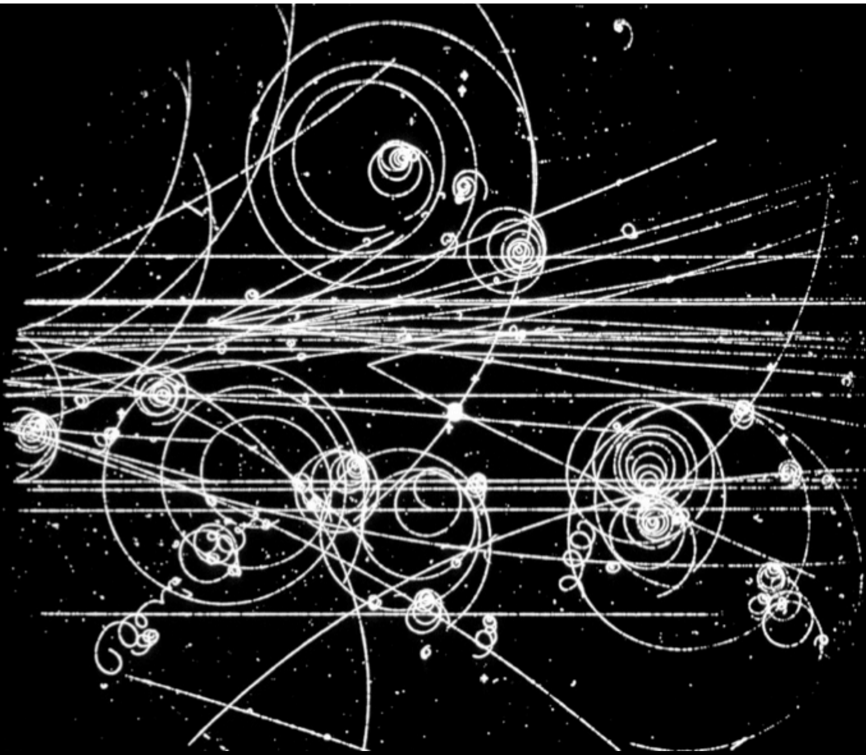
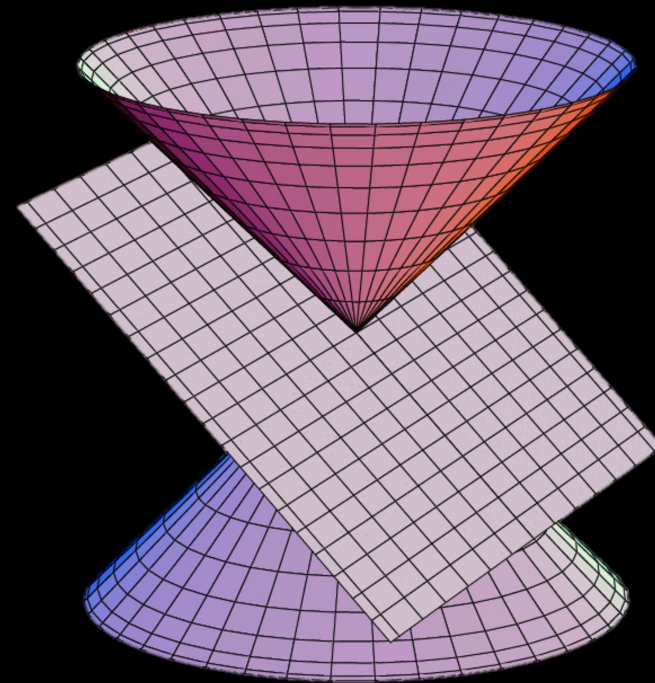




