Chemistry 1B
Fall 2016

sessions 5-6

Chapter 12

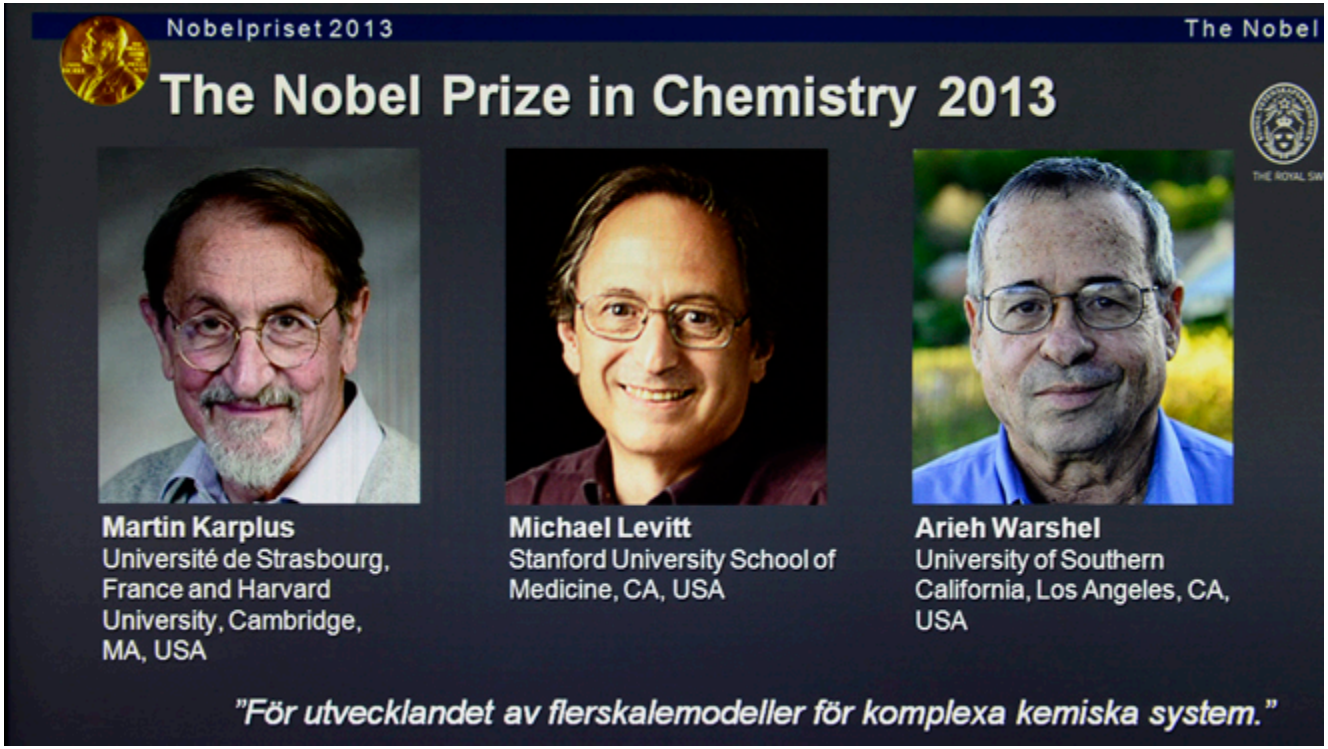
pp. 557-569

*(569-571)

What can you do to become famous?

[and win a cool $1.2 million]?]

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 Newtownian 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."

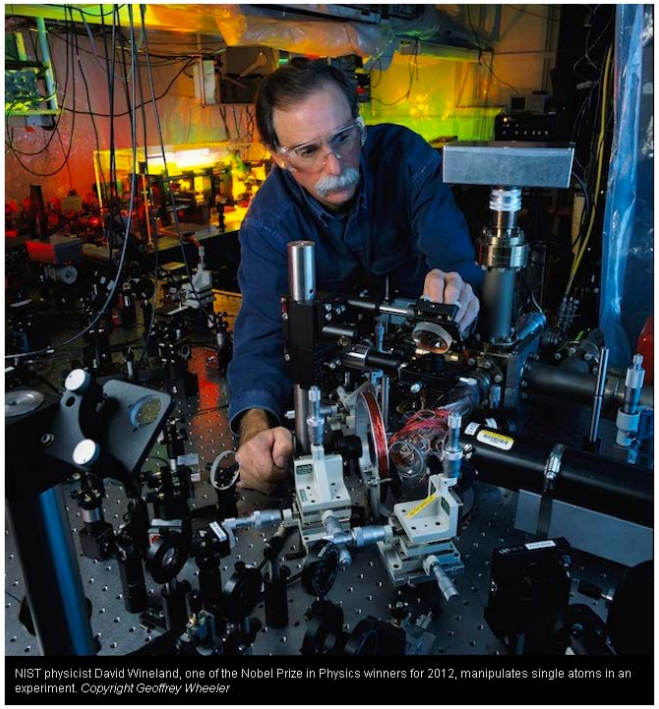
Molecular Mechanics at UCSC

Prof Ilan Benjamin
Prof. Yuan Ping

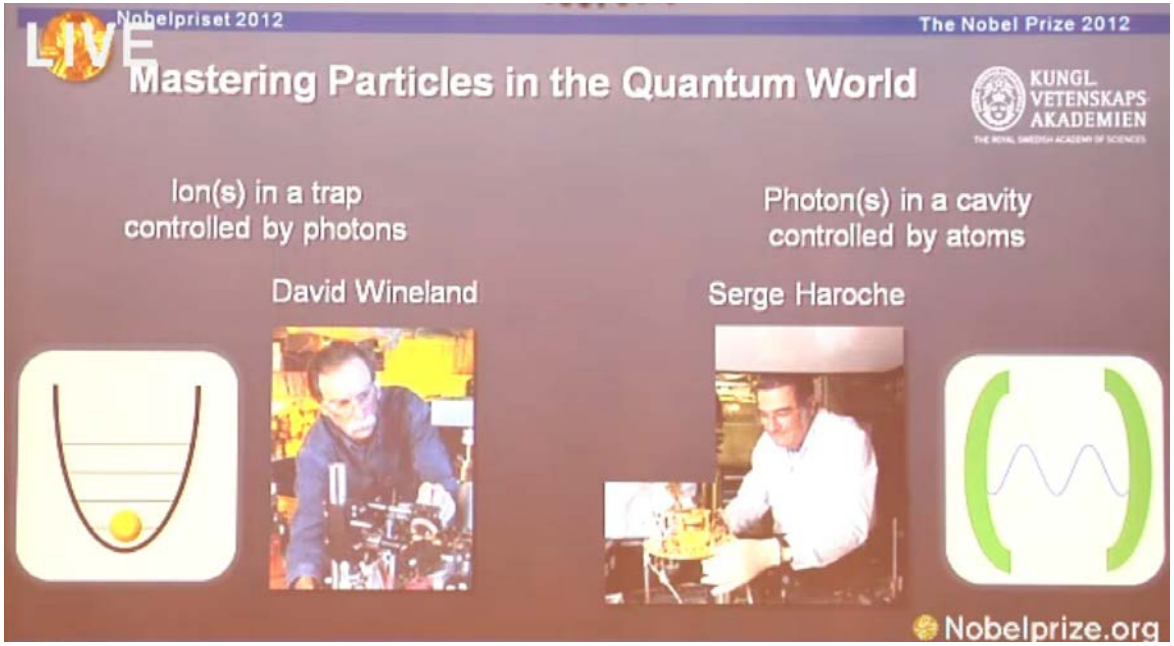
2012 Nobel in QUANTUM physics

Nobel Awarded to Scientists Who Learned to Control Quantum Systems

By ScienceNow October 9, 2012 | 2:41 pm | Categories: Physics



NIST physicist David Wineland, one of the Nobel Prize in Physics winners for 2012, manipulates single atoms in an experiment. *Copyright Geoffrey Wheeler*



- electron spin, "the 4th quantum number and the Pauli exclusion principle

- effective nuclear charge, Z_{eff}
  the "net" attraction for an electron in a many-electron atom

- knowledge of the principal quantum number (n) and Z_{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

- **how does increased atomic number (Z) and the presence of other electrons affect orbital energies?**

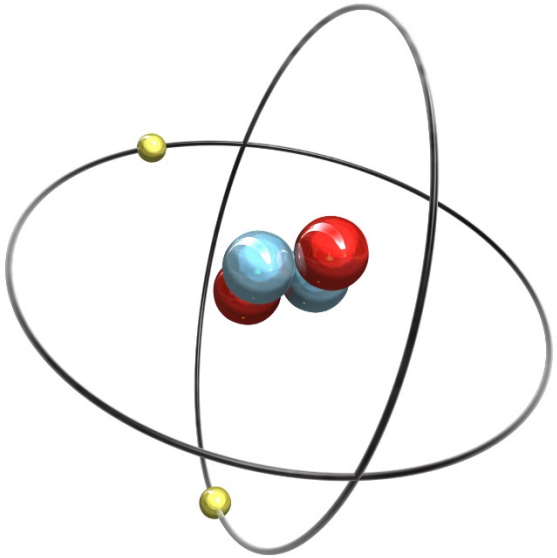
- **how does one "fill up" the available orbitals in many-electron atoms**

Chemistry 1B -AL

multi-electron atoms

Electron Spin

Electronic Configurations

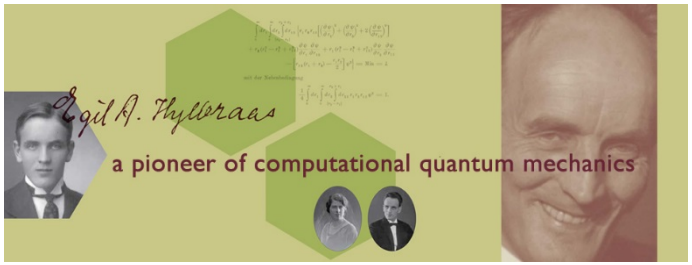


☒

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

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** ✓



Quantal/Experimental

Year	Method		$-E$
1924	experimental, Lyman (1924)	*exp*	2.9035
1998	exp., Bergeson *et al.* (1998)		2.903 693 775
1929	var., 38 param., Hylleraas (1929)		2.9037
1993	relativ. Drake (1993)	*calc*	2.903 700 023

but solutions are very complex .

$$\Psi(s,u,t) = \mathcal{N}e^{-(1/2)s} \sum_{l,m,n} C_{l,m,n} s^{l-m} u^{m-n} t^{n}. \quad (2)$$

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.

this video

- electron spin, "the 4th quantum number and the Pauli exclusion principle

- effective nuclear charge, Z_{eff}
  the "net" attraction for an electron in a many-electron atom

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in next class

- knowledge of the principal quantum number (n) and Z_{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

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

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)*

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?

HW#3: 23

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.upscale.utoronto.ca/GeneralInterest/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 $E_n = -\frac{m_e e^4}{8h^2\varepsilon_0^2}\frac{Z^2}{n^2} = -(2.18\times10^{-18}\ J)\frac{Z^2}{n^2}$. 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 (σ=shielding of nuclear charge) of the _____.

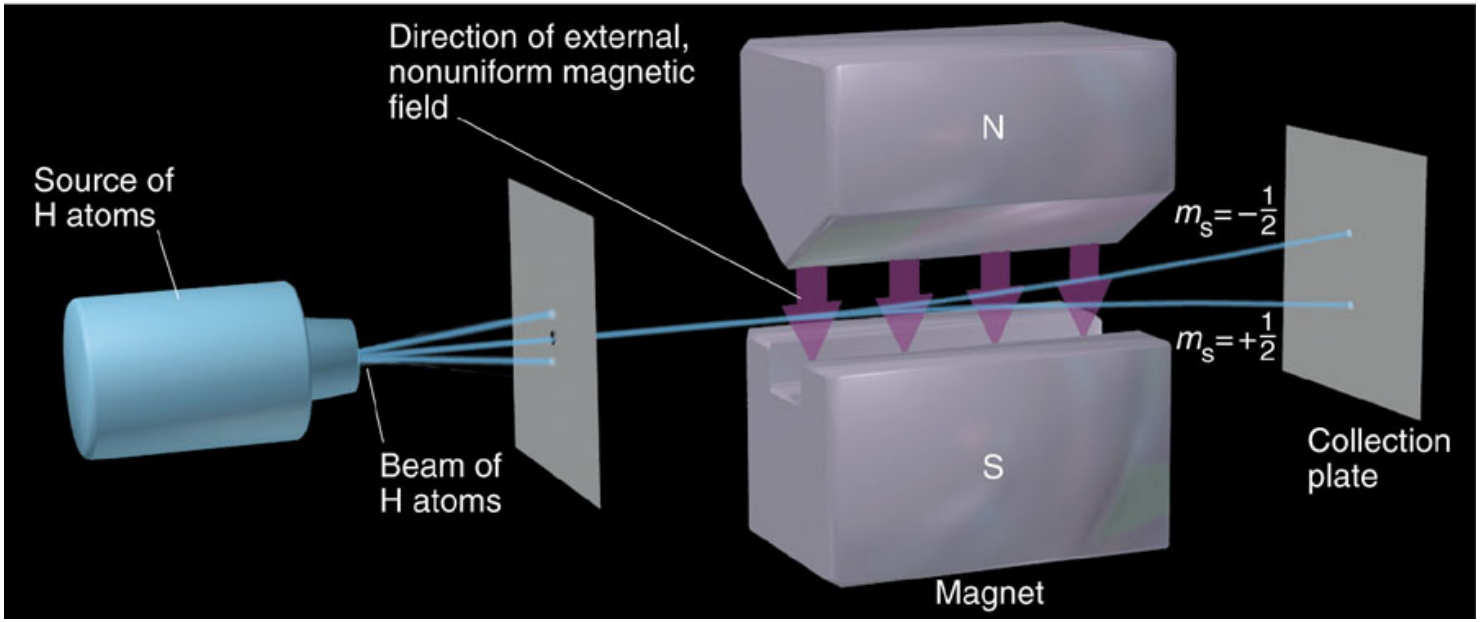
2. In a helium atom Z_{eff} for an electron will be _____ the +2 charge on the nucleus.

