

Chemistry 1B-02 Session 5-6  
Fall 2016

**Chemistry 1B**  
**Fall 2016**

sessions 5-6

Chapter 12

pp. 557-569

\*(569-571)

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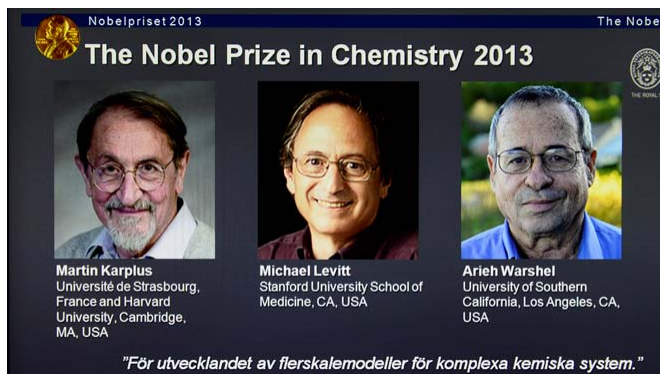
What can you do to become famous?

*[and win a cool \$1.2 million?]*

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# Chemistry 1B-02 Session 5-6 Fall 2016

## STUDY QUANTUM MECHANICS



When scientists wanted to simulate complex chemical processes on computers, they used to have to choose between software that was based on classical Newtonian physics or ones based on **quantum** physics. But the academy said the three laureates developed computer models that "opened a gate between these two worlds."

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## Molecular Mechanics at UCSC



Prof Ilan Benjamin  
Prof. Yuan Ping

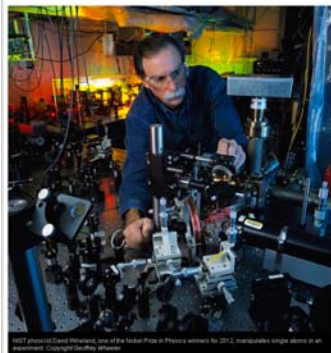
4

# Chemistry 1B-02 Session 5-6 Fall 2016

## 2012 Nobel in QUANTUM physics

Nobel Awarded to Scientists Who Learned to Control Quantum Systems

By Education 22 October 9, 2012 2:47 pm Categories: Physics



Nobelpriset 2012 The Nobel Prize 2012

### Mastering Particles in the Quantum World

ION(s) in a trap controlled by photons


Photon(s) in a cavity controlled by atoms

David Wineland Serge Haroche

Nobelprize.org

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## aims for lectures 5-6: many electron atoms

- electron spin, “the 4<sup>th</sup> quantum number and the Pauli exclusion principle
- effective nuclear charge,  $Z_{\text{eff}}$   
the “net” attraction for an electron in a many-electron atom 
- knowledge of the principal quantum number ( $n$ ) and  $Z_{\text{eff}}$  for and atom’s valence electrons leads to an understanding of:
  - $E_{2s} < E_{2p}$
  - $E_{3p} < E_{3d}$
  - $E_{3d}$  vs  $E_{4s}$
- Hund’s Rule and electron configuration in many-electron atoms  
the Aufbau Principle

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*new considerations for many-electron atoms  
(somewhat different 'order' of presentation than Zumdahl)*

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- **how does increased atomic number ( $Z$ ) and the presence of other electrons affect orbital energies?**
- **how does one “fill up” the available orbitals in many-electron atoms**

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Chemistry 1B -AL

multi-electron atoms

Electron Spin

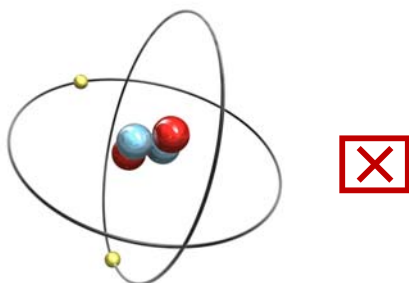
Electronic Configurations

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*did the Schrodinger equation "work" for helium ??*

---



$$\mathcal{H}_{\text{helium}} \Psi = E_{\text{helium}} \Psi \quad ???$$

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*many-electron atoms and Schrödinger Equation (pp 557-558)*

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Although the Schrödinger equation,  $\mathcal{H}\Psi = E\Psi$ , for polyelectronic atoms (and molecules) cannot be solved exactly (mathematically)

Numerical computer calculations give solutions that **agree perfectly with experiment** ✓



Year	Quantal/Experimental Method	$-E$
1924	experimental, Lyman (1924)	2.9035
1998	exp., Bergeson <i>et al.</i> (1998)	<u>2.903 693 775</u>
1929	var., 38 param., Hylleraas (1929)	2.9037
1993	relativ. Drake (1993)	<u>2.903 700 023</u>

but solutions are very complex .

$$\Psi(s, u, t) = N e^{-\Omega/2s} \sum_{l,m,n} C_{l,m,n} s^{l-m} u^{m-n} t^n \quad (2)$$

so- We can (and will!!) use the hydrogen-like orbitals as a very good approximation to the exact solutions of the Schrödinger equation for many-electron atoms.

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# Chemistry 1B-02 Session 5-6 Fall 2016

## aims for sessions 5-6: many electron atoms

### this video

- electron spin, “the 4<sup>th</sup> quantum number and the Pauli exclusion principle
- effective nuclear charge,  $Z_{\text{eff}}$   
the “net” attraction for an electron in a many-electron atom

### in next class

- knowledge of the principal quantum number (n) and  $Z_{\text{eff}}$  for and atom’s valence electrons leads to an understanding of:
  - $E_{2s} < E_{2p}$
  - $E_{3p} < E_{3d}$
  - $E_{3d}$  vs  $E_{4s}$
- Hund’s Rule and electron configuration in many-electron atoms  
the Aufbau Principle

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## worksheet III sections I.1-2 and II.1-3

Chemistry 1B-AL Fall 2016, Study Guide and Worksheet III

**Learning Objectives and Worksheet III**  
Chemistry 1B-AL Fall 2016

Lectures (5-6) Many Electron Atoms and the Aufbau Principle

Read pp. 557-569 (you will not be responsible for the material on pp-569-571; however the CHEM1B-AL staff would be more than happy to discuss these concepts with you)

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Atomic orbital **APPROXIMATION**

To describe the electronic structure of atoms we will be using a model that is an approximation to the actual (exact) solutions to the Schrödinger equation. In this model the many-electron wavefunction is “built” up by placing electrons into “hydrogen-like” atomic orbitals.

