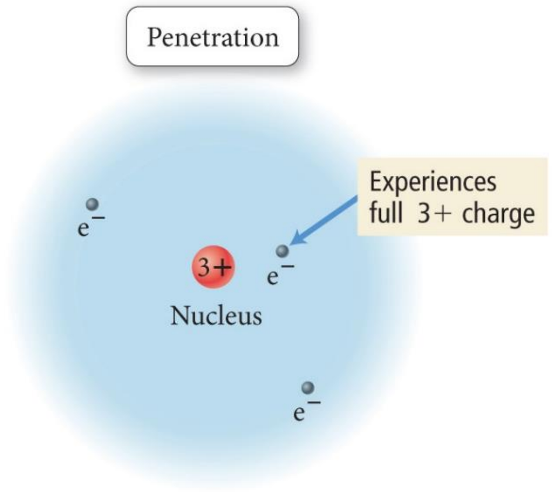
- Coulomb's Law gives the potential energy between two charged particles (q_1 & q_2)
  - E(+) = repulsion (increases energy of a system…destabilizing effect)
  - E(–) = attraction (**decreases** energy of a system…**stabilizing** effect…energetically **FAVORABLE**)
- $|E|$ is proportional to magnitude of charges and inversely proportional to distance (r) between the charged particles
- Important: we'll be coming back to Coulomb's law when we talk about ionic compounds/lattice energy

Two Orbital Effects that Impact Electron Energies

- in general, anything that helps to bring electrons closer to the nucleus and allows them to interact more with the positive charge will serve to ***lower*** the energy and lead to a ***more stable*** (i.e., happy) system

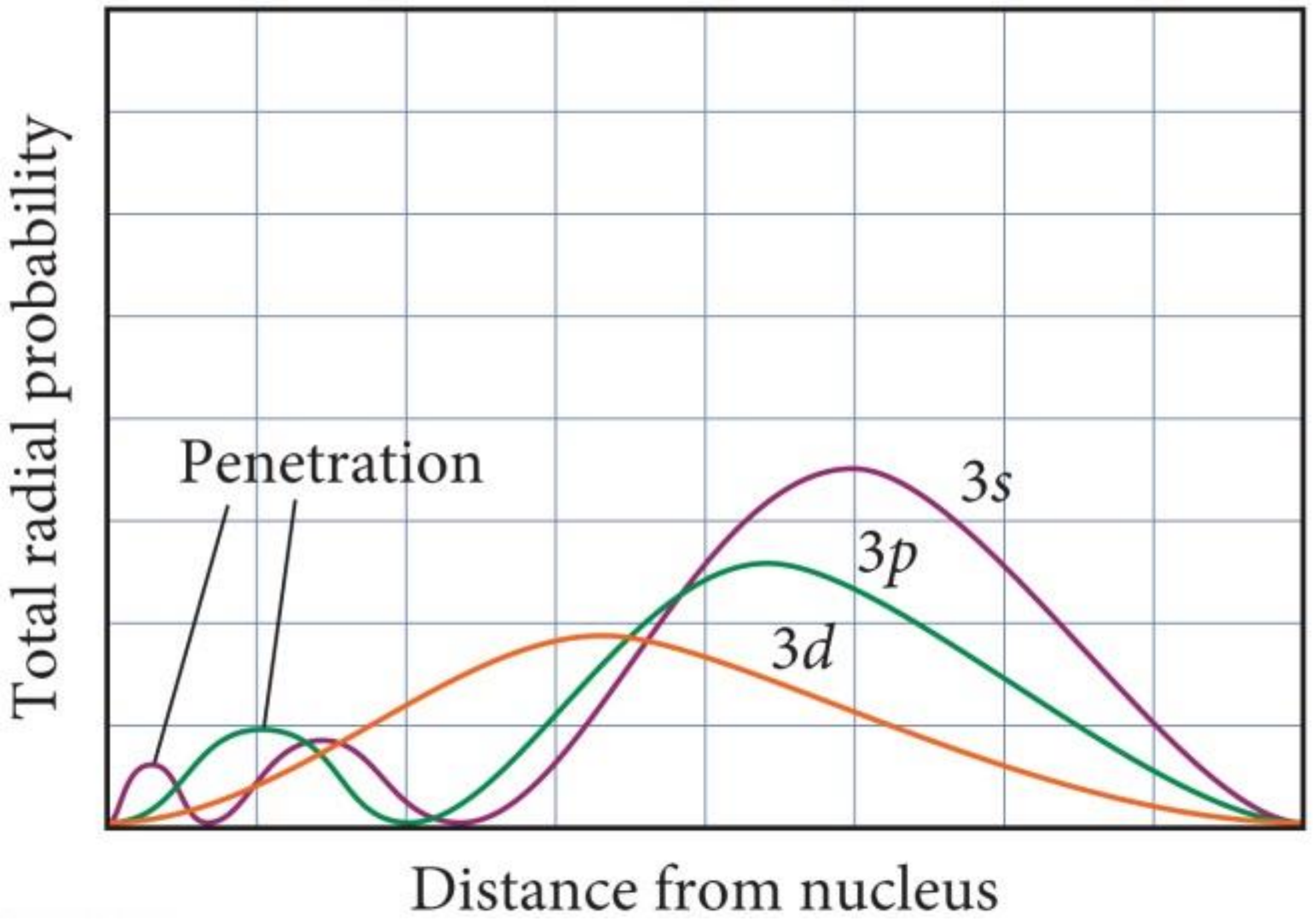
1. shielding
   - electrons in energy levels with larger values of n do not "feel" the full effects of the nucleus because of charge shielding from inner electrons
2. **orbital penetration =** how close the e^-s in an orbital gets to the nucleus
   - more penetration = electrons closer to nucleus
   - s-orbitals penetrate more than p-orbitals (which penetrate more than d-orbitals which penetrate more than f-orbitals)
   - orbital penetration for a given value of n:
     - ns > np > nd > nf…
   - the more the electrons penetrate, the closer to the nucleus, and the lower (i.e., more negative) the energy (see Coulomb's law)