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

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

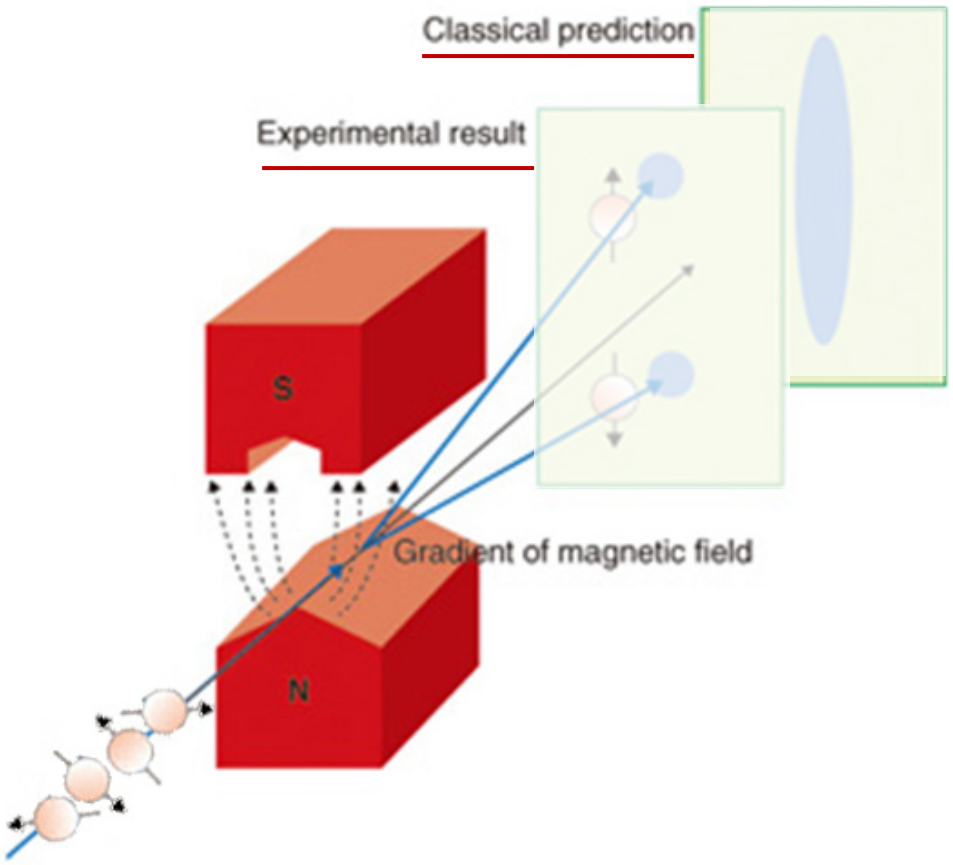
3. In the ground state of the Li atom has configuration _____. The electron in the 2s orbital has the higher (less negative) energy both because

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



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

the 4th quantum number: spin

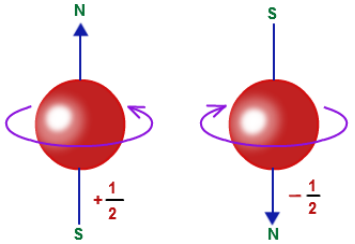


https://www.ntt-review.jp/archive/ntttechnical.php?contents=ntr201209fa4_s.html

the electron has two possible spin states with spin quantum numbers

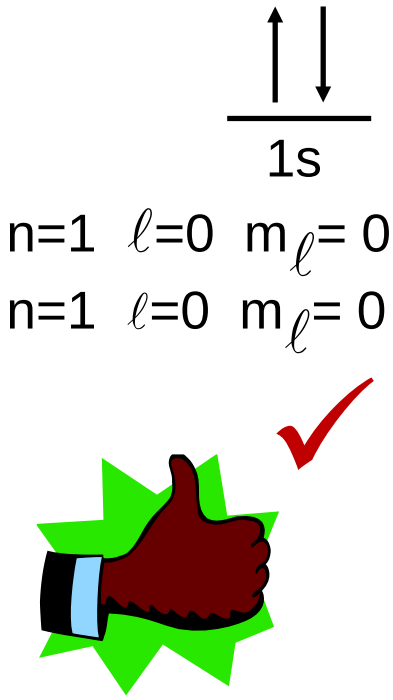
m_s=+½ or m_s=–½

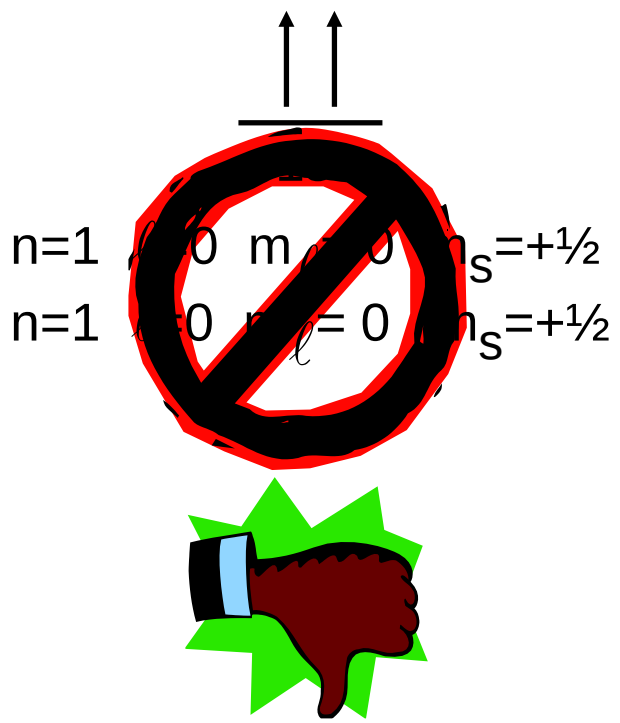
spin up and spin down



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

no two electrons can have the same four quantum numbers:





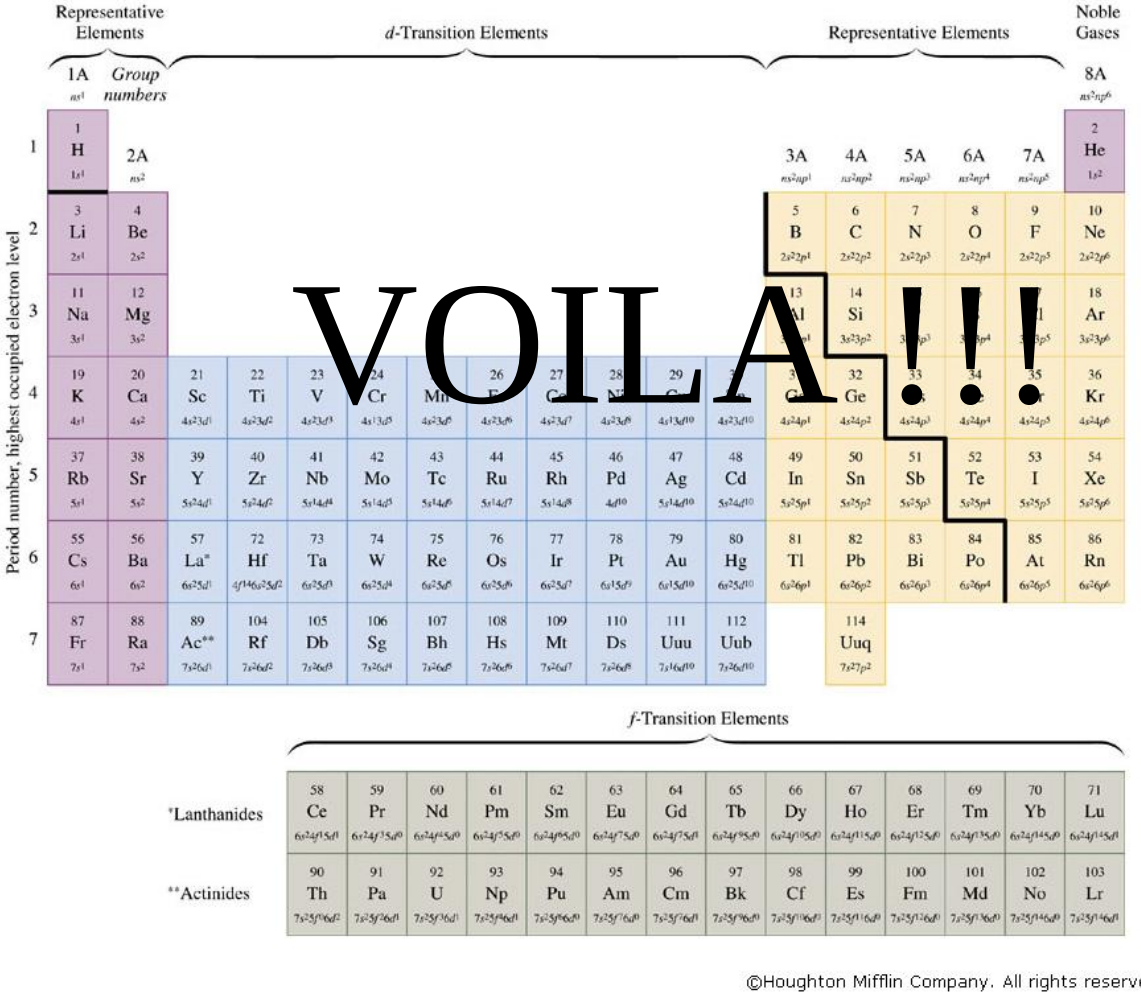
He, Li, Be, B, C, N, O, F, Ne …….

- greater nuclear charge (Z) than hydrogen (Z=1)

- more electrons than hydrogen (one-electron)

- 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.

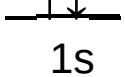
- This description allows us to understand the **energies** of electrons in atoms and ions, the **relative sizes** of atoms and ions, and the **chemical reactivity** and other properties of various elements.

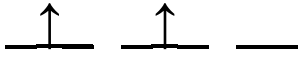


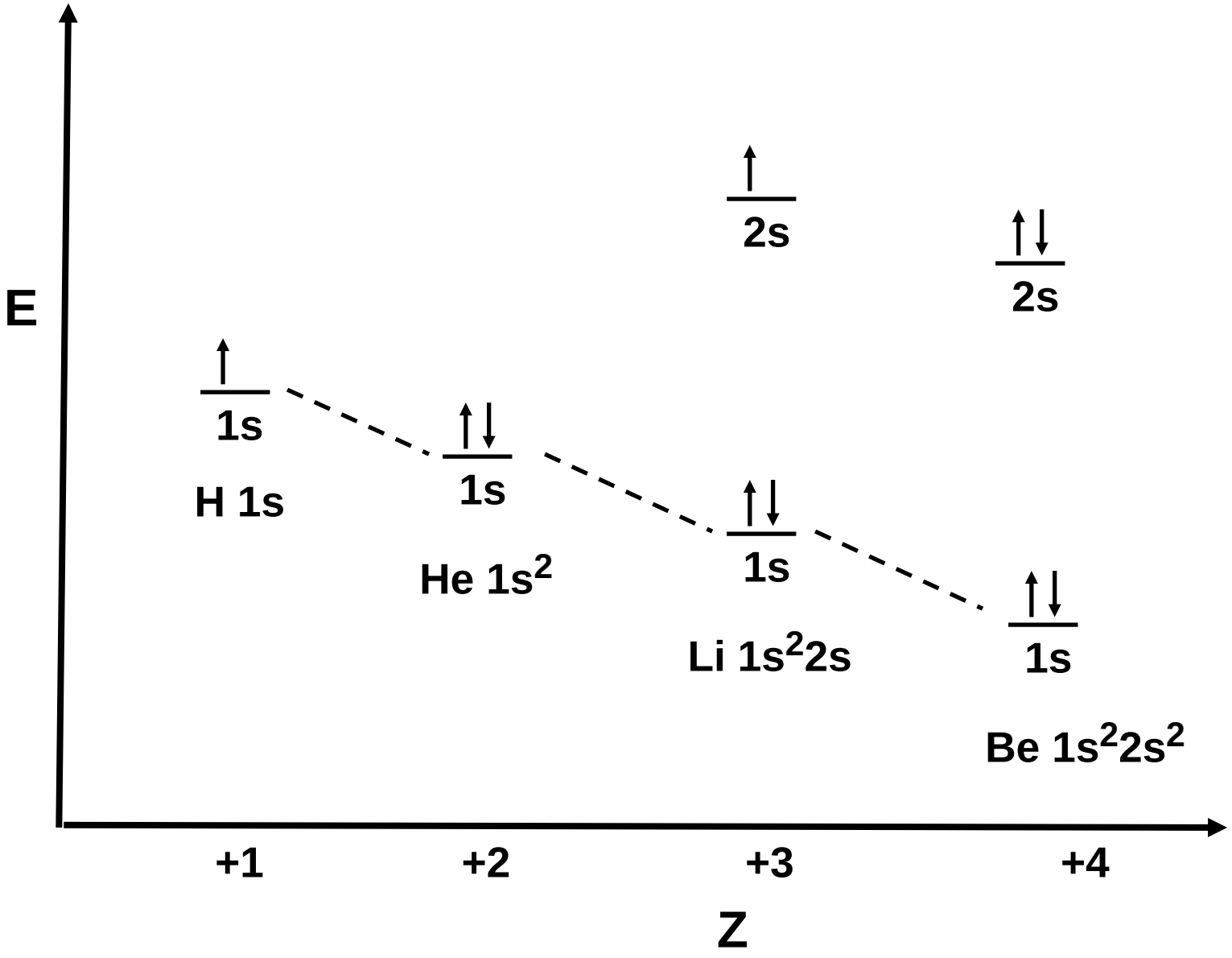
VOILA!!!