I. Pauli Exclusion Principle (PEP)

1. What did the Stern-Gerlach experiment indicate?

2. What is Pauli Exclusion Principle as related to allowed orbital occupancy?

Addition information on Stern-Gerlach and electron “spin” (University of Toronto):  
<http://www.usgcarlab.utoronto.ca/Gerlach/Steve/Harrison/SternGerlach/SternGerlach.html>

II. Energies of orbitals in many-electron atoms

1. In the hydrogen atom, and for all 1-electron ions, the energy of an electron in an orbital with quantum numbers  $n, l, m_l, m_s$  is given by  $E_n = -\frac{m_e e^4 Z^2}{8h^2 n^2} = -(2.18 \times 10^{-18} \text{ J}) \frac{Z^2}{n^2}$ . For the energy of an electron in a many electron atom the nuclear charge  $Z$  is replaced by \_\_\_\_\_ which takes into account both  $Z$ , the \_\_\_\_\_ of the nucleus, and the repulsion (or-shielding of nuclear charge) of the \_\_\_\_\_.

2. In a helium atom  $Z_{\text{eff}}$  for an electron will be \_\_\_\_\_ the +2 charge on the nucleus.

1

2. In a helium atom  $Z_{\text{eff}}$  for an electron will be \_\_\_\_\_ the +2 charge on the nucleus.

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Chemistry 1B-AL Fall 2016, Study Guide and Worksheet III

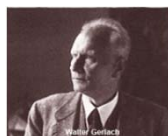
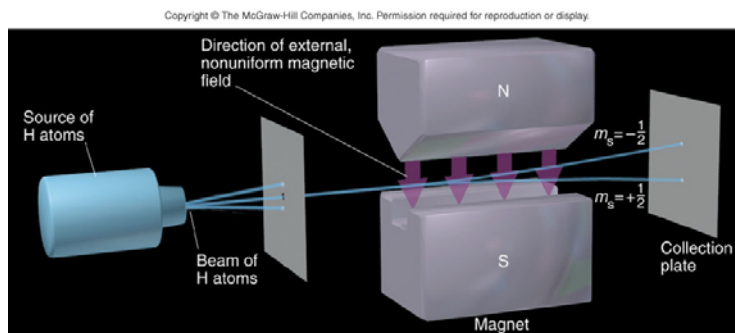
3. In the ground state of the Li atom has configuration \_\_\_\_\_ the electron in the 2s orbital has the higher (less negative) energy both because \_\_\_\_\_

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## Stern-Gerlach Experiment

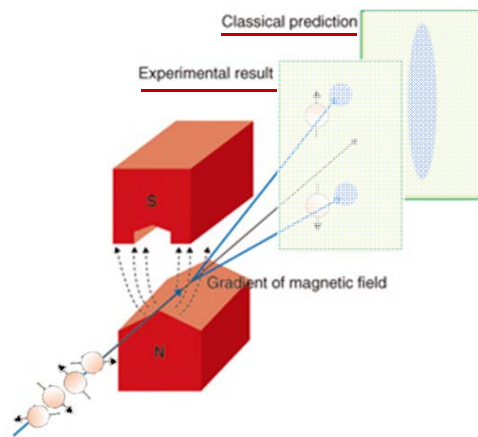
- Stern-Gerlach experiment (fig. 8-1 Silberberg)



<https://quantum-reality.net/2015/11/03/the-stern-gerlach-experiment/>

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## the 4<sup>th</sup> quantum number: spin

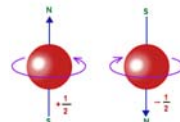


[https://www.ntt-review.jp/archive/ntttechnical.php?contents=ntr201209fa4\\_s.html](https://www.ntt-review.jp/archive/ntttechnical.php?contents=ntr201209fa4_s.html)

the electron has two possible spin states with spin quantum numbers

$$m_s = +\frac{1}{2} \text{ or } m_s = -\frac{1}{2}$$

spin up and spin down



<http://www.quantum-field-theory.net/discovery-electron-spin/>

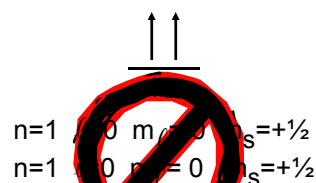
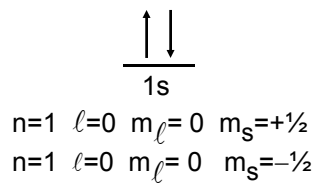
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## Pauli exclusion principle (PEP) (sec 12.10)

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no two electrons can have the same four quantum numbers:



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## many-electron atoms

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He, Li, Be, B, C, N, O, F, Ne .....

- greater nuclear charge ( $Z$ ) than hydrogen ( $Z=1$ )
- more electrons than hydrogen (one-electron)

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*where we are heading !!! chapter 12*

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- Quantum mechanics describes many-electron atoms by filling hydrogen-like orbitals with the atom's electrons in a manner consistent with the Pauli Exclusion Principle.
- This description allows us to understand the **energies** of electrons in atoms and ions, the **relative sizes** of atoms and ions, and the **chemical reactivity** and other properties of various elements.

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*voila*

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VOILA!!!

Representative Elements		f-Transition Elements										Representative Elements					Noble Gases	
1A Group numbers												3A	4A	5A	6A	7A	8A	
1	H																He	
2	Li	Be											B	C	N	O	F	Ne
3	Na	Mg											Al	Si	P	S	Cl	Ar
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba	La*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Fr	Ra	Ac**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Uub	Uuq					

\*Lanthanides  
\*\*Actinides

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## *electronic configuration*

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**electronic configuration:** specification of which orbitals the electrons occupy in an atom (or molecule) [*and possibly the spins of electrons*]

e.g. for H:  $1s$  or  $\frac{\uparrow}{1s}$

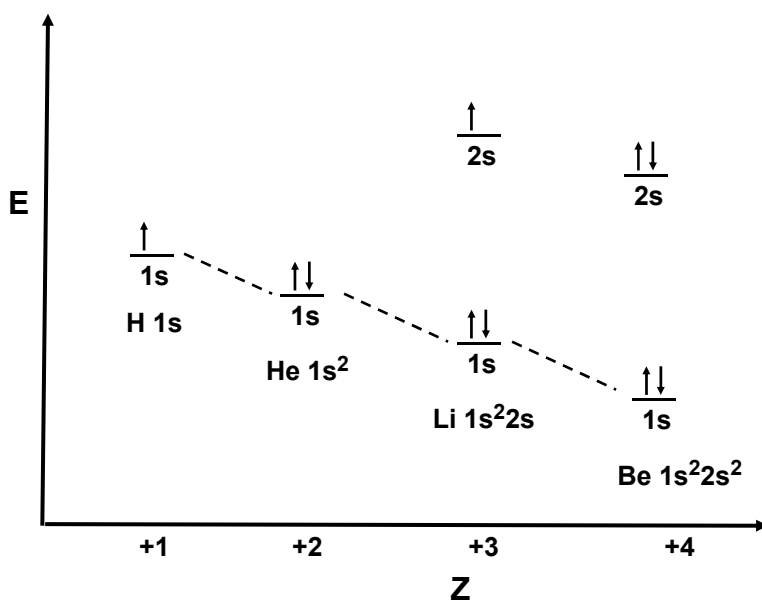
He:  $1s^2$  or  $\frac{\uparrow\downarrow}{1s}$