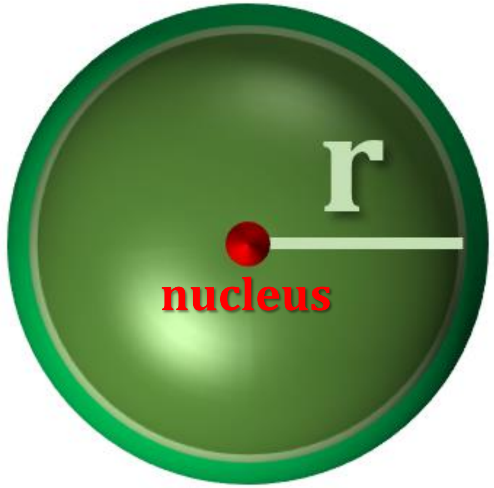




Orbital Penetration: s vs. p vs. d

a **radial distribution function** for an atomic orbital shows the total probability of finding an electron within **a thin spherical shell** at a distance ***r*** from the **nucleus**





<u>**WITHIN THE SAME ATOM**</u> we see some general trends

- the **3s** electrons penetrate more deeply than the **3p** or **3d** electrons
- the **3s** electrons are less shielded from the nucleus than the **3p** or **3d** electrons
- the **3s** electrons experience a greater ***effective nuclear charge*** than the **3p** or 3d electrons and are lower in energy than the **3p** or **3d** electrons
- orbital energies: **3s** < **3p** < **3d**

Writing Orbital Diagrams and Electron Configurations

Orbital Diagrams

- individual atomic orbitals are represented as boxes with sublevels labelled
- electrons in orbitals are represented by up- or down-arrows (half-arrows) to show electron spin (m_s = + ½ or – ½)
- electrons are filled into the orbitals following specific rules until all of the atom's electrons are housed in orbitals
  - **Aufbau Principle:** lowest energy orbitals are filled first
  - **Hund's rule:** When filling individual orbitals of a given sublevel, electrons fill them singly first with parallel spins
- two electrons sharing an orbital MUST have opposite spins
  - **Pauli Exclusion Principle:** No two electrons in an atom can have the same four quantum numbers