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 

He: $1s^2$ or 

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


E
2s
2s
1s
1s
H 1s
1s
He 1s2
1s
Li 1s22s
Be 1s22s2
+1
+2
+3
+4
Z

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

n and Z

$$E_n = -\frac{m_e e^4}{8h^2 \varepsilon_0^{\,2}} \frac{Z^2}{n^2} = -\left(2.18 \times 10^{-18}\ J\right) \frac{Z^2}{n^2}$$

$$\bar{r} \approx (5.29 \times 10^{-11} m)\ \frac{n^2}{Z}$$

- Holds **EXACTLY** for 1-electon atoms and ions:
  H, He^{+}, Li^{2+},Be^{3+}, ...
  Here Z is "regular" nuclear charge with Z=1, 2, 3, 4,

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

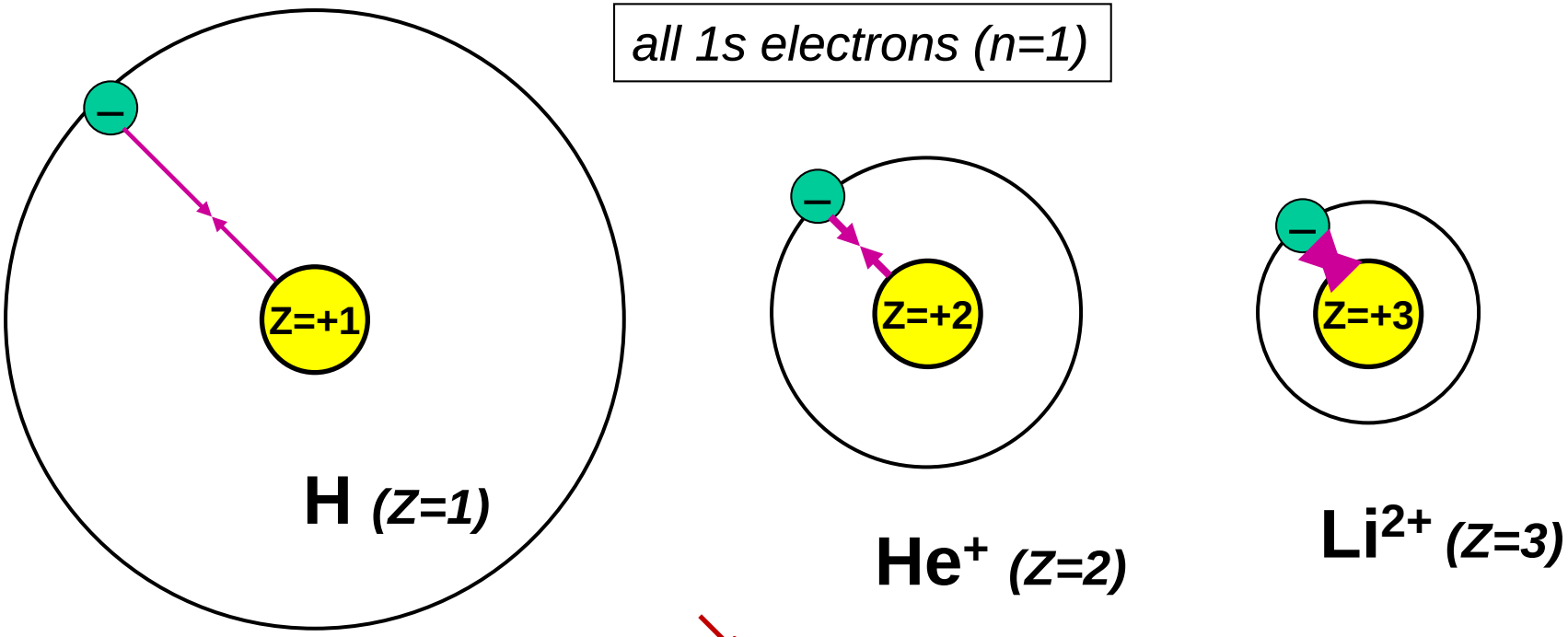
- ionization energy **(IE)** : the energy required to remove an electron from an atom, ion, or molecule in the gas phase

- X (g) + IE → $X^+(g) + e^-$ (absorbs energy IE: *endothermic,* **+** *sign for IE*)

- **IE_n** for state n is energy difference between state **n** and state **n**→∞

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

- 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



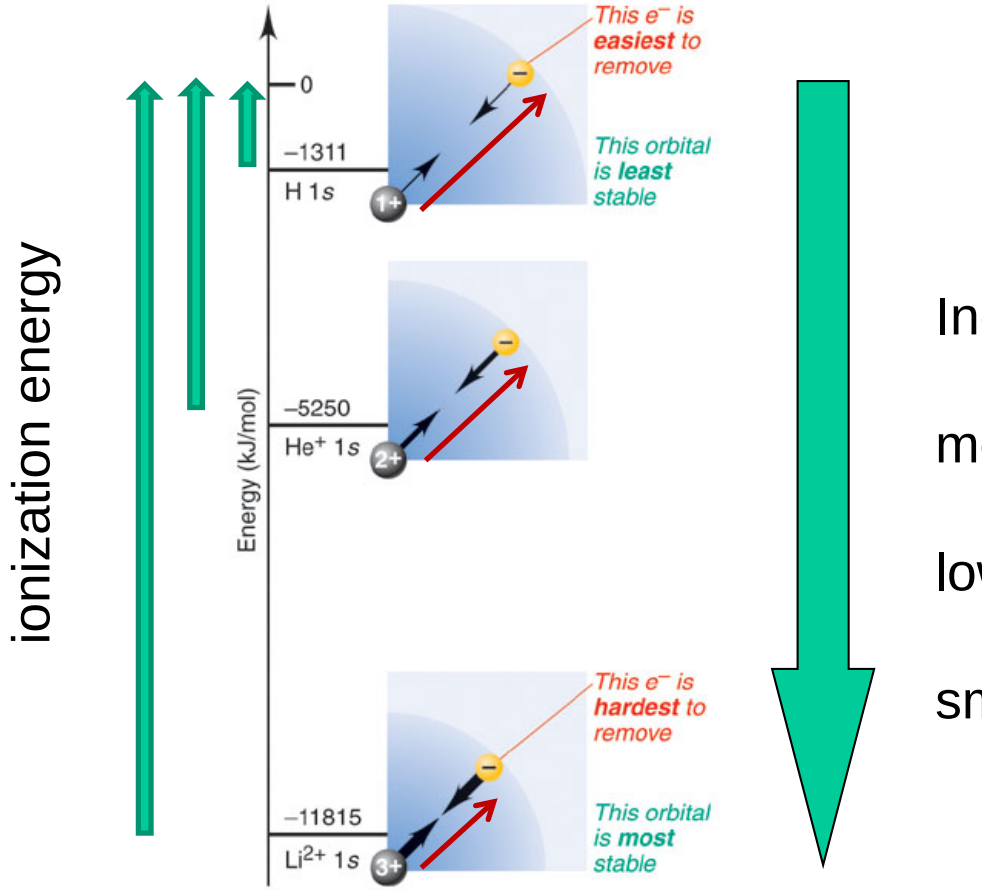
$$E_n = -\frac{m_e e^4}{8h^2 \varepsilon_0{}^2}\frac{Z^2}{n^2} = -\left(2.18\times10^{-18}\ J\right)\frac{Z^2}{n^2}$$

"Bohr" radius in gas phase

$$\bar{r}_{avg} \approx (0.529\times10^{-10}\text{m})\ \frac{n^2}{Z}$$

increase Z
- more attraction
- lower *(more negative)* energy (*ie higher IE*)
- smaller r_{avg}

Silberberg Figure 8.3
Energy of H 1s vs He^+ 1s vs Li^{2+} 1s (still 1 electron)



Increase Z

more attraction

lower energy (ie higher IE)

smaller average radius

Important Factoids in Understanding Effective Nuclear Charge

- **Energy dependence on n and Z_{eff}**

$$E_n \approx -(2.18\times10^{-18}\ \text{J})\frac{Z_{eff}^{\ 2}}{n^2}$$

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

Z_{eff} = Z – (effect of electron repulsions)

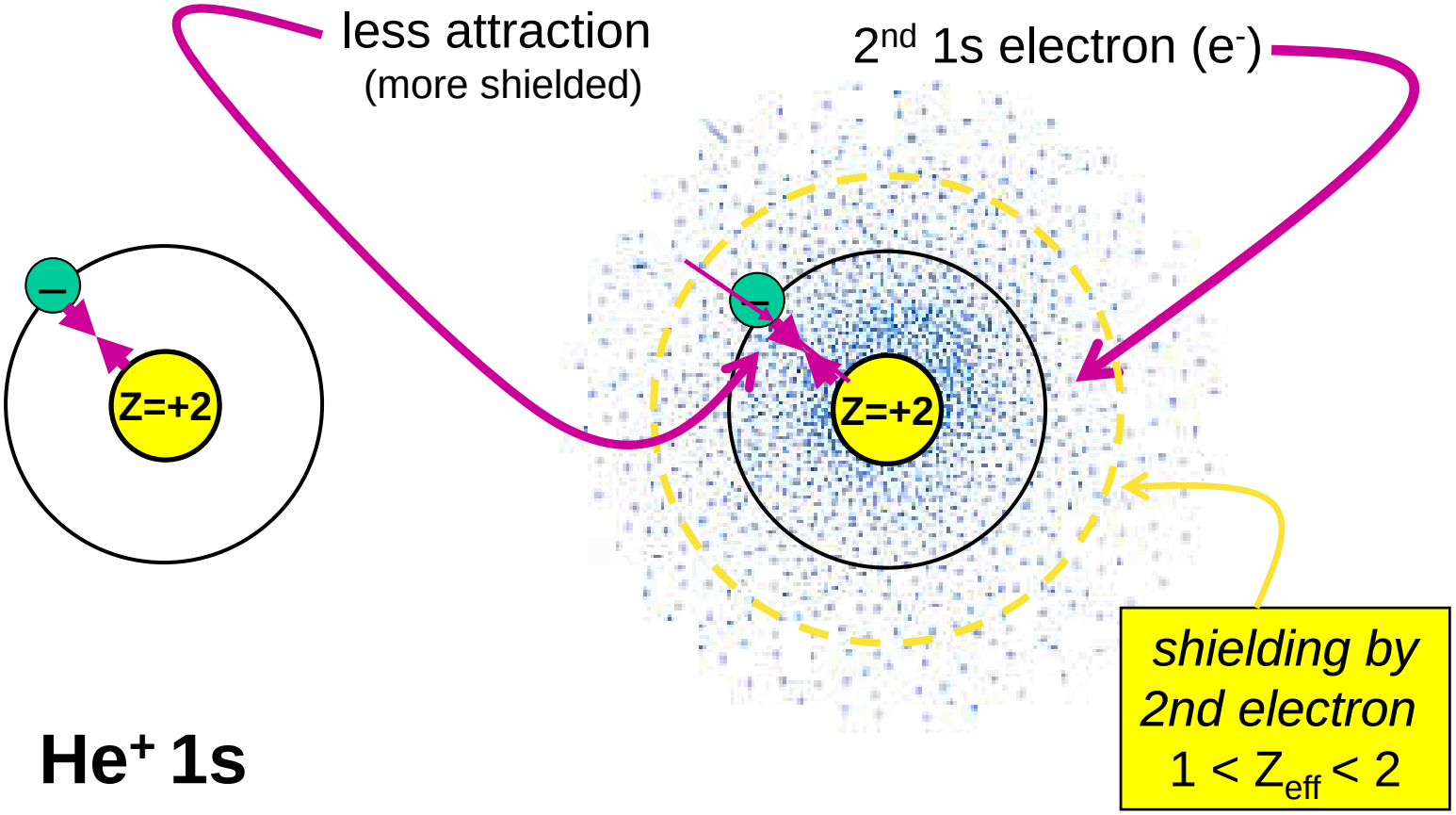
Z_{eff} = Z – (shielding of other electrons)

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

- **electrons in same shell:**

He^+ $1s$ vs He $1s^2$

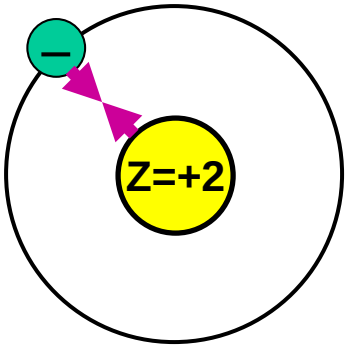
the two 1s electrons shield one another from the Z=+2 nuclear pull



more shielding → lower Z_{eff} → larger average radius

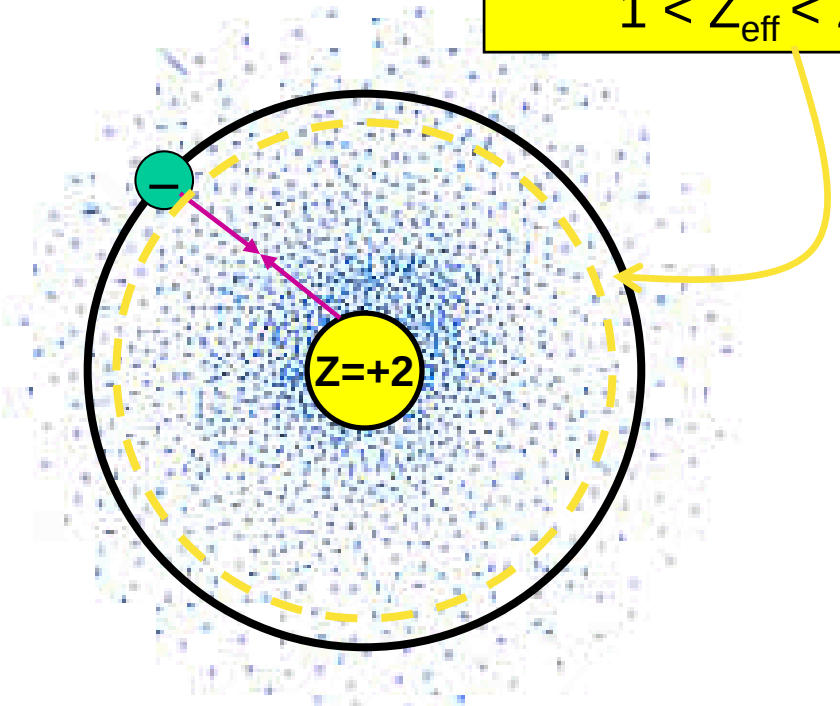
He^+ vs He (what **net** positive charge does a 1s electron 'see' ?)