C:  $1s^2 2s^2 2p^2$   $\frac{\uparrow}{\quad} \frac{\uparrow}{\quad} \text{---}$   
2p

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## *configurations (for 1s and 2s levels) ground states (preview)*

---



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*remembering from H atom*

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- Dependence of energy and average radius of electron in a hydrogen orbital on:

**n and Z**

$$E_n = -\frac{m_e e^4}{8h^2 \epsilon_0^2} \frac{Z^2}{n^2} = -(2.18 \times 10^{-18} \text{ J}) \frac{Z^2}{n^2}$$
$$\bar{r} \approx (5.29 \times 10^{-11} \text{ m}) \frac{n^2}{Z}$$

- Holds **EXACTLY** for 1-electron atoms and ions:  
H, He<sup>+</sup>, Li<sup>2+</sup>, Be<sup>3+</sup>, ...  
Here Z is “regular” nuclear charge with Z=1, 2, 3, 4,

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*ionization energy (section problem (HW2 #11, S3))*

---

- ionization energy (**IE**): the energy required to remove an electron from an atom, ion, or molecule in the gas phase
- X (g) + IE → X<sup>+</sup>(g) + e<sup>-</sup> (absorbs energy IE:  
*endothermic, + sign for IE*)

- IE<sub>n</sub>** for state n is energy difference between state n and state n → ∞

$$(IE)_n = (E_\infty - E_n) = -E_n = +(2.18 \times 10^{-18} \text{ J}) \frac{Z^2}{n^2}$$

- similar to the work function Φ in the photoelectric effect, except IE refers to gas phase ionization where Φ refers to removal of electron from the solid

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*what happens when other electrons are present: effective nuclear charge (p 559)*

## Important Factors in Understanding Effective Nuclear Charge

- Energy dependence on  $n$  and  $Z_{\text{eff}}$

$$E_n \approx - (2.18 \times 10^{-18} \text{ J}) \frac{Z_{\text{eff}}^2}{n^2}$$

- $Z_{\text{eff}}$  and shielding (*attraction-repulsion*)

$$Z_{\text{eff}} = Z - \underbrace{\quad}_{\text{(effect of electron repulsions)}}$$

$$Z_{\text{eff}} = Z - \text{(shielding of other electrons)}$$

*1s electron 'feels' full  $Z=+2$  nuclear attraction*

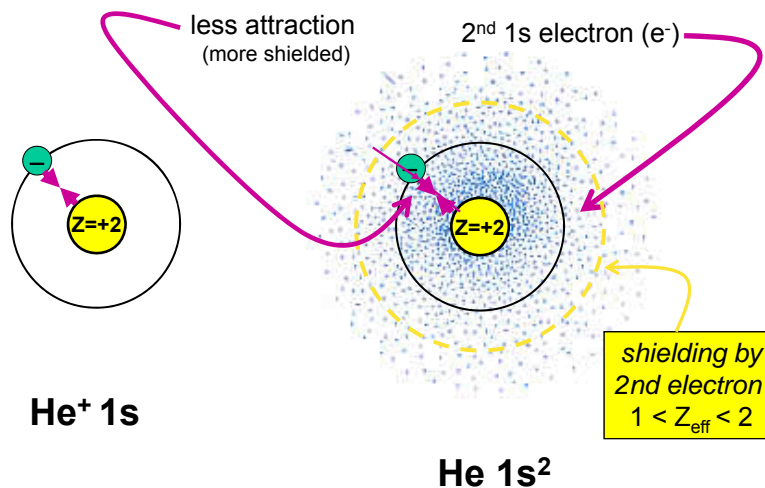
- electrons in same shell:



*the two 1s electrons shield one another from the  $Z=+2$  nuclear pull*

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*He<sup>+</sup> vs He (what positive charge does a 1s electron 'see'?)*



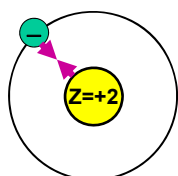
more shielding  $\rightarrow$  lower  $Z_{\text{eff}}$   $\rightarrow$  larger average radius

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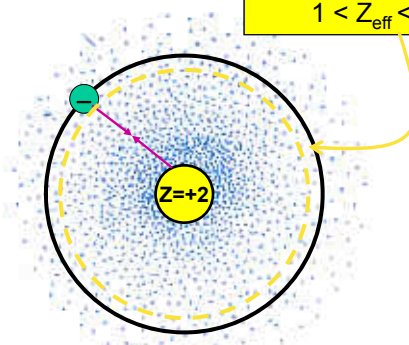
*He<sup>+</sup> vs He (what **net** positive charge does a 1s electron 'see'?)*

no shielding  $Z_{\text{eff}} = 2$



**He<sup>+</sup> 1s**

shielding of electron  
by 2nd 1s electron  
 $1 < Z_{\text{eff}} < 2$



**He 1s<sup>2</sup>**

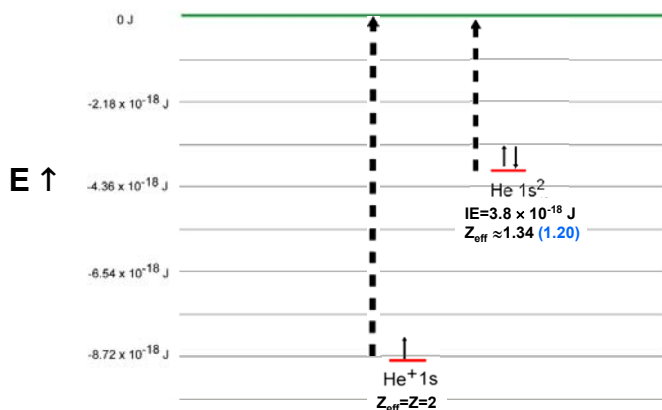
lower  $Z_{\text{eff}} \rightarrow$  larger average radius  
lower  $Z_{\text{eff}} \rightarrow$  lower attractive forces

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*Energy of He 1s<sup>2</sup> vs He<sup>+</sup> 1s (HO fig 12.2)*