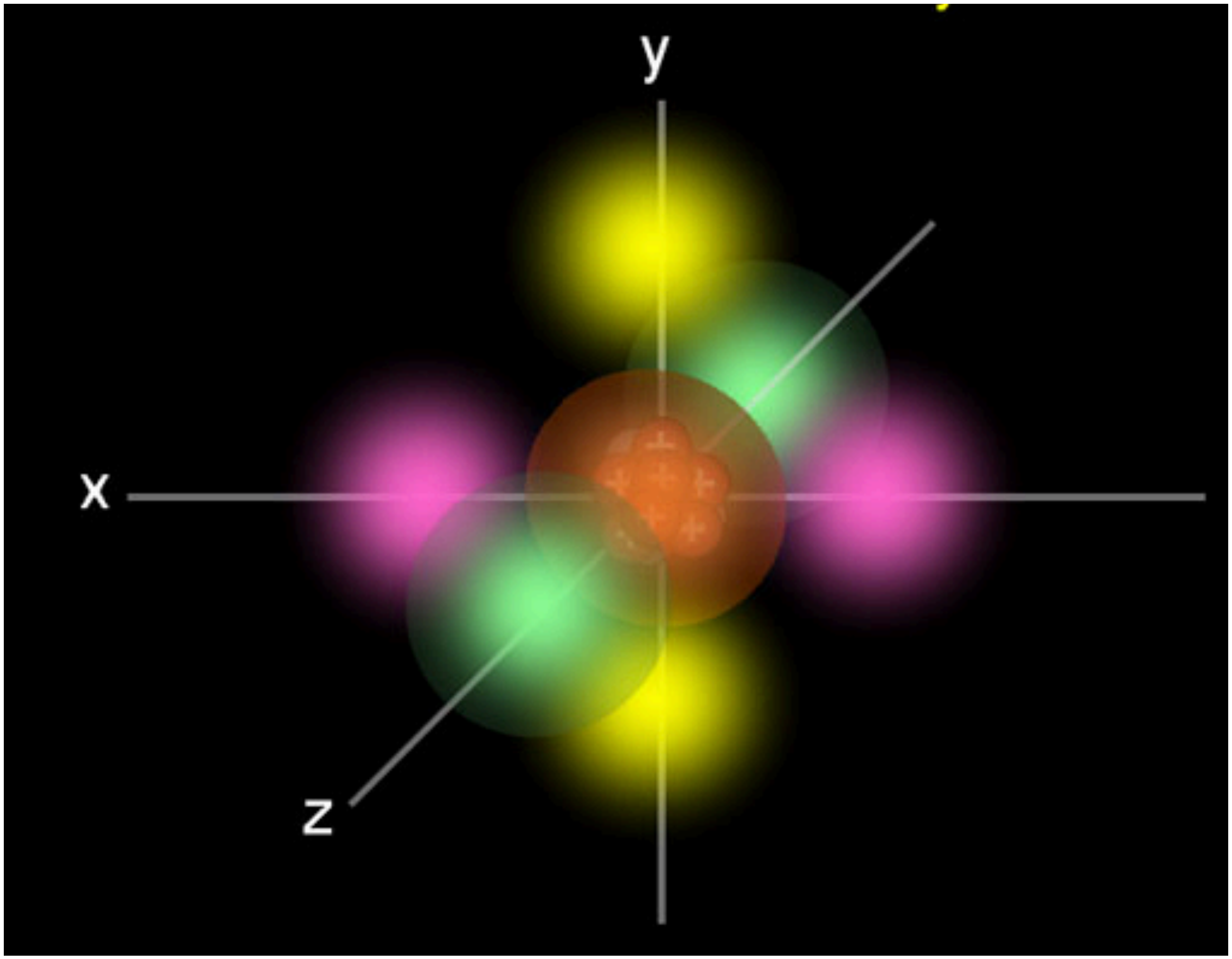
Modern Physics (Phys. IV): 2704

Professor Jasper Halekas
Van Allen 70
MWF 12:30-1:20 Lecture

Announcements

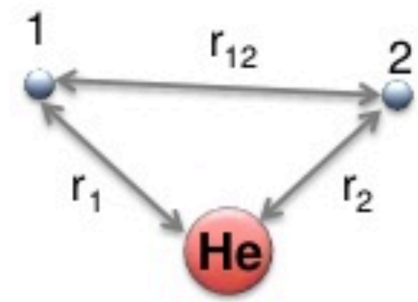
- HW #9 Due Friday
- Lab Q7 (Electron Spin Resonance) this week

Multi-Electron Atoms



Schrödinger Equation for Multi-Electron Atoms

Once we have two or more electrons, the Schrodinger equation **cannot** be solved exactly: *fundamental challenge for quantum chemistry!*



fixed nucleus at origin

Helium atom hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m_e}\nabla_1^2 - \frac{\hbar^2}{2m_e}\nabla_2^2 - \frac{2e^2}{4\pi\varepsilon_0 r_1} - \frac{2e^2}{4\pi\varepsilon_0 r_2} + \frac{e^2}{4\pi\varepsilon_0 r_{12}}$$

electron kinetic energy | **electron-nuclear coulombic attraction** | **electron repulsion**