no shielding $Z_{eff} = 2$



He^+ 1s

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

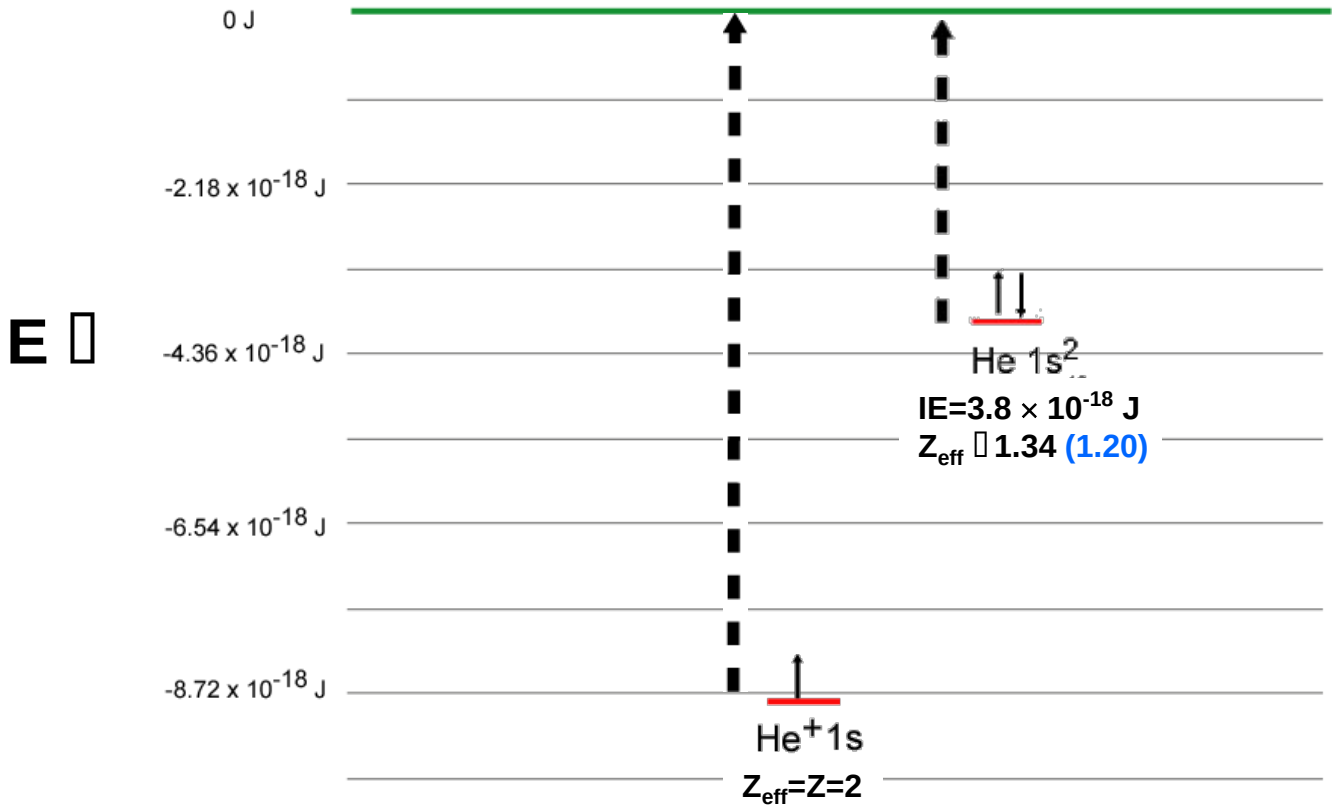


He $1s^2$

lower Z_{eff} → larger average radius
lower Z_{eff} → lower attractive forces

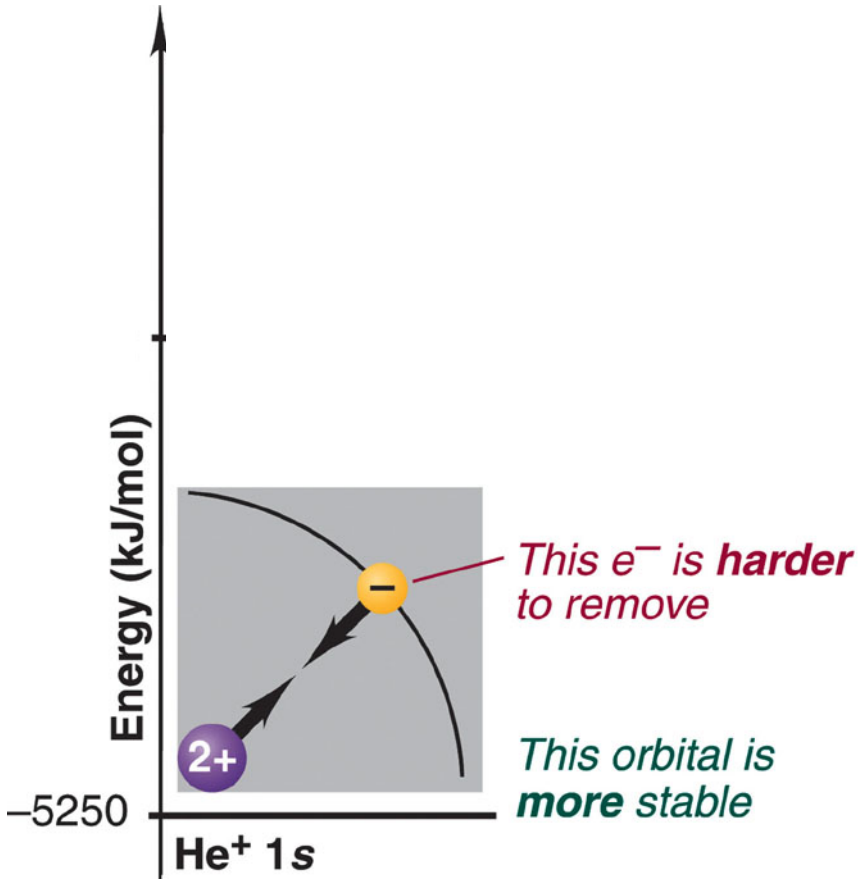
Z_{eff} and Ionization Energies

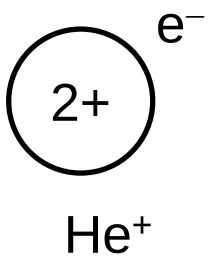
Z_{eff} (He^+ 1s) > Z_{eff} (He $1s^2$)



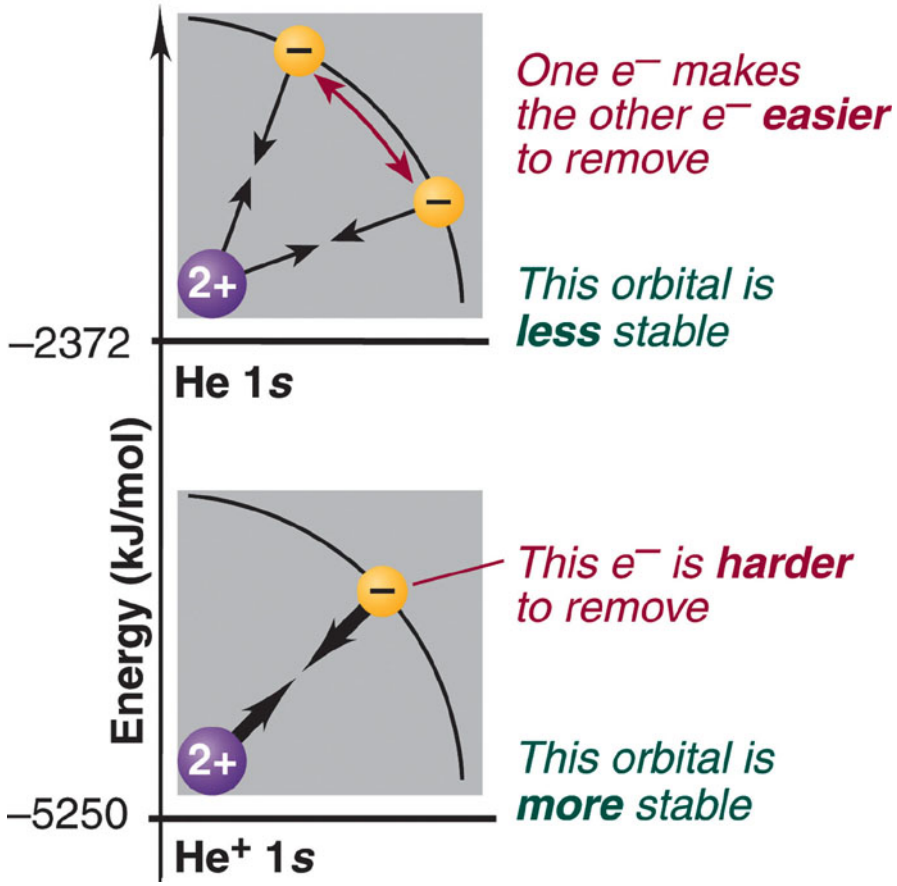
$$IE \approx (2.18\times10^{-18}\ J)\frac{Z_{eff}^{\ 2}}{n^2} \qquad Z_{eff} \approx \left[\frac{n^2\ IE}{2.18\times10^{-18}J}\right]^{1/2}$$

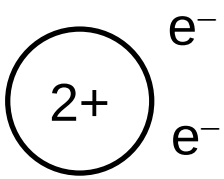
this is approximate way to calculate Z_{eff} ; other techniques give slightly different numbers


Energy (kJ/mol)
–5250
2+
He+ 1s
This e– is harder to remove
This orbital is more stable

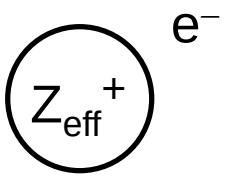

e–
2+
He+

Silberberg figure 8.4A: energy of He $1s^2$ vs He^+ 1s (same shell shielding) Zumdahl (p. 556-8) [558-559]$_{7th}$

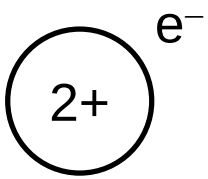




actual He atom



Zumdahl's 'hypothetical' He atom



He^+

what about shielding if the electrons are in different shells

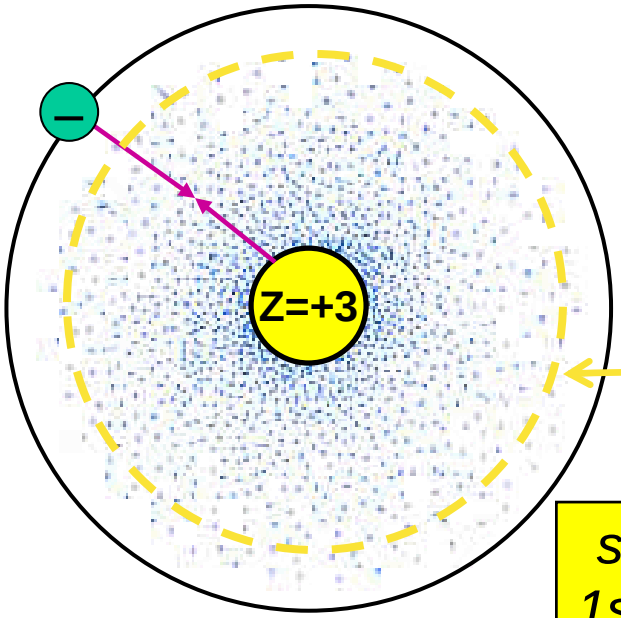
$$Li^{2+}\ 2s \quad vs \quad Li\,[1s^2]\,2s$$

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 ?

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

2s electron



$$IE_{experimental} = 0.86 \times 10^{-18}\,J$$

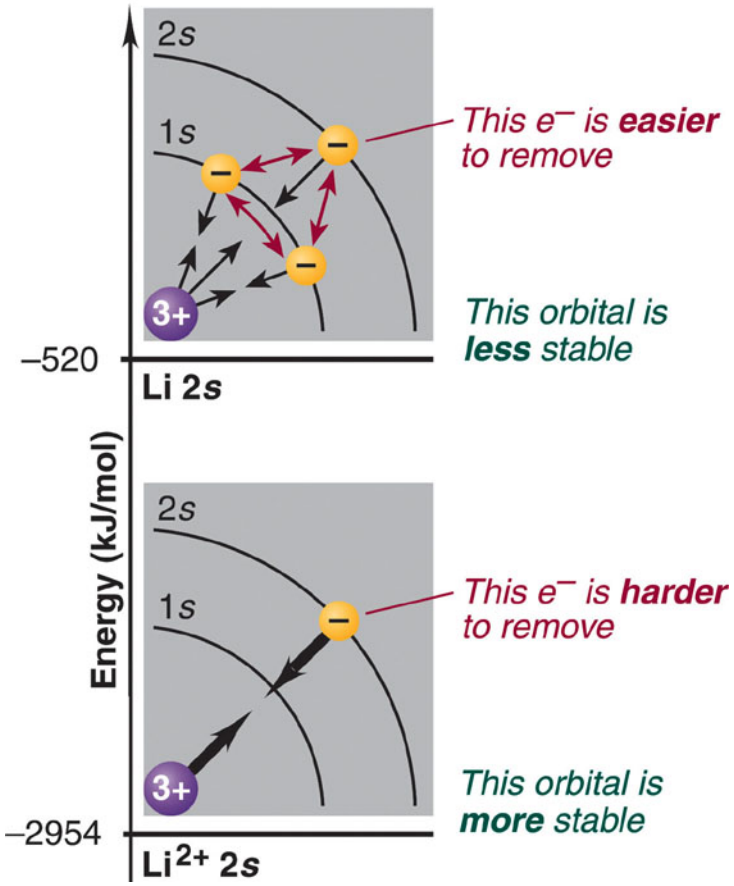
$$(Z_{eff})_{2s} \approx \left[\frac{n^2\ IE_{2s}}{2.18 \times 10^{-18}\,J} \right]^{1/2} = 1.26$$

shielding by $1s^2$ electrons

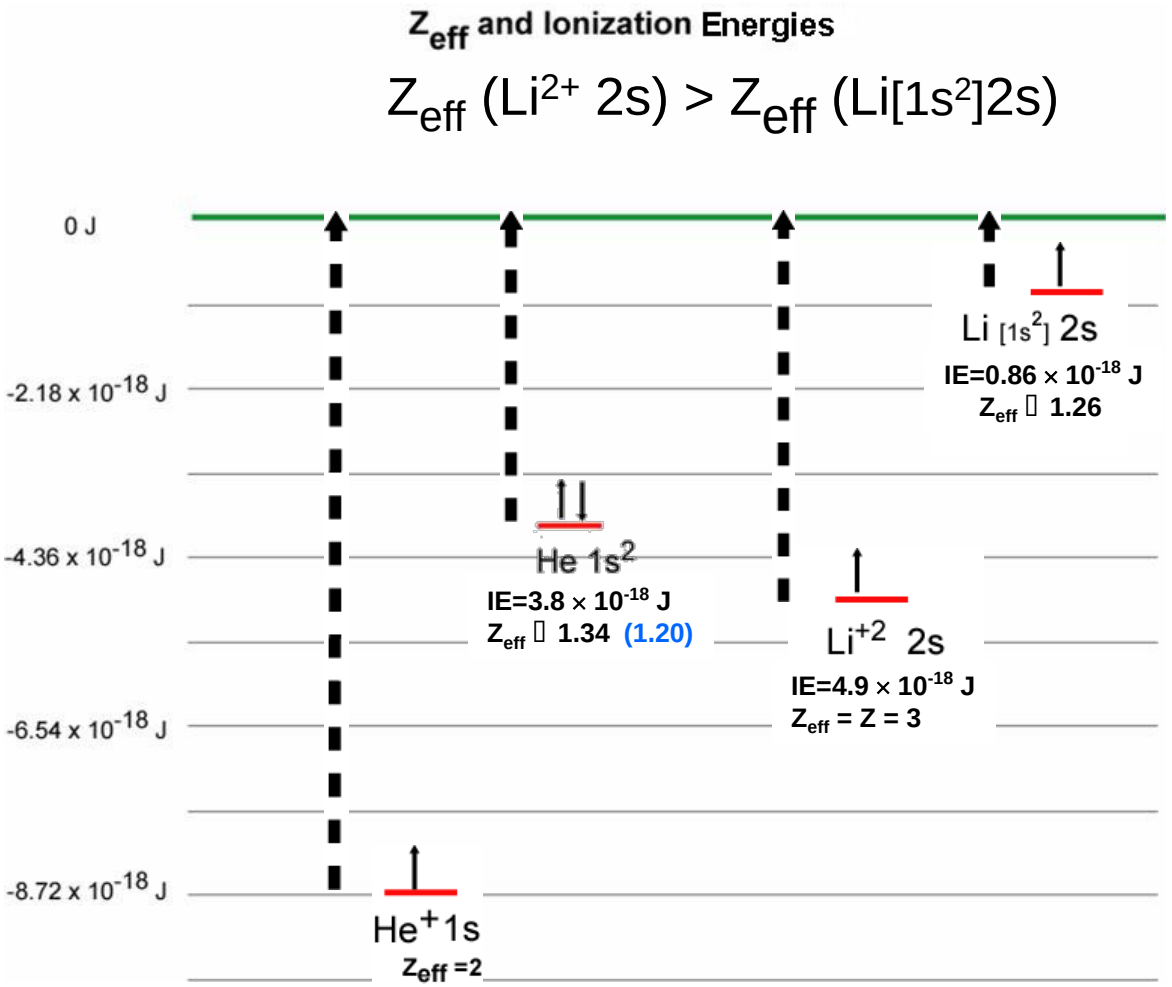
$Z_{eff} \approx 1.26$

Li $1s^2 2s$

figure 8.4 B (Silb) shielding by inner shell electrons



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



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

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

how would one expect the shielding of 1s electron
for another 1s electron [same shell] to compare to
the shielding of a 1s electron for a 2s electron [different shells] ?