**$Z_{\text{eff}}$  and Ionization Energies**

$Z_{\text{eff}}(\text{He}^+ 1s) > Z_{\text{eff}}(\text{He } 1s^2)$

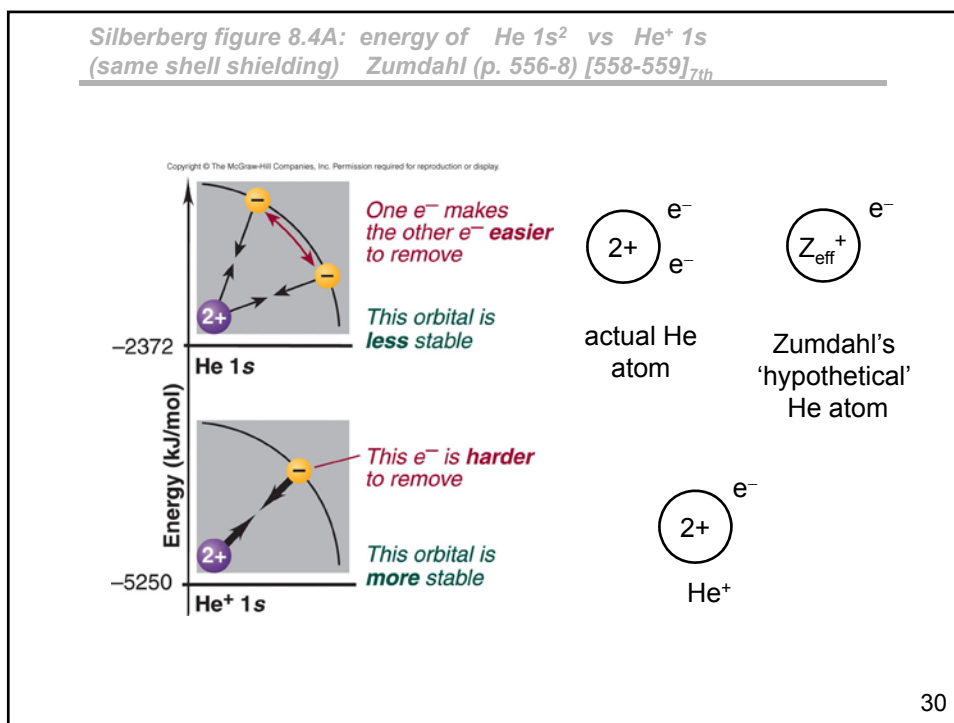
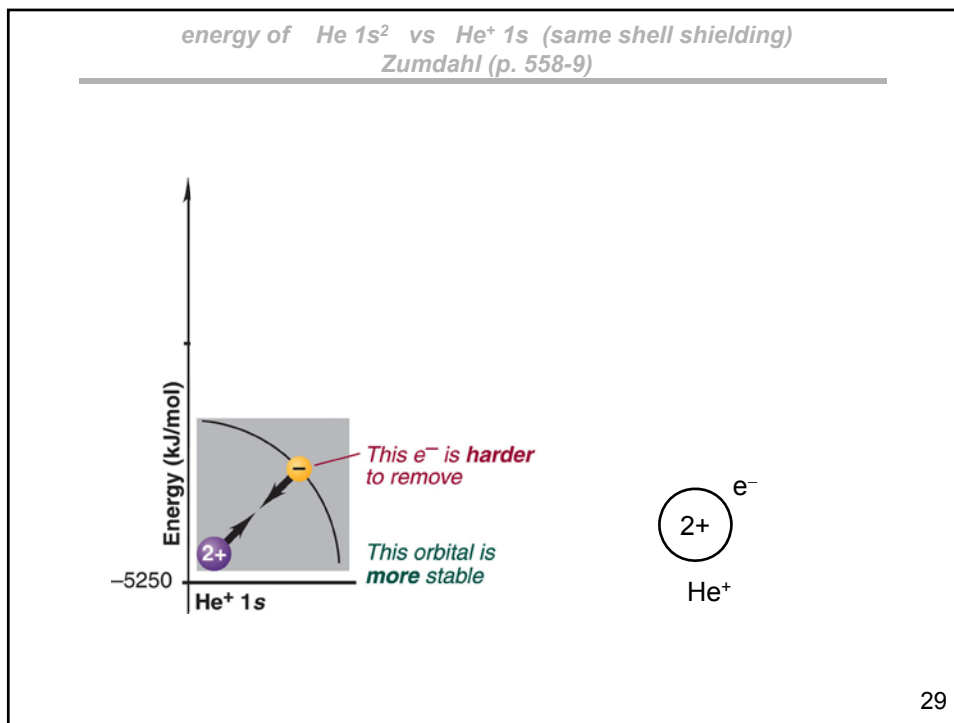


$$IE \approx (2.18 \times 10^{-18} \text{ J}) \frac{Z_{\text{eff}}^2}{n^2} \quad Z_{\text{eff}} \approx \left[ \frac{n^2 IE}{2.18 \times 10^{-18} \text{ J}} \right]^{1/2}$$

*this is approximate way to calculate  $Z_{\text{eff}}$ ;  
other techniques give slightly different numbers*

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Fall 2016

$Z_{\text{eff}}$ : effective nuclear charge

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what about shielding if the electrons are in different shells



shielding the 2s electron

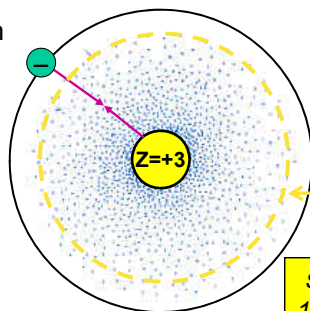
would you expect electrons in an inner shell to provide less or greater shielding effects than electrons in the same shell ?

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$Z_{\text{eff}}$  for 2s electron in  $\text{Li } 1s^2 2s$

---

2s electron



$\text{Li } 1s^2 2s$

$$\text{IE}_{\text{experimental}} = 0.86 \times 10^{-18} \text{ J}$$

$$(Z_{\text{eff}})_{2s} \approx \left[ \frac{n^2 \text{IE}_{2s}}{2.18 \times 10^{-18} \text{ J}} \right]^{1/2} = 1.26$$

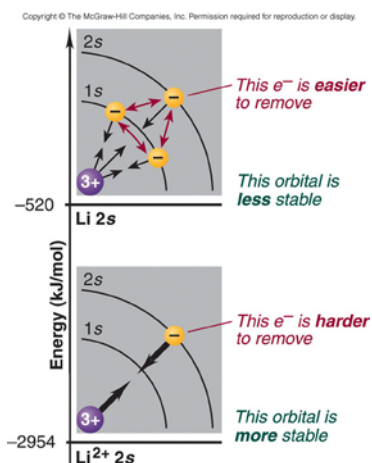
shielding by  
 $1s^2$  electrons  
 $Z_{\text{eff}} \approx 1.26$