Pauli Exclusion Principle

Electrons in an atom are arranged in individual "orbitals" each having a set of quantum numbers (n, l, m_l, m_s)

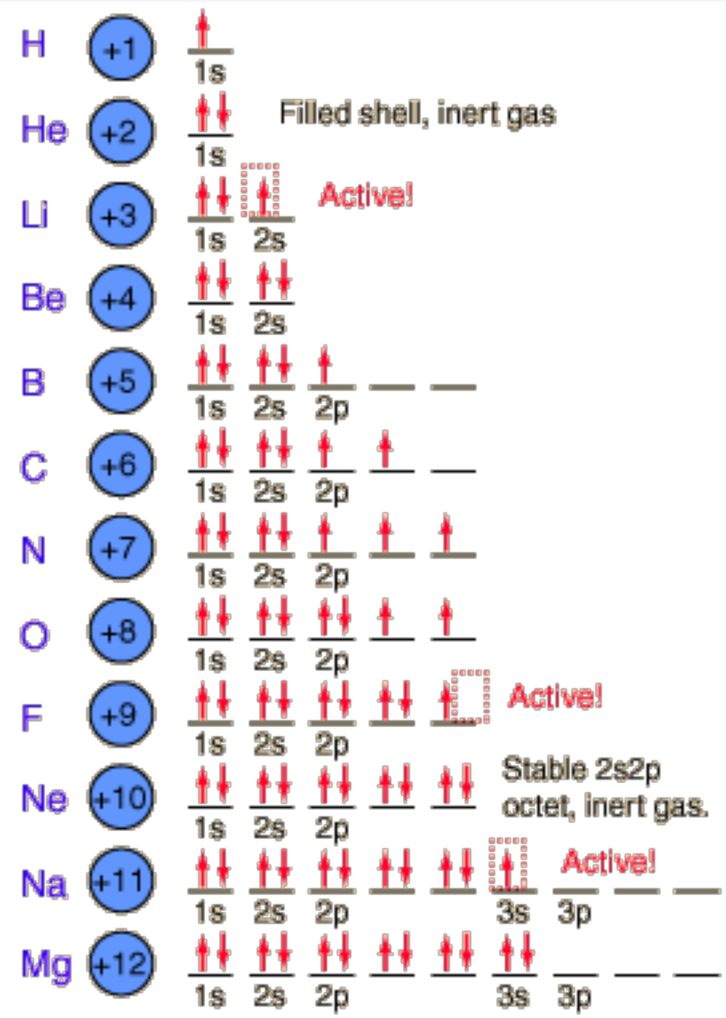
No two occupied electron orbitals can have the same set of quantum numbers.

State	Principal quantum number n	Orbital quantum number	Magnetic quantum number	Spin quantum number	Maximum number of electrons	
1s	1	0	0	$+\frac{1}{2}, -\frac{1}{2}$	2	
2s	2	0	0	$+\frac{1}{2}, -\frac{1}{2}$	2	8
2p	2	1	-1,0,+1	$+\frac{1}{2}, -\frac{1}{2}$	6	
3s	3	0	0	$+\frac{1}{2}, -\frac{1}{2}$	2	18
3p	3	1	-1,0,+1	$+\frac{1}{2}, -\frac{1}{2}$	6	
3d	3	2	-2,-1,0,1,2	$+\frac{1}{2}, -\frac{1}{2}$	10	

Shell name	Subshell name	Subshell max electrons	Shell max electrons
K	1s	2	**2**
L	2s	2	2 + 6 = **8**
	2p	6	
M	3s	2	2 + 6 + 10 = **18**
	3p	6	
	3d	10	