shielding of same shell **? <<<** shielding of outer shell by inner shell

He $1s^2$ vs Li$1s^2$2s

How so ? *[$Z_{eff}=Z_{nucleus}$-shielding of other electrons]*

He : $Z_{eff}(1s) \approx 1.34 = +2 -$ shielding of other 1s electron

shielding of other 1s electron $=$ **0.66**

Li : $Z_{eff}(2s) \approx 1.26 = +3 -$ shielding of two 1s electrons

shielding of each inner shell 1s electron $= \frac{1.74}{2} =$ **0.87**

DONE FOR NOW !!

http://www.tunnel.ru/i/post/350182/3501828039/2063662981/at948236225.gif

- Stern-Gerlach electron spin +½ and –½
- Pauli Exclusion Principle (PEP)
- effective nuclear charge: Z_{eff}
  - $+Z_{\text{nuclear chage}}$ – repulsion (shielding) by other electrons
  - shielding greater from electron in inner shell than electron in same shell [from electrons 'inside' or closer to nucleus]
  - $E_n \approx -\frac{m_e e^4}{8h^2 \varepsilon_0^{\,2}} \frac{Z_{eff}^2}{n^2} = -(2.18\times10^{-18}\ \text{J}) \frac{Z_{eff}^2}{n^2}$ $\qquad \bar{r} \approx (5.29\times10^{-11}\text{m}) \frac{n^2}{Z_{eff}}$

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

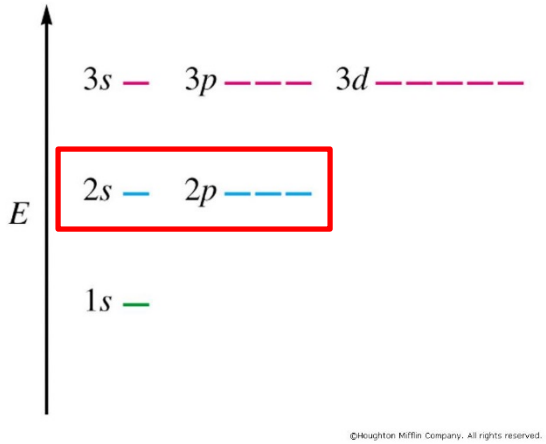


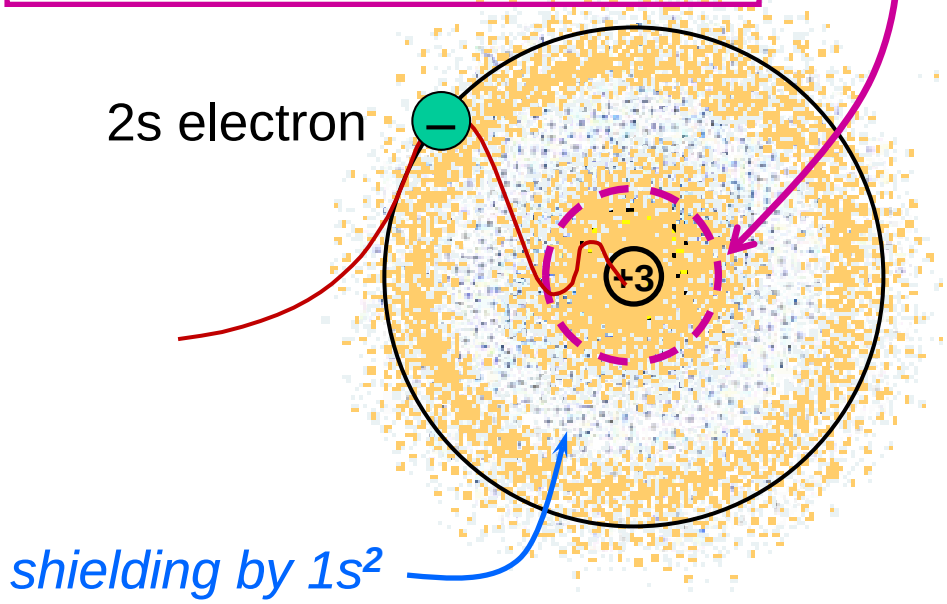
fig. 12.23 for 1-electron atoms and ions

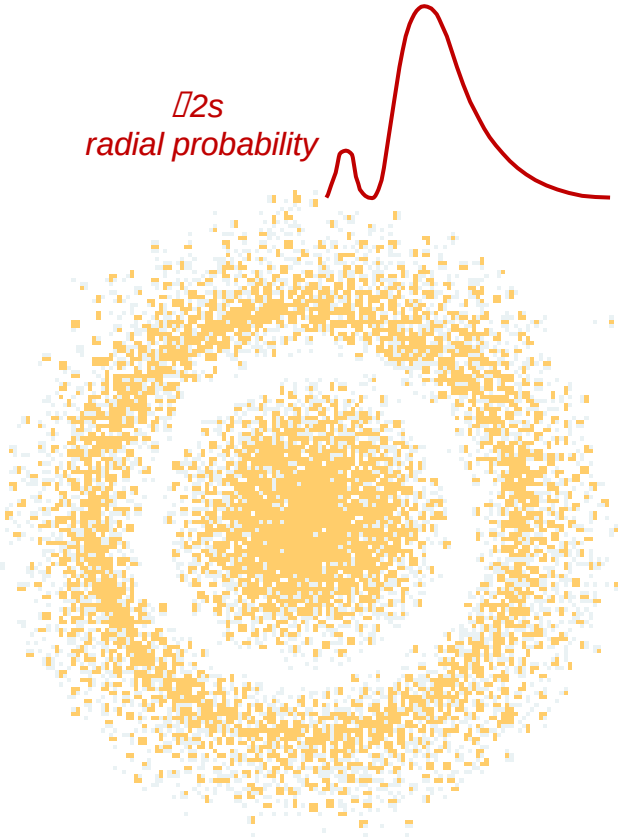
now Z_{eff}

and the effect of penetration of inner shell electron density by electrons in the same shell (e.g. 2s electron vs 2p electron)

Z_{eff} for 2s vs 2p: 2p and 2s have SAME energy in 1-electon ion

‘penetration’ by 2s electron of $1s^2$ shielding GIVES INCREASED Zeff





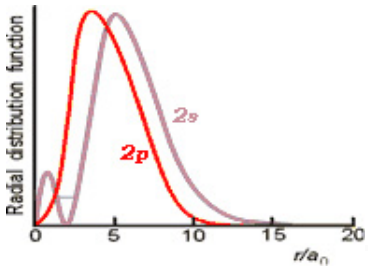
Li $1s^2$2s

Z_{eff} ≈ 1.26

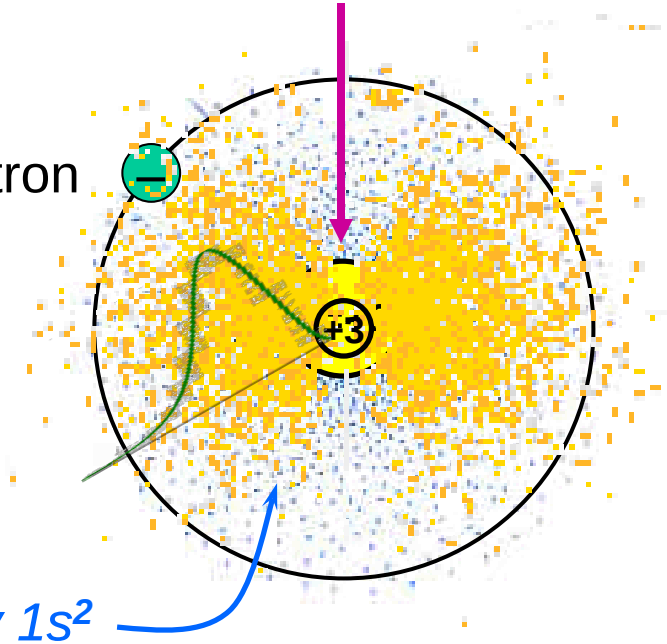
actual 2s electron density (one radial node; one inner maximum in radial probability)

Z_{eff} for 2s vs 2p

no (less) ‘penetration’ of $1s^2$ shielding
by 2p electron GIVES relatively smaller Z_{eff}



2p electron



shielding by $1s^2$

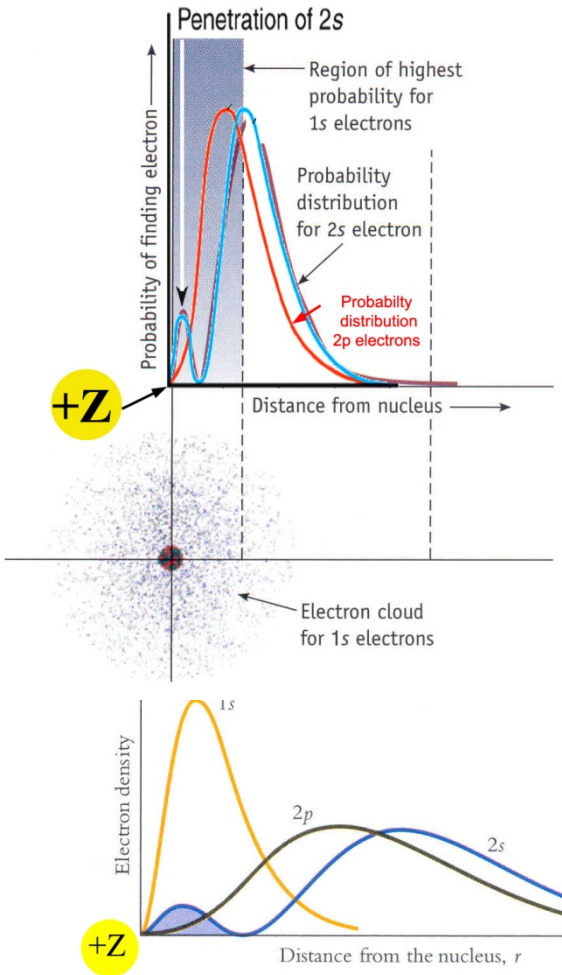
Li $1s^2 2p$

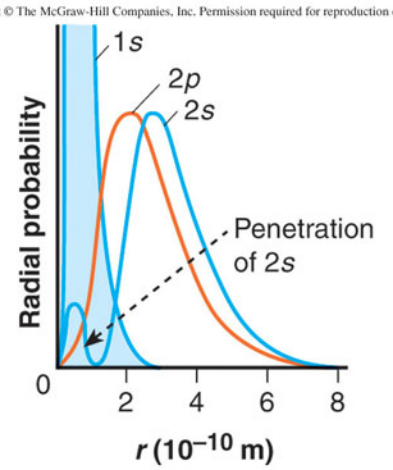
actual 2p electron density
(no radial nodes;
no ‘inner maxima’ in radial probability)

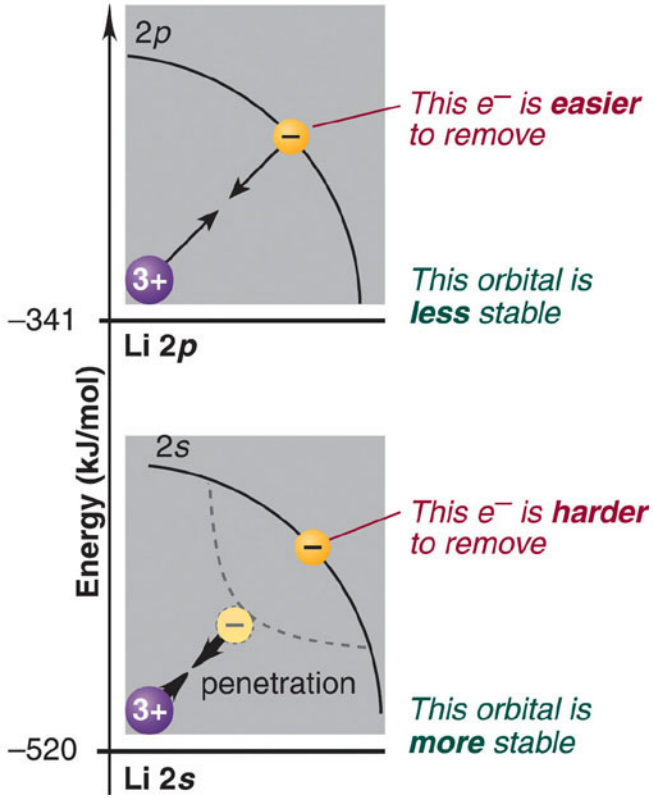
Z_{eff} for 2s > Z_{eff} for 2p

$E_{2s} < E_{2p}$

Z_{eff} for 2s vs 2p (handout fig. 12.4)