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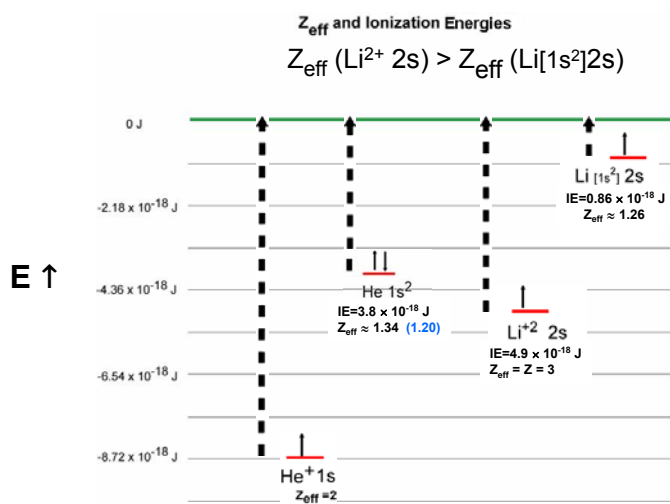
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*figure 8.4 B (Silb) shielding by inner shell electrons*



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*Energy of  $Li^{2+} 2s$  vs  $Li [1s^2] 2s$  (HO Fig. 12.3)*



$$Z_{\text{eff}} \approx \left[ \frac{n^2 \text{IE}}{2.18 \times 10^{-18} \text{J}} \right]^{1/2}$$

*this is approximate way to calculate  $Z_{\text{eff}}$ ; other techniques give slightly different numbers*

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*take home material from: Video03*

- Stern-Gerlach electron spin  $+\frac{1}{2}$  and  $-\frac{1}{2}$
- Pauli Exclusion Principle (PEP)
- effective nuclear charge:  $Z_{\text{eff}}$ 
  - $+Z_{\text{nuclear charge}} - \text{repulsion (shielding) by other electrons}$
  - shielding greater from electron in inner shell than electron in same shell [from electrons 'inside' or closer to nucleus]
  - $E_n \approx -\frac{m_e e^4}{8h^2 \epsilon_0^2} \frac{Z_{\text{eff}}^2}{n^2} = -(2.18 \times 10^{-18} \text{ J}) \frac{Z_{\text{eff}}^2}{n^2}$       $\bar{r} \approx (5.29 \times 10^{-11} \text{ m}) \frac{n^2}{Z_{\text{eff}}}$

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*in many-electron atoms  
how do the energies of the 2s and 2p orbitals compare?*

In 1-electron atoms (H-atom) and 1-electron ions ( $\text{He}^+$ ,  $\text{Li}^{2+}$  ...), a 2s and 2p orbital will have the .. **SAME** .. energy

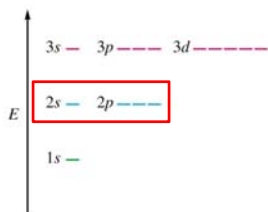


fig. 12.23 for 1-electron atoms and ions

**now  $Z_{\text{eff}}$**   
**and the effect of penetration of inner shell electron density by electrons in the same shell (e.g. 2s electron vs 2p electron)**

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*Z<sub>eff</sub> for 2s vs 2p: 2p and 2s have SAME energy in 1-electron ion*

---

'penetration' by 2s electron of 1s<sup>2</sup> shielding GIVES INCREASED Z<sub>eff</sub>

**Li 1s<sup>2</sup>2s**  
**Z<sub>eff</sub> ≈ 1.26**

*2s*  
radial probability

actual 2s electron density  
(one radial node;  
one inner maximum in radial probability)

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*Z<sub>eff</sub> for 2s vs 2p*

---

no (less) 'penetration' of 1s<sup>2</sup> shielding by 2p electron GIVES relatively smaller Z<sub>eff</sub>

**Li 1s<sup>2</sup>2p**

Z<sub>eff</sub> for 2s > Z<sub>eff</sub> for 2p  
E<sub>2s</sub> < E<sub>2p</sub>

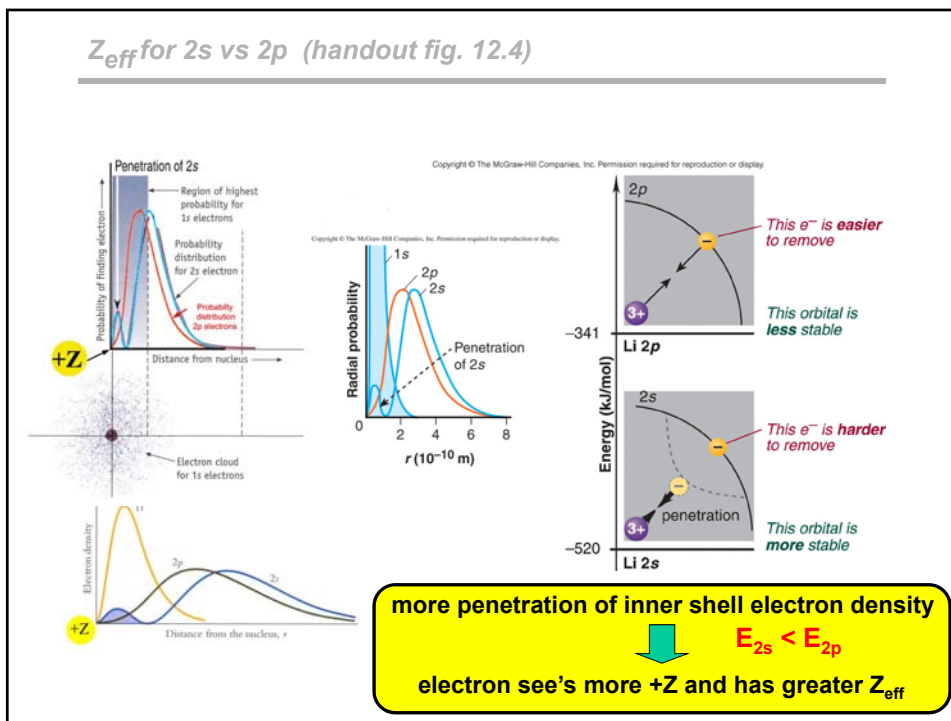
Radial distribution function

actual 2p electron density  
(no radial nodes;  
no 'inner maxima' in radial probability)

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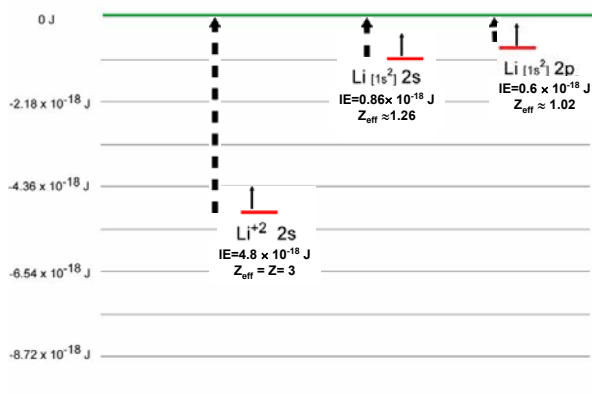
## $Z_{\text{eff}}$ for 2s vs 2p (handout fig. 12.4)