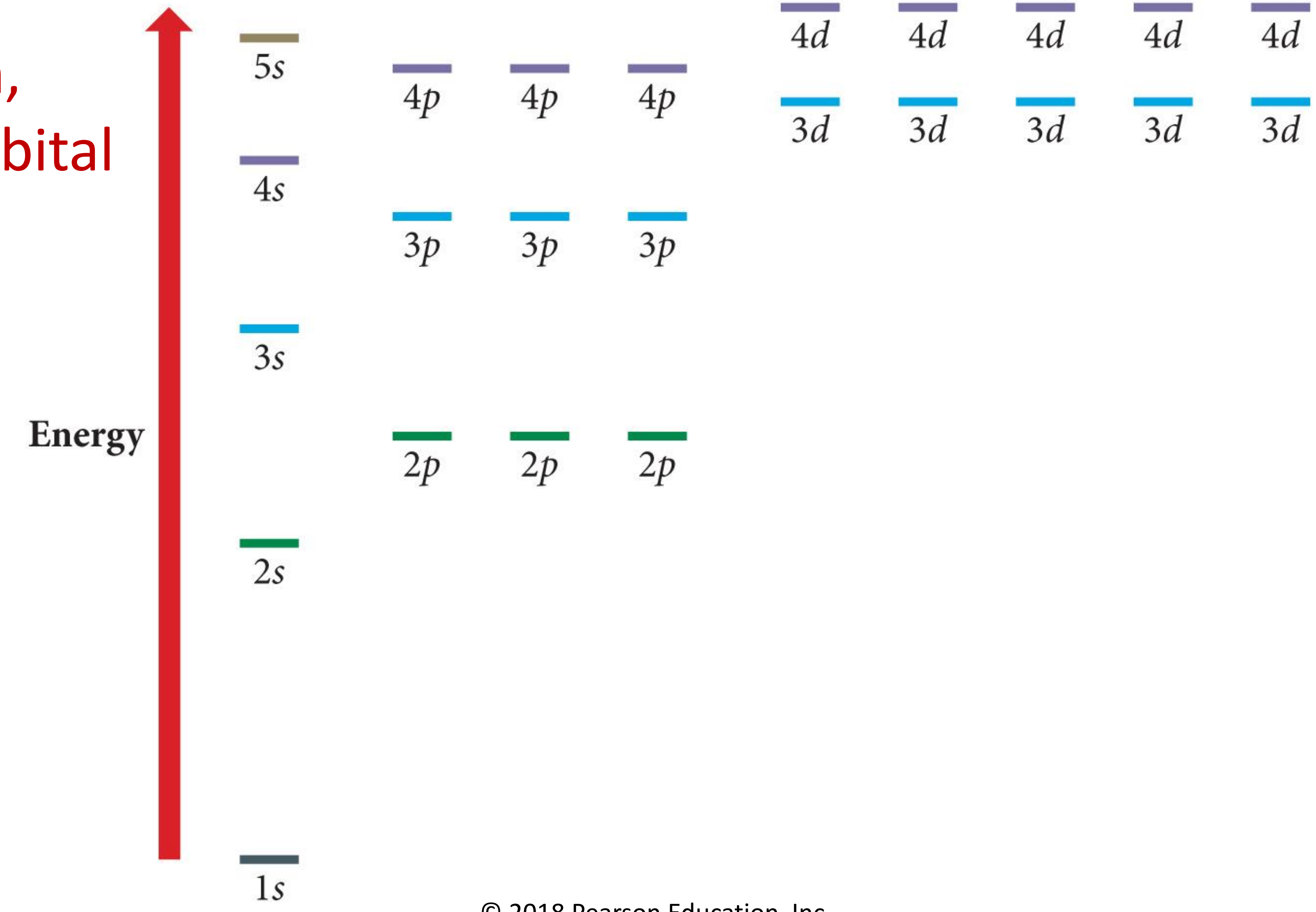
Electron Configurations

- only number of electrons in each sublevel are shown in order of increasing energy
- SPECIFIC (and unexpected) order of filling sublevels (next slide)

	electron configuration	orbital diagram
H Z = 1	$1s^1$	[↿] 1s
He Z = 2	$1s^2$	[↿⇂] 1s
Li Z = 3	$1s^2\,2s^1$	[↿⇂] 1s [↿] 2s
C Z = 6	$1s^2\,2s^2\,2p^2$	[↿⇂] 1s [↿⇂] 2s [↿][↿][ ] 2p

General Energy Ordering of Orbitals for Multi-electron Atoms

at higher values of n, significant overlap of orbital energies



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

Try This On Your Own

- Give the full electron configuration for nickel (Z = 28)
- Give the orbital diagram of the last two sublevels
- Determine the number of unpaired electrons in a nickel atom