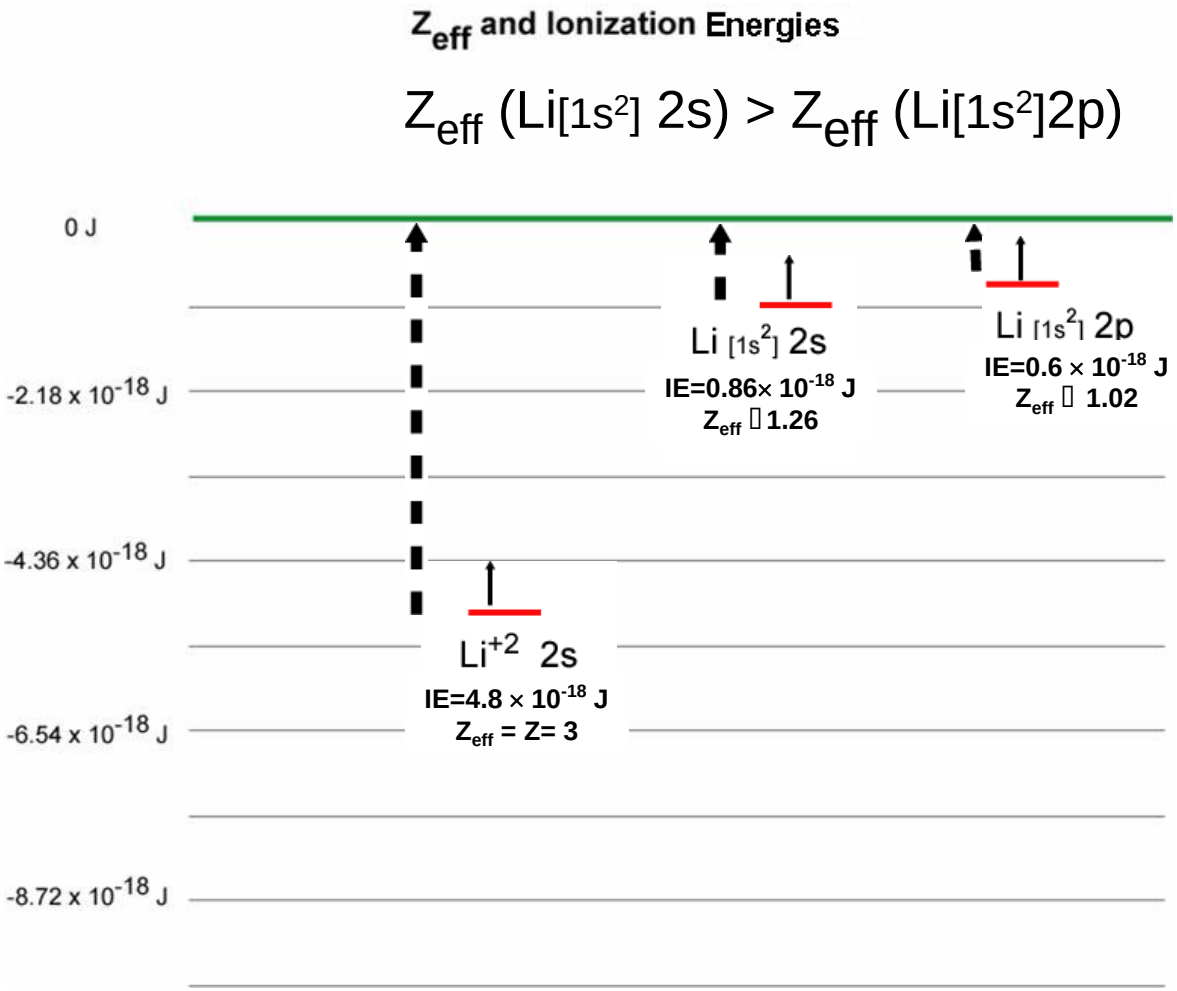


more penetration of inner shell electron density

$E_{2s} < E_{2p}$

electron see's more +Z and has greater Z_{eff}

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



- **Configurations and valence-level orbital diagrams**
- **Hund's rule**
- **2nd row aufbau fig 8.8 (Sil)**

- **Increasing Z_{eff} due to increasing penetration effects (figure HO 12Z.6);** ➡

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

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

- **4s vs 3d (Z_{eff} vs n)** ➡

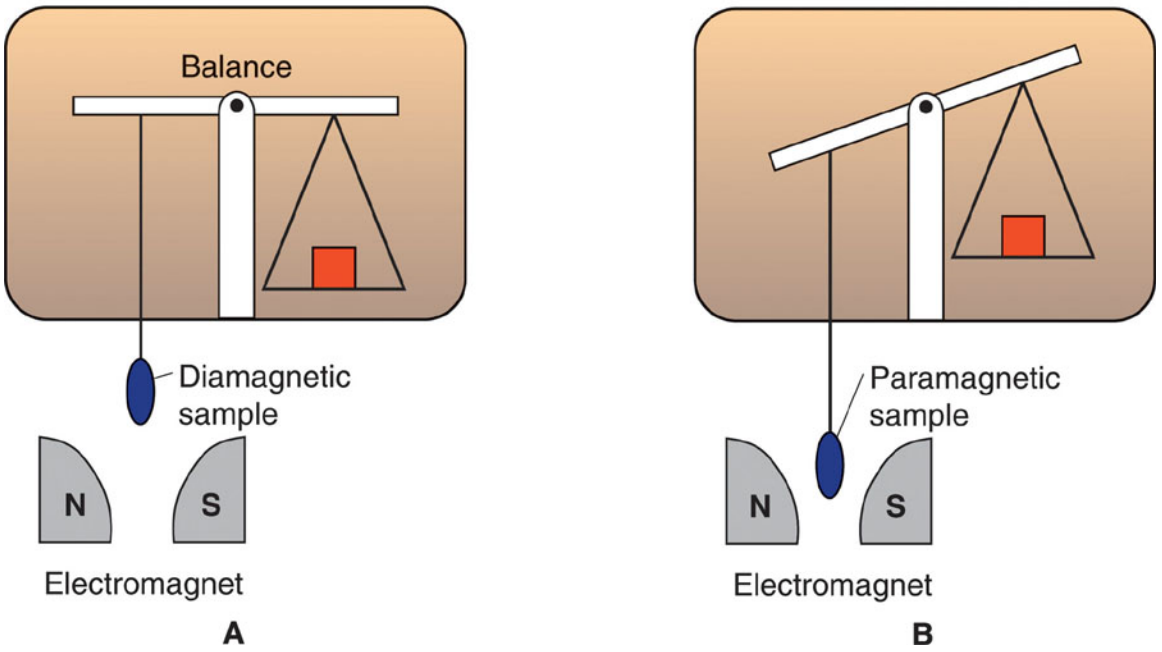
- **Orbital energy ordering** ➡ **fig 8.6 (Silb) (figure 8.13, Silb)** ➡

- **Hund's rule**
  - **Energy ordering**
  - **Unambiguous [closed shell, 1e, (n-1)e's**
    e.g. p^1, p^5, d^1,d^9]
  - **Ambiguous [e.g. p^2,p^3,p^4, $d^2 \rightarrow d^8$]**

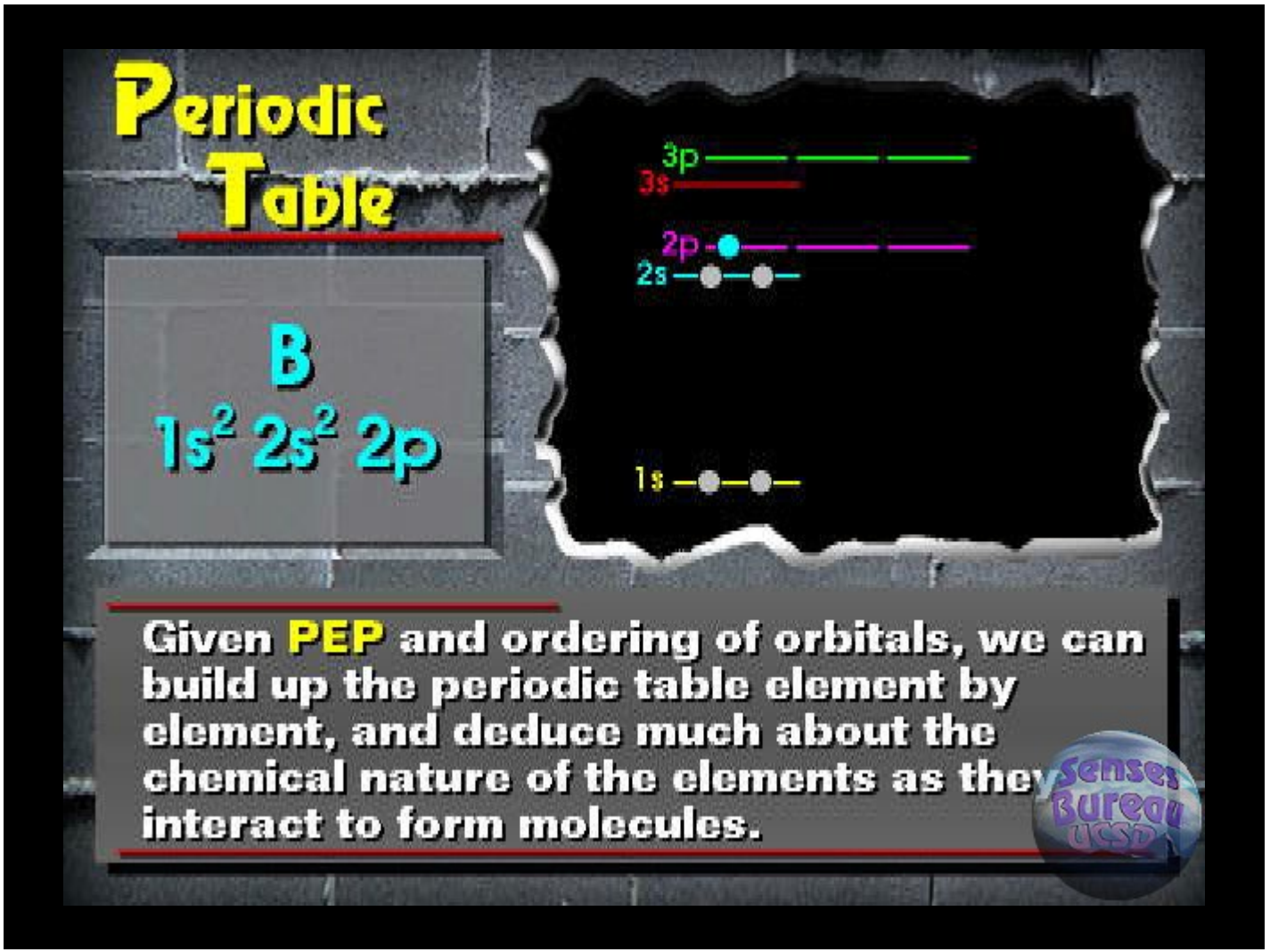
- **Examples (periodic table)**
  - **ground state**
  - **excited state**
  - **not allowed configuration**
  - **transition metal cations**
  - **"exceptions"**

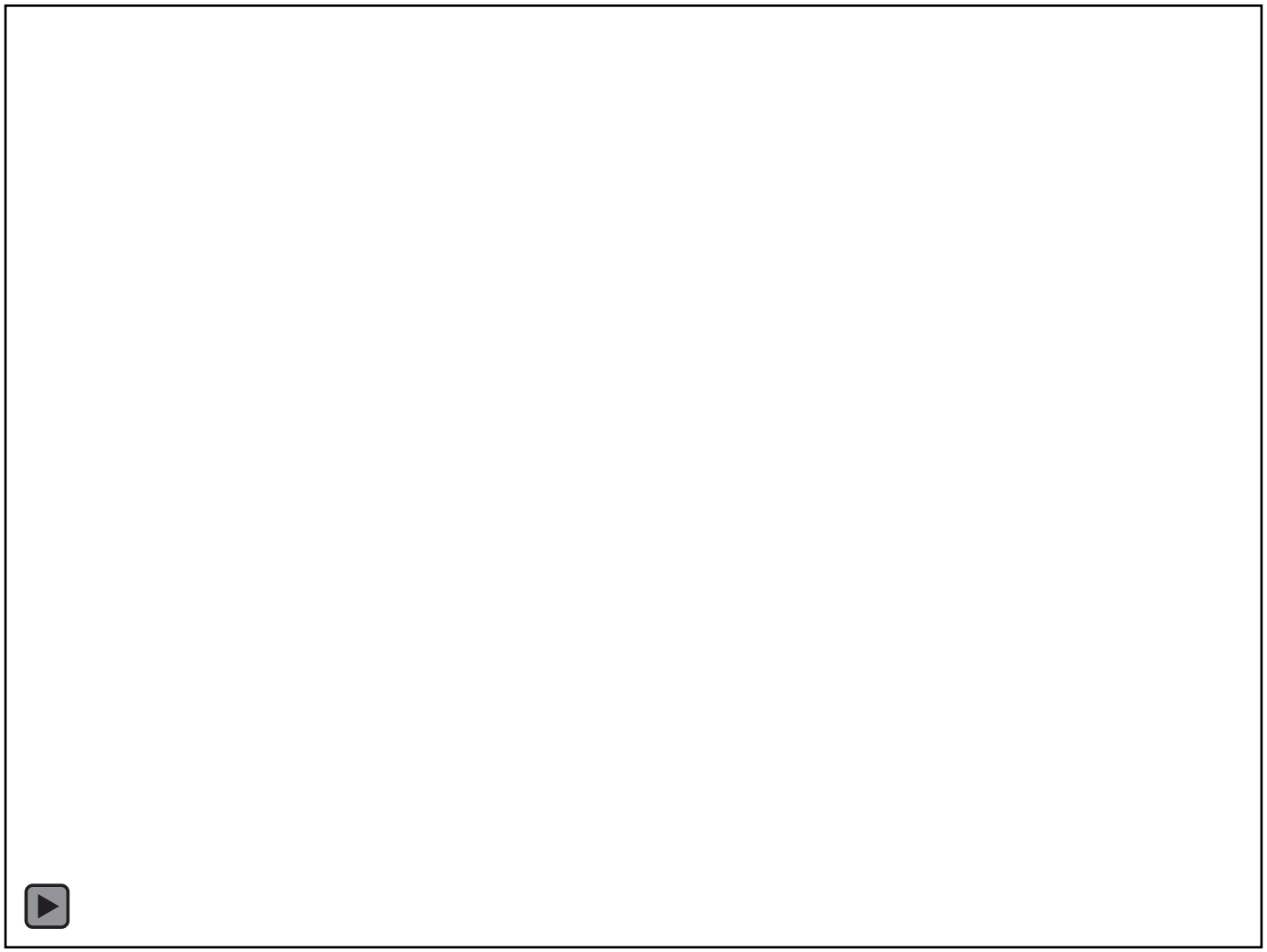
Diamagnetic
- pushed out of magnet
- no unpaired electrons