## Energy of Li $[1s^2] 2s$ vs Li $[1s^2] 2p$ (HO Fig. 12.5): penetration

$Z_{\text{eff}}$  and Ionization Energies

$$Z_{\text{eff}}(\text{Li}[1s^2] 2s) > Z_{\text{eff}}(\text{Li}[1s^2] 2p)$$



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*how do the energies of the 2s and 2p orbitals compare in many-electron atoms?*

---

- Configurations and valence-level orbital diagrams →
- Hund's rule →
- 2<sup>nd</sup> row aufbau [fig 8.8 \(Sil\)](#) →

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*3s, 3p, 3d, 4s orbital energy ordering*

---

- Increasing  $Z_{\text{eff}}$  due to increasing penetration effects ([figure HO 12Z.6](#)); →

$$(Z_{\text{eff}})_{3s} > (Z_{\text{eff}})_{3p} > (Z_{\text{eff}})_{3d}$$

$$(E)_{3s} < (E)_{3p} < (E)_{3d}$$

- 4s vs 3d ( $Z_{\text{eff}}$  vs n) →
- Orbital energy ordering [fig 8.6 \(Silb\)](#)  
[\(figure 8.13, Silb\)](#) →

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## Fall 2016

### configurations

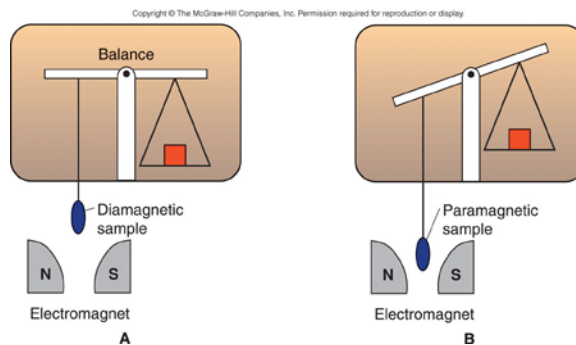
- **Hund's rule**
  - Energy ordering
  - Unambiguous [closed shell, 1e, (n-1)e's  
e.g. p<sup>1</sup>, p<sup>5</sup>, d<sup>1</sup>, d<sup>9</sup>] →
  - Ambiguous [e.g. p<sup>2</sup>, p<sup>3</sup>, p<sup>4</sup>, d<sup>2</sup>→d<sup>8</sup>] →
- **Examples ([periodic table](#))** →
  - ground state
  - excited state
  - not allowed configuration
  - transition metal cations
  - "exceptions" →

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### unpaired electrons and magnetic properties (Gouy balance)

**Diamagnetic**  
• pushed out of magnet  
• no unpaired electrons

**Paramagnetic**  
• pulled into magnet  
• unpaired electrons



Gouy Balance

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*the Periodic Table*

**Periodic Table**

**B**  
 $1s^2 2s^2 2p$

3p  
3s  
2p  
2s  
1s

Given **PEP** and ordering of orbitals, we can build up the periodic table element by element, and deduce much about the chemical nature of the elements as they interact to form molecules.

senses  
surreal  
dissip



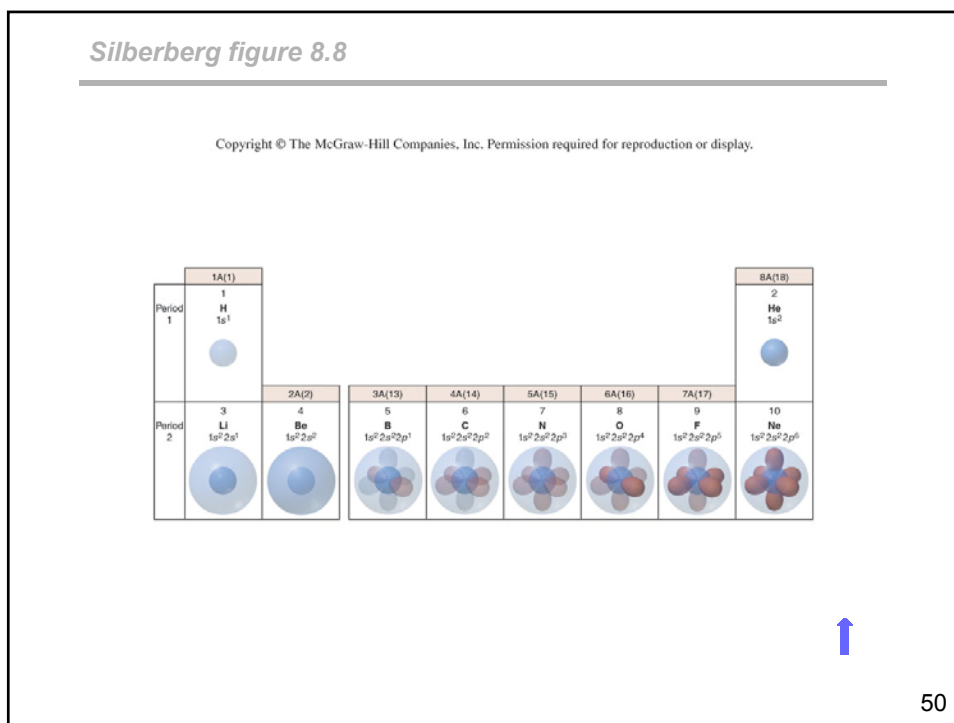
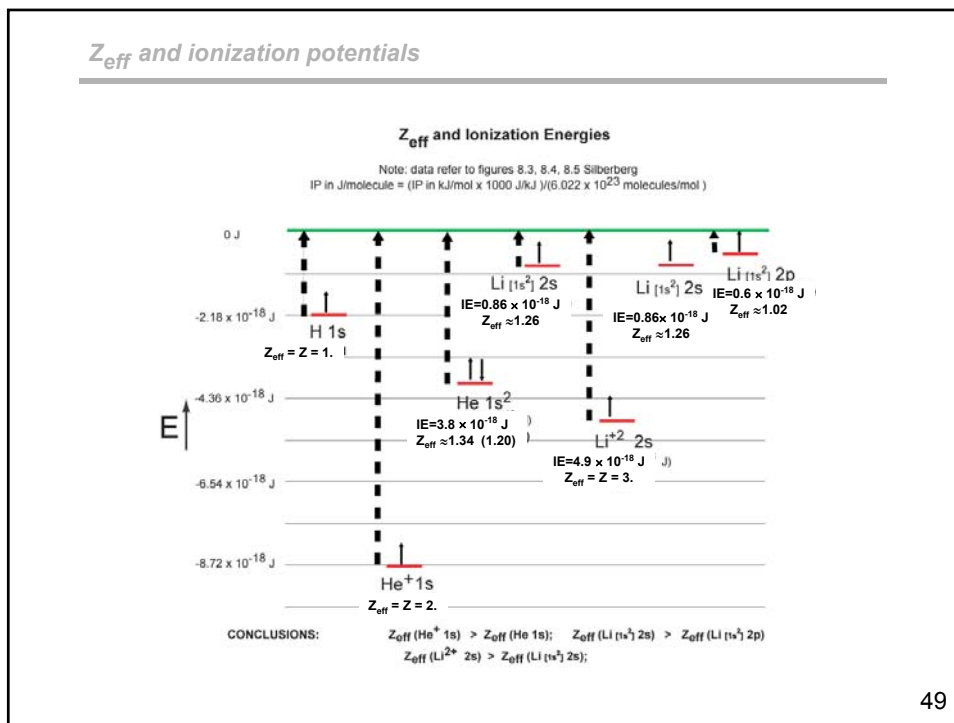
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end of material sessions 5-6