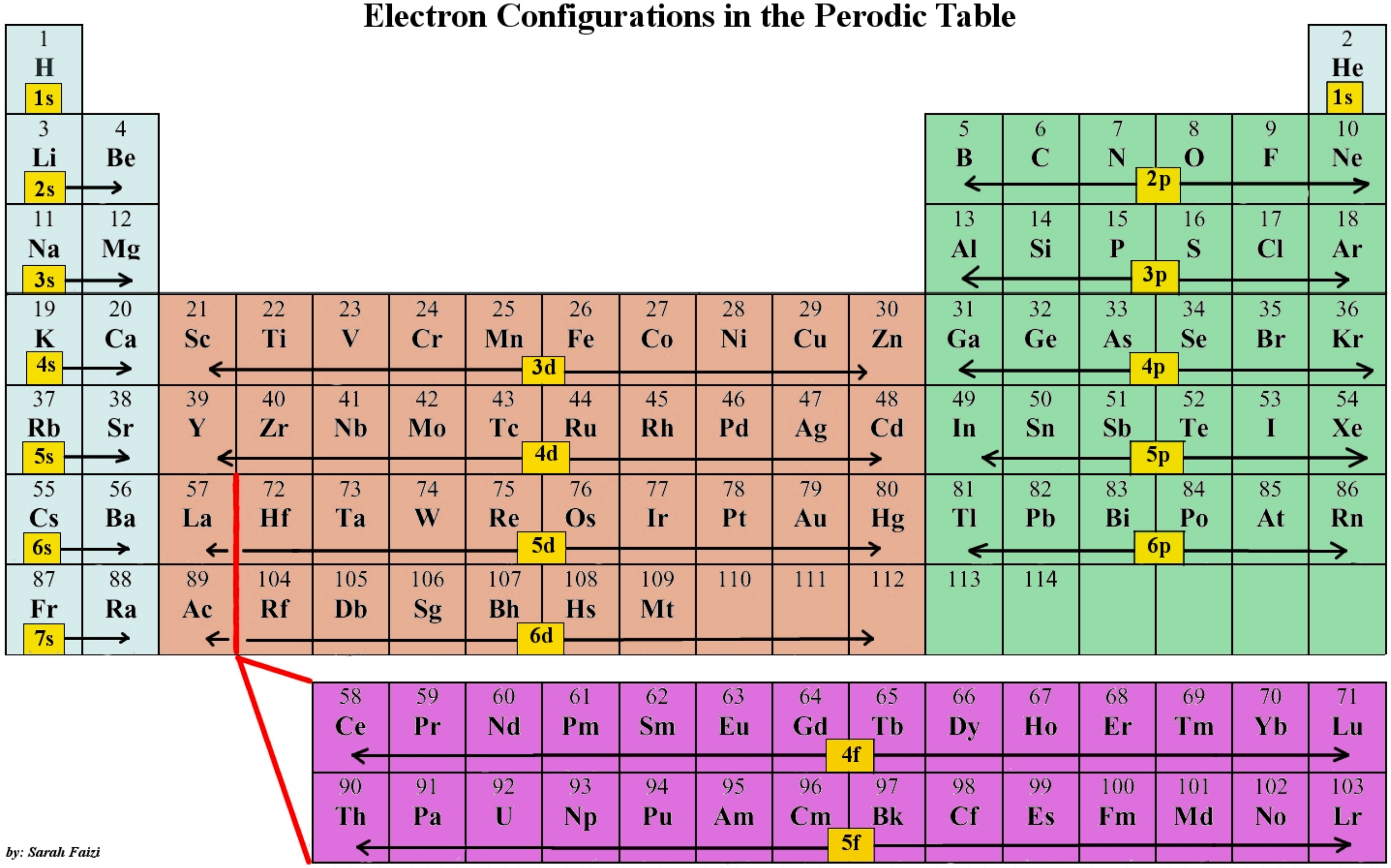
Orbital Filling

Atom	1s	2s	2p	2p	2p	Electronic configuration
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	↑↓	↑↓	↑↓	↑↓	↑↓	$1s^2 2s^2 2p^6$