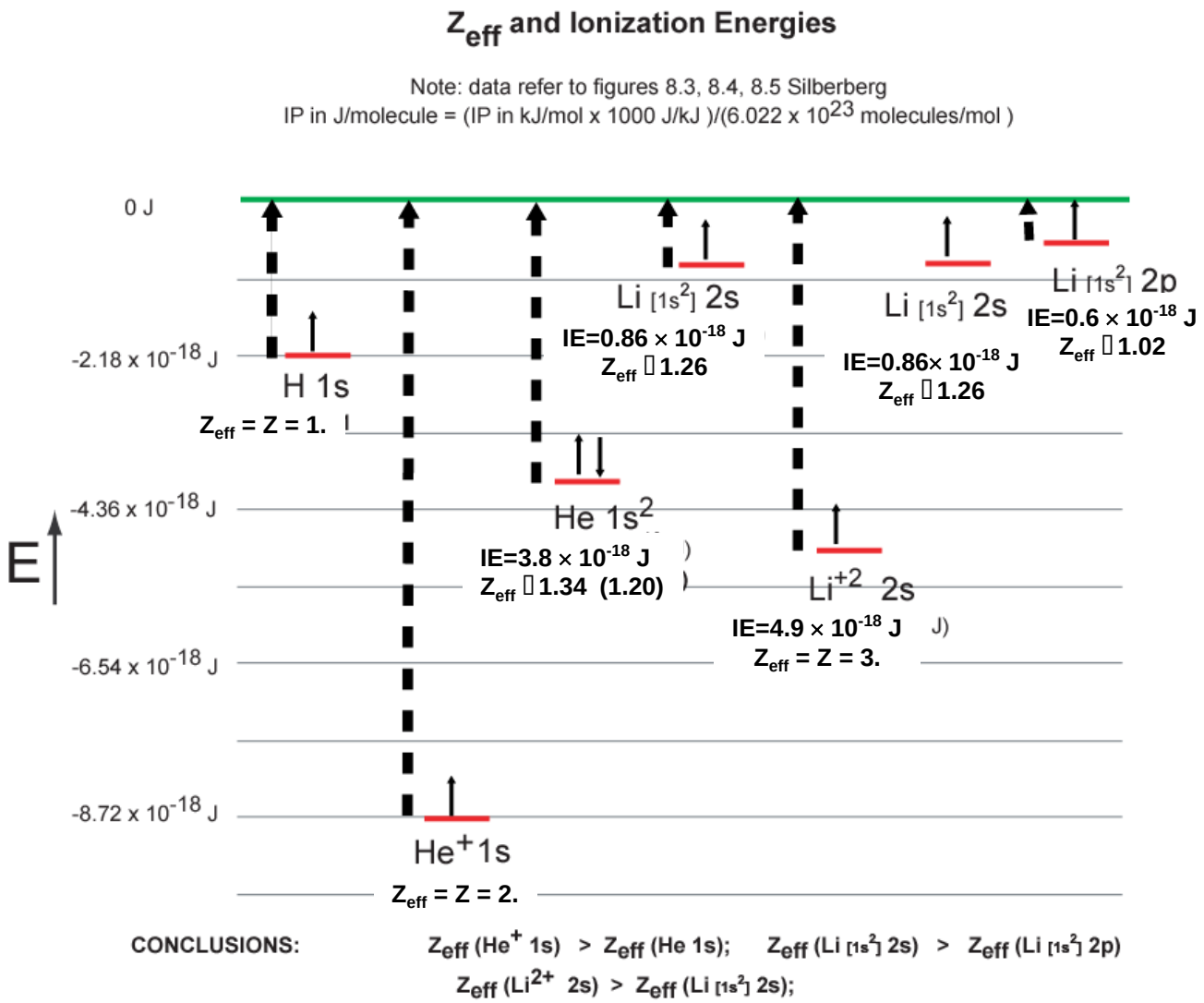
Paramagnetic
- pulled into magnet
- unpaired electrons



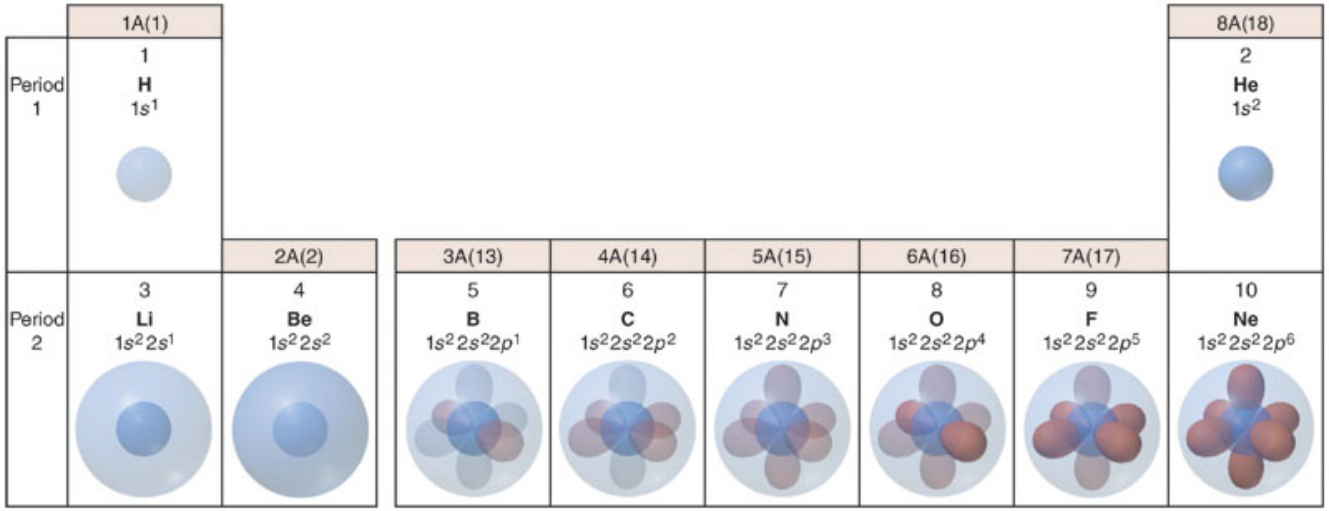
Gouy Balance


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 Bureau UCSD

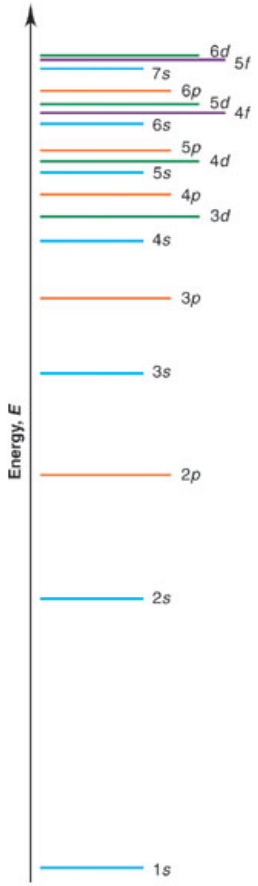



Z_{eff} and Ionization Energies
Note: data refer to figures 8.3, 8.4, 8.5 Silberberg
IP in J/molecule = (IP in kJ/mol x 1000 J/kJ)/(6.022 x 10^{23} molecules/mol)
0 J
-2.18 x 10^{-18} J
-4.36 x 10^{-18} J
-6.54 x 10^{-18} J
-8.72 x 10^{-18} J
E
H 1s
Z_{eff} = Z = 1.
Li [$1s^2$] 2s
IE=0.86 × 10^{-18} J
Z_{eff} 1.26
Li [$1s^2$] 2s
IE=0.86× 10^{-18} J
Z_{eff} 1.26
Li [$1s^2$] 2p
IE=0.6 × 10^{-18} J
Z_{eff} 1.02
He $1s^2$
IE=3.8 × 10^{-18} J
Z_{eff} 1.34 (1.20)
Li^{+2} 2s
IE=4.9 × 10^{-18} J
Z_{eff} = Z = 3.
He^+ 1s
Z_{eff} = Z = 2.
CONCLUSIONS:
Z_{eff} (He^+ 1s) > Z_{eff} (He 1s); Z_{eff} (Li [$1s^2$] 2s) > Z_{eff} (Li [$1s^2$] 2p)
Z_{eff} (Li^{2+} 2s) > Z_{eff} (Li [$1s^2$] 2s);

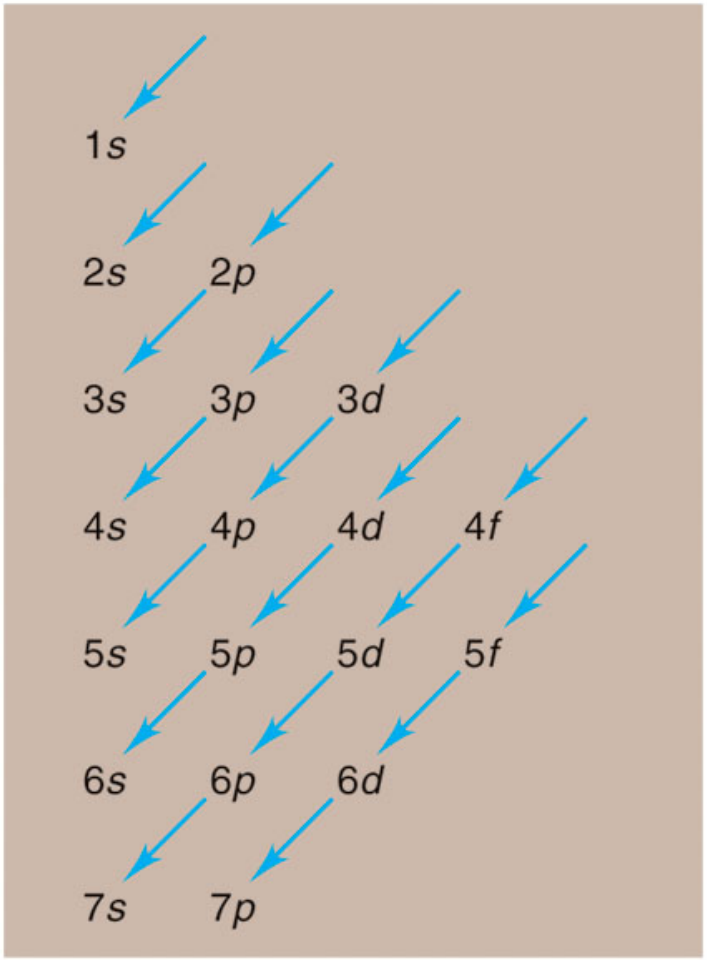
Silberberg figure 8.8



Silberberg figure 8.6



Silberberg figure 8.13



Zumdahl figure 12.29

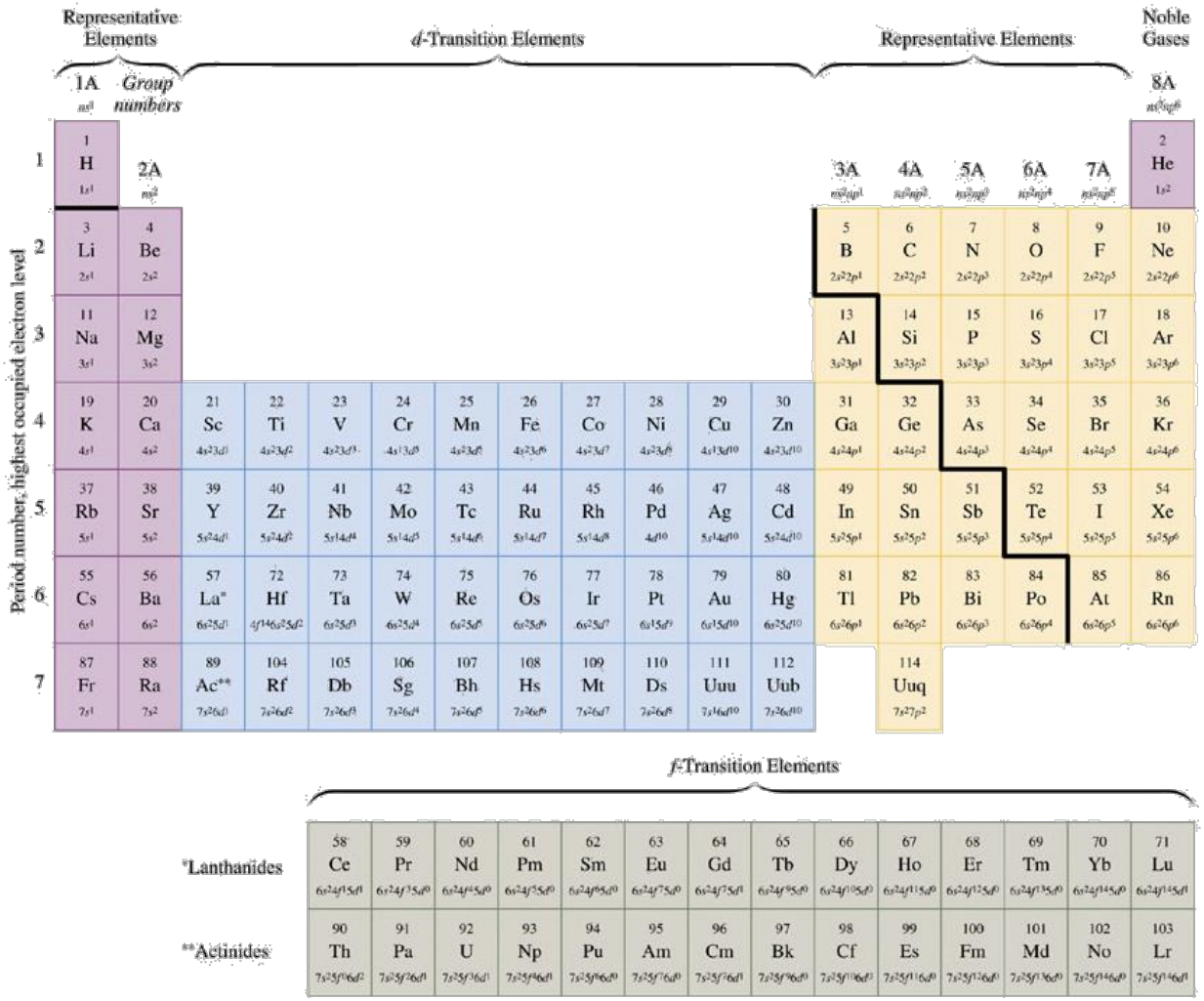
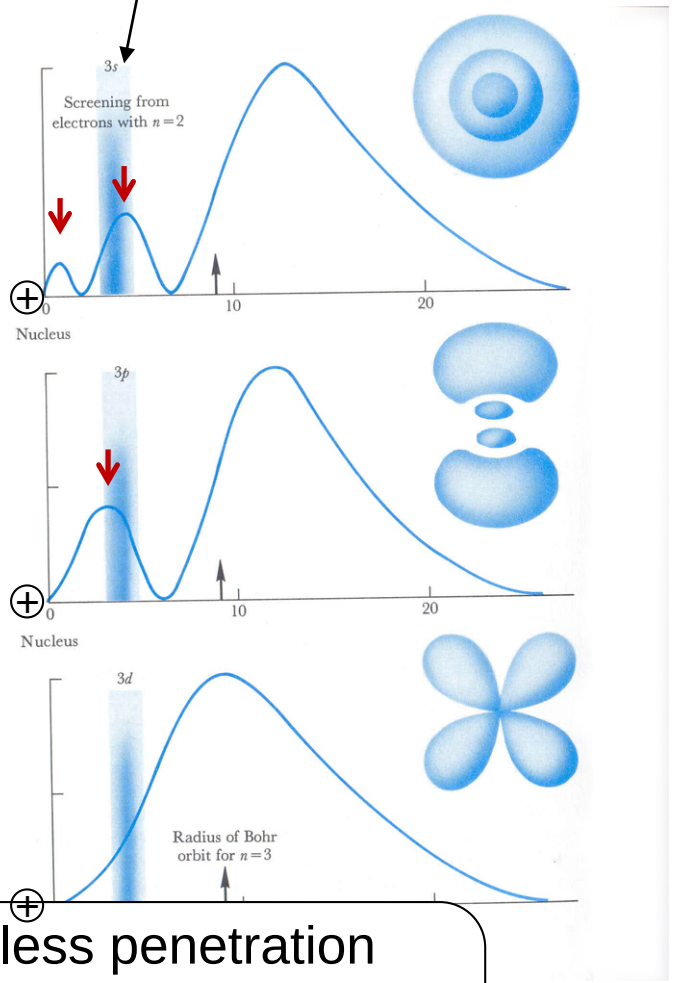