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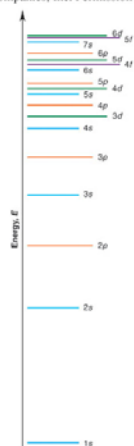
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# Chemistry 1B-02 Session 5-6 Fall 2016

Silberberg figure 8.6

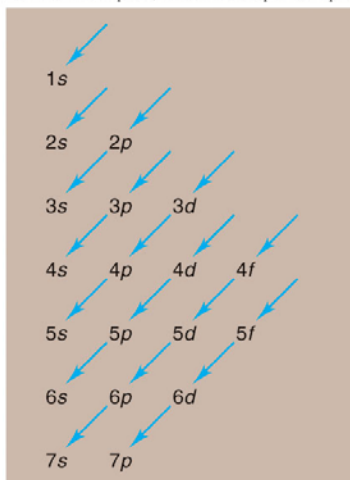
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Silberberg figure 8.13

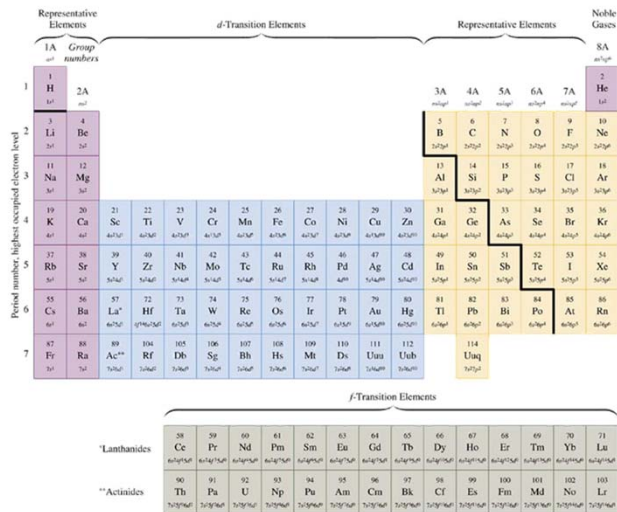
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Zumdahl figure 12.29

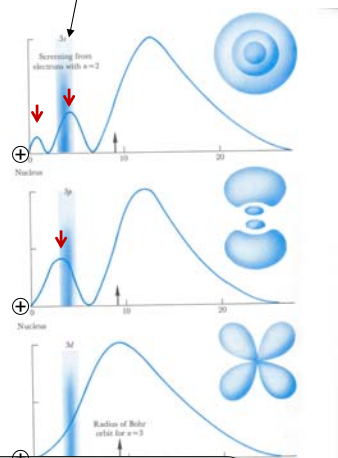


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Figure HO 8.6: penetration of 3s vs 3p vs 3d; **radial nodes =  $n-l-1$**

screening by  $n=2$  electrons



**3s:** 2 radial nodes  
2 "inner electron density maxima"

**3p:** 1 radial node  
1 "inner maxima"

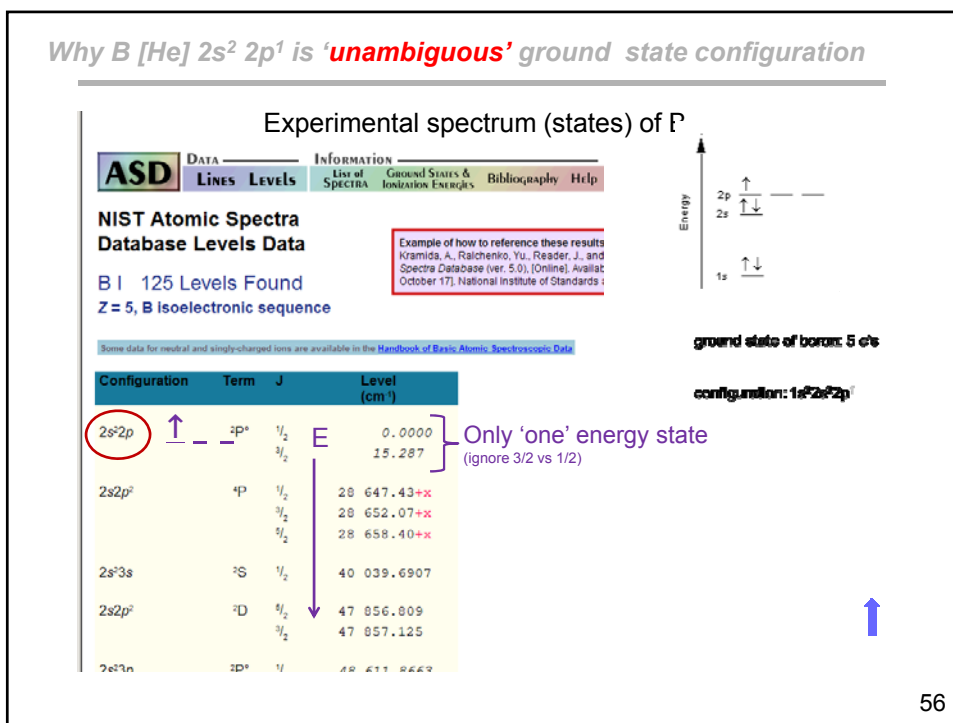
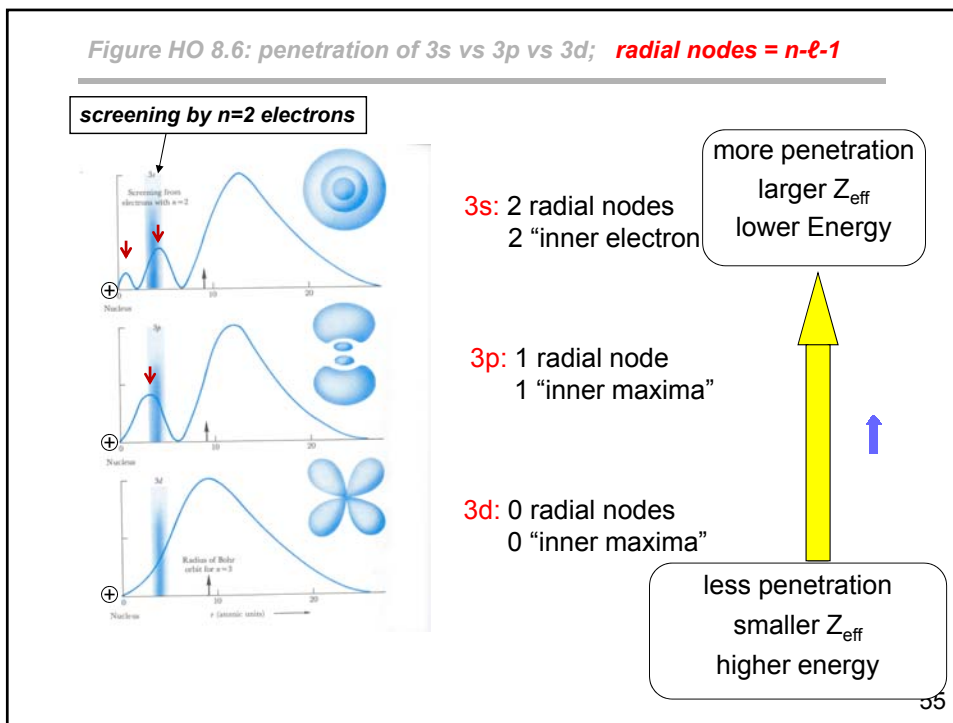
**3d:** 0 radial nodes  
0 "inner maxima"