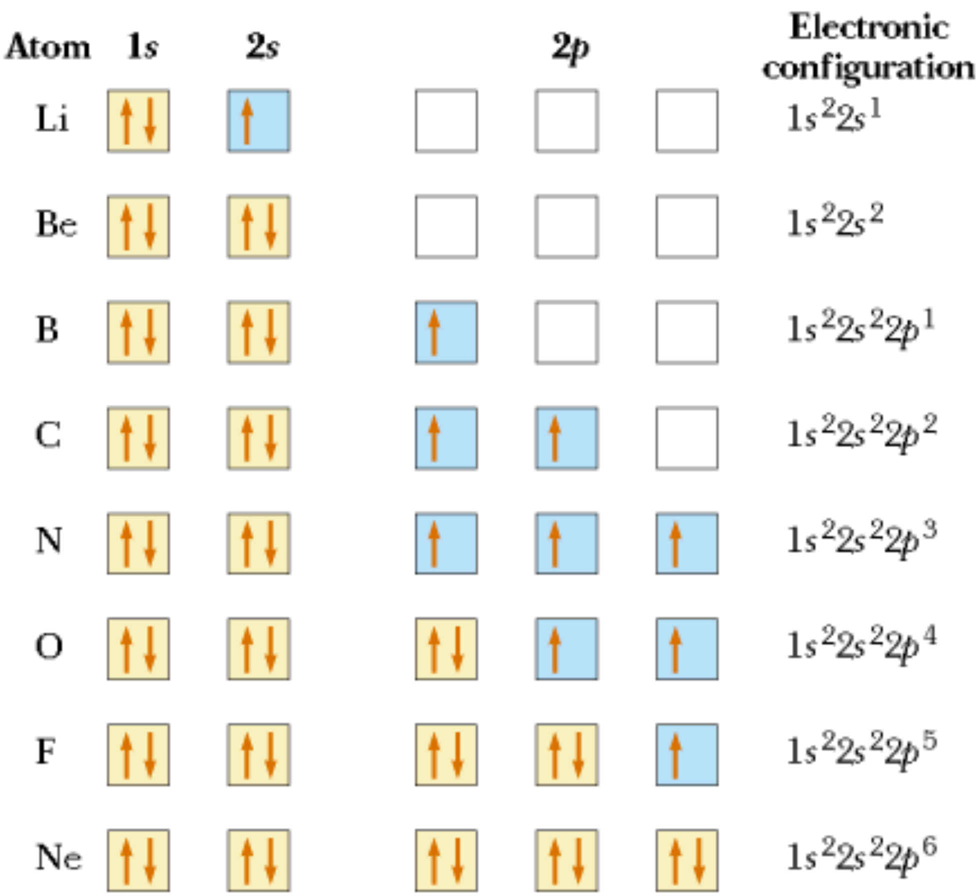


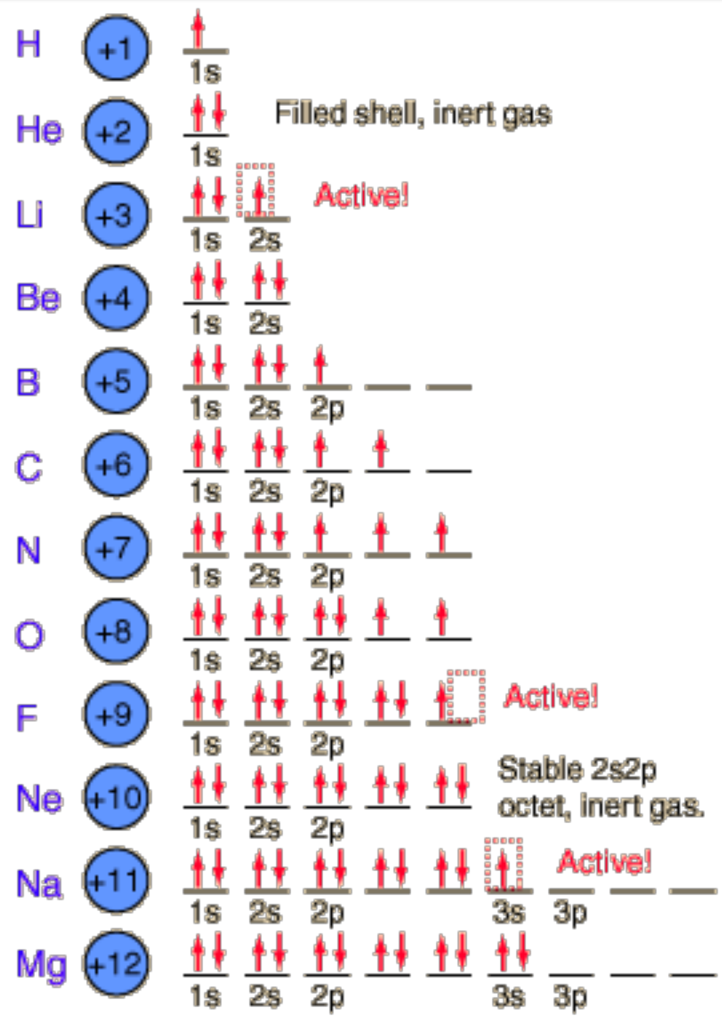
Periodic Table

Electron Configurations in the Perodic Table



Orbital Filling