Figure HO 8.6: penetration of 3s vs 3p vs 3d; ***radial nodes = n-ℓ-1***

screening by n=2 electrons



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

3p: 1 radial node
1 "inner maxima"

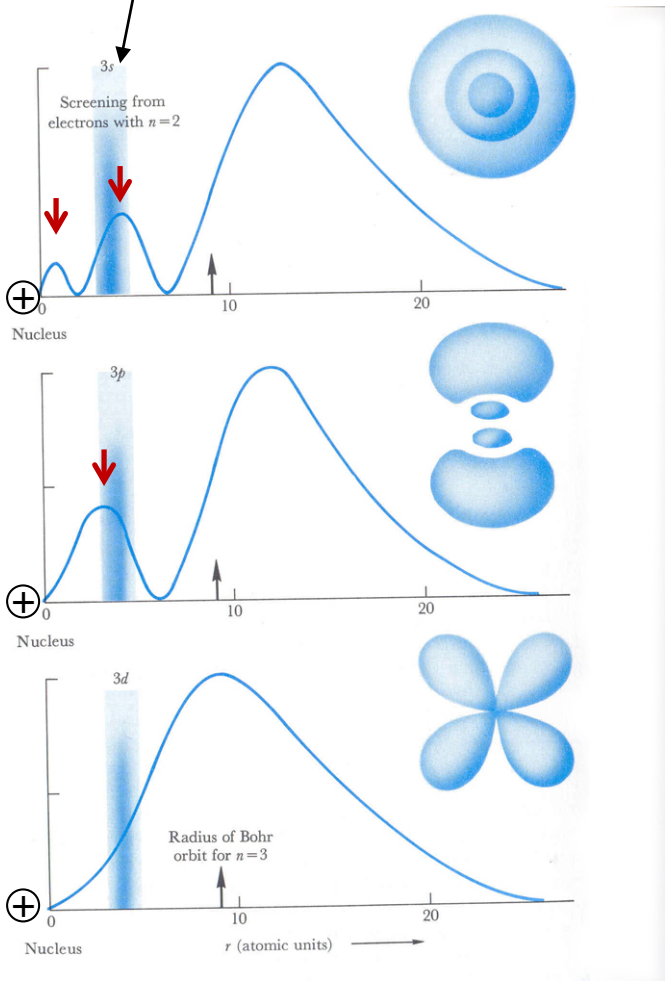
3d: 0 radial nodes
0 "inner maxima"

less penetration
smaller Z_{eff}
higher energy

more penetration
larger Z_{eff}
lower Energy

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

3p: 1 radial node
1 "inner maxima"

3d: 0 radial nodes
0 "inner maxima"

more penetration
larger Z_{eff}
lower Energy

less penetration
smaller Z_{eff}
higher energy

Why B [He] $2s^2\ 2p^1$ is '***unambiguous***' ground state configuration

Experimental spectrum (states) of B

ASD DATA — LINES LEVELS — INFORMATION — 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

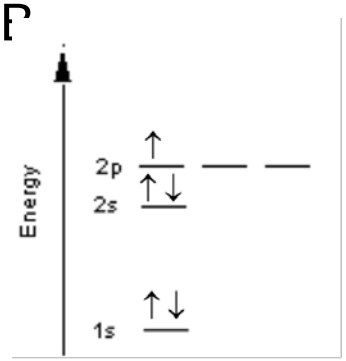
Example of how to reference these results
Kramida, A., Ralchenko, Yu., Reader, J., and
Spectra Database (ver. 5.0), [Online]. Availab
October 17]. National Institute of Standards

Some data for neutral and singly-charged ions are available in the Handbook of Basic Atomic Spectroscopic Data

Configuration	Term	J	Level (cm^{-1})
$2s^2 2p$	$^2P°$	$^1/_2$	0.0000
		$^3/_2$	15.287
$2s2p^2$	^4P	$^1/_2$	28 647.43+x
		$^3/_2$	28 652.07+x
		$^5/_2$	28 658.40+x
$2s^2 3s$	^2S	$^1/_2$	40 039.6907
$2s2p^2$	^2D	$^5/_2$	47 856.809
		$^3/_2$	47 857.125
$2s^2 3p$	$^2P°$	$^1/$	48 611.8663

E

Only 'one' energy state
(ignore 3/2 vs 1/2)



ground state of boron: 5 e's

configuration: $1s^2 2s^2 2p^1$

Why B [He] $2s^2\ 2p^1$ is '***unambiguous***' ground state configuration

Experimental spectrum (states) of B

ASD — Data: Lines, Levels — Information: 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

Example of how to reference these results
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		$^3/_2$	15.287
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		$^3/_2$	28 652.07+x
		$^5/_2$	28 658.40+x
$2s^2 3s$	^2S	$^1/_2$	40 039.6907
$2s2p^2$	^2D	$^5/_2$	47 856.809
		$^3/_2$	47 857.125
$2s^2 3p$	$^2P°$	$^1/$	48 611.8663

E

Only 'one' energy state
(ignore 3/2 vs 1/2)

Excited states have excited [He] $2s^1\ 2p^2$ configuration

Why C [He] $2s^2\ 2p^2$ is '**ambiguous**' ground state configuration

Experimental spectrum (states) of C

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

NIST Atomic Spectra Database Levels Data

Example of how to referenc
Kramida, A., Ralchenko, Yu.,
Spectra Database (ver. 5.0), [
October 17]. National Institute

C I 282 Levels Found

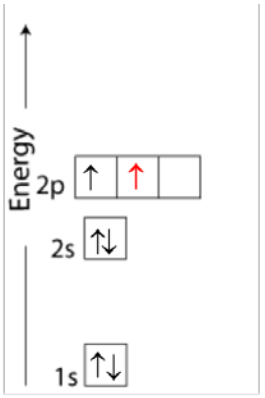
Z = 6, C isoelectronic sequence

Some data for neutral and singly-charged ions are available in the Handbook of Basic Atomic Spectrosc

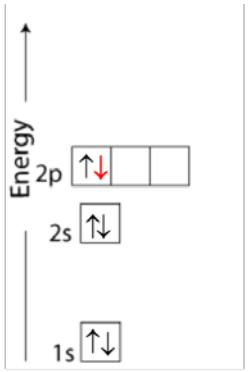
Configuration	Term	J		Level (cm^{-1})
$2s^2 2p^2$	^3P	0	E	0.00
		1		16.40
		2		43.40
$2s^2 2p^2$	^1D	2		10 192.63
$2s^2 2p^2$	^1S	0		21 648.01
$2s 2p^3$	$^5S°$	2		33 735.20
$2s^2 2p 3s$	$^3P°$	0		60 333.43
		1		60 352.63
		2		60 393.14

Ground energy state
(ignore 0 vs 1 vs 2)

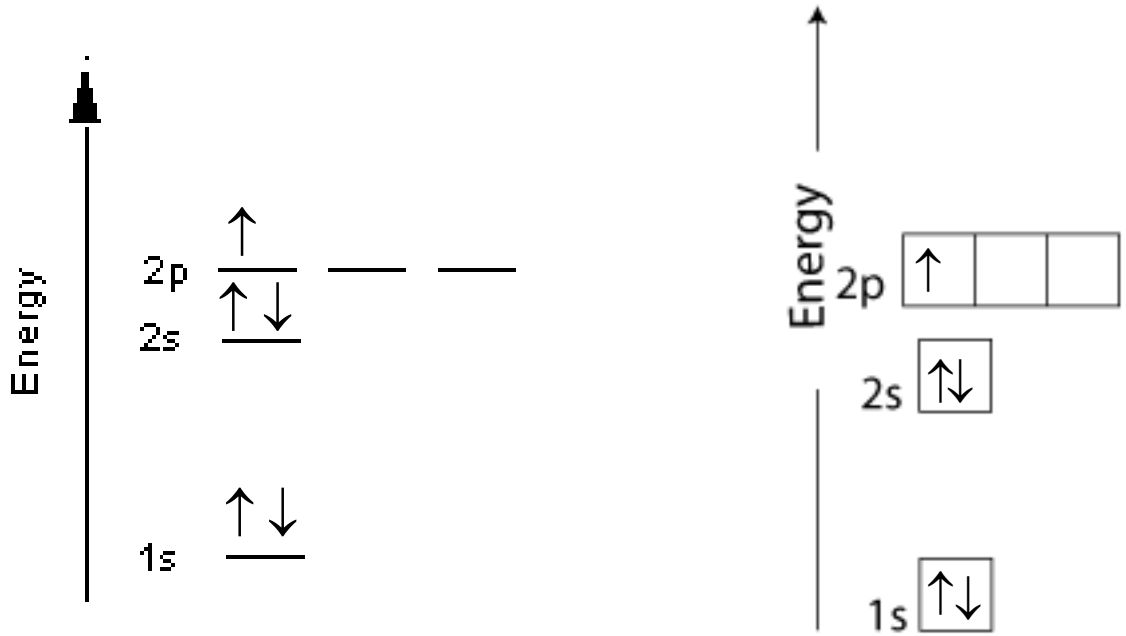
Excited states with same [He] $2s^2\ 2p^2$ configuration



lowest energy: ground state



higher energy: excited state



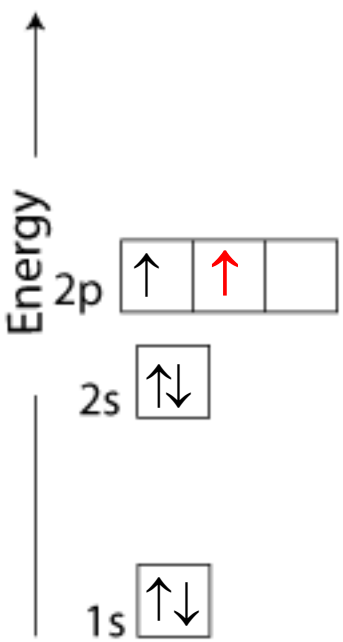
ground state of boron: 5 e's

configuration: $1s^2 2s^2 2p^1$ or [He] $2s^2 2p^1$

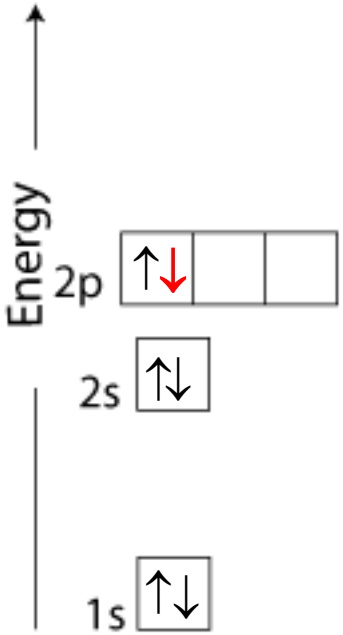
Friedrich Hund

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

carbon 6e's: $1s^2 2s^2 2p^2$ or $[He]2s^2 2p^2$



lowest energy: ground state



higher energy: excited state

E_{3d} vs E_{4s} a contest between n and Z_{eff} !!!

$$E_n \approx -(2.18\times10^{-18}\ \text{J})\frac{Z_{eff}^2}{n^2}$$

smaller n ⇒ lower (more negative) energy

larger Z_{eff} ⇒ lower (more negative) energy

who wins for lower energy?

3d vs 4s

n: 3 4 **3d wins for lower energy**

Z_{eff}: smaller larger **4s wins for lower energy**

0 radial nodes 3 radial nodes

and the energy winner is :

in neutral atoms Z_{eff} wins: $\mathbf{E_{4s} < E_{3d}}$

but in positive ions (e.g. Fe^{3+}) n wins: $\mathbf{E_{3d} < E_{4s}}$

The Aufbau Principle that we have been using is extremely useful in describing electronic configurations in atoms and ions. However since it is an 'approximation' to the actual (Schrödinger) wavefunctions, exceptions may be observed.

extra stability of half- or filled-shells:

^{23}V: $[^{18}Ar]\ 4s^2 3d^3$ ↑ ↑ ↑ _ _ *as expected*

^{24}Cr: $[^{18}Ar]\ 4s^2 3d^4$ ↑ ↑ ↑ ↑ _ *expected*

but **$[^{18}Ar]\ 4s^1$ ↑ $3d^5$ ↑ ↑ ↑ ↑ ↑** *observed (half-filled)*

^{28}Ni: $[^{18}Ar]\ 4s^2 3d^8$

~~^{29}Cu: $[^{18}Ar]\ 4s^2 3d^9$~~

but: ^{29}Cu: $[^{18}Ar]\ 4s^1 3d^{10}$

filled

half-filled

In chemistry 1B-02 you will NOT be responsible for memorizing exceptions but just to 'explain' a given exception