less penetration  
smaller  $Z_{\text{eff}}$   
higher energy

more penetration  
larger  $Z_{\text{eff}}$   
lower Energy

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# Chemistry 1B-02 Session 5-6 Fall 2016

## Why B [He] 2s<sup>2</sup> 2p<sup>1</sup> is 'unambiguous' ground state configuration

Experimental spectrum (states) of B

**ASD** DATA INFORMATION  
 LINES LEVELS LIST OF SPECTRA GROUND STATES & IONIZATION ENERGIES BIBLIOGRAPHY HELP

**NIST Atomic Spectra Database Levels Data**

B I 125 Levels Found  
 Z = 5, B Isoelectronic sequence

Some data for neutral and singly-charged ions are available in the [Handbook of Basic Atomic Spectroscopic Data](#).

Configuration	Term	J	Level (cm <sup>-1</sup> )
$2s^2 2p$	↑ - - <sup>2</sup> P°	1/2	0.0000
		3/2	15.287
$2s^2 2p^2$	↑ - ↑ <sup>4</sup> P	1/2	20 647.43+*
		3/2	20 652.07+*
		5/2	28 658.40+*
$2s^2 3s$	<sup>3</sup> S	1/2	40 039.6907
$2s^2 2p^2$	↑ ↓ <sup>3</sup> D	3/2	47 056.009
		5/2	47 057.125
$2s^2 3p$	<sup>3</sup> P°	1/2	48 611.8669

} Only 'one' energy state (ignore 3/2 vs 1/2)  
} Excited states have excited [He] 2s<sup>1</sup> 2p<sup>2</sup> configuration

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## Why C [He] 2s<sup>2</sup> 2p<sup>2</sup> is 'ambiguous' ground state configuration

Experimental spectrum (states) of C

**ASD** DATA INFORMATION  
 LINES LEVELS LIST OF SPECTRA GROUND STATES & IONIZATION ENERGIES BIBLIOGR

**NIST Atomic Spectra Database Levels Data**

C I 282 Levels Found  
 Z = 6, C isoelectronic sequence

Some data for neutral and singly-charged ions are available in the [Handbook of Basic Atomic Spectroscopic Data](#).

Configuration	Term	J	Level (cm <sup>-1</sup> )
$2s^2 2p^2$	↑ ↑ - <sup>3</sup> P	0	0.00
		1	16.40
		2	43.40
$2s^2 2p^2$	↑ ↓ - <sup>1</sup> D	2	10 192.63
		3	10 200.00
$2s^2 2p^2$	↑ ↓ ↑ <sup>1</sup> S	0	21 648.01
		1	21 655.00
$2s^2 2p^3$	<sup>4</sup> S°	2	33 735.20
$2s^2 2p^3 s$	<sup>3</sup> P°	0	60 333.43
		1	60 352.63
		2	60 393.14

} Ground energy state (ignore 0 vs 1 vs 2)  
} Excited states with same [He] 2s<sup>2</sup> 2p<sup>2</sup> configuration

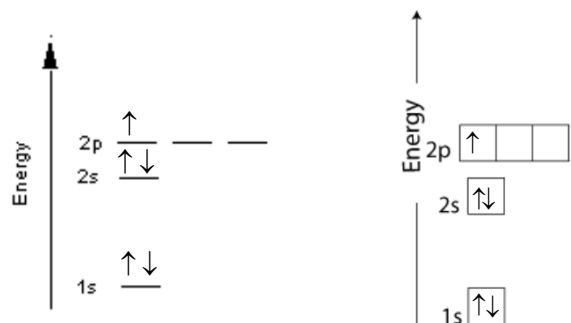
**lowest energy: ground state**

**higher energy: excited state**

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## *n=1 and n=2 energy diagram for multi-electron atoms*



ground state of boron: 5 e<sup>-</sup>s

configuration:  $1s^2 2s^2 2p^1$  or  $[\text{He}] 2s^2 2p^1$



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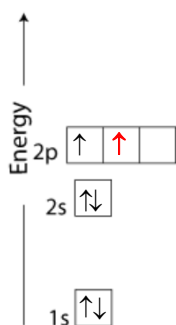
## *Hund's Rule*



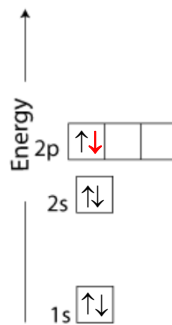
**Friedrich Hund**

for a given configuration, the lowest energy state will have the maximum number of electrons with parallel spins

carbon 6e<sup>-</sup>s:  $1s^2 2s^2 2p^2$  or  $[\text{He}] 2s^2 2p^2$



*lowest energy: ground state*



*higher energy: excited state*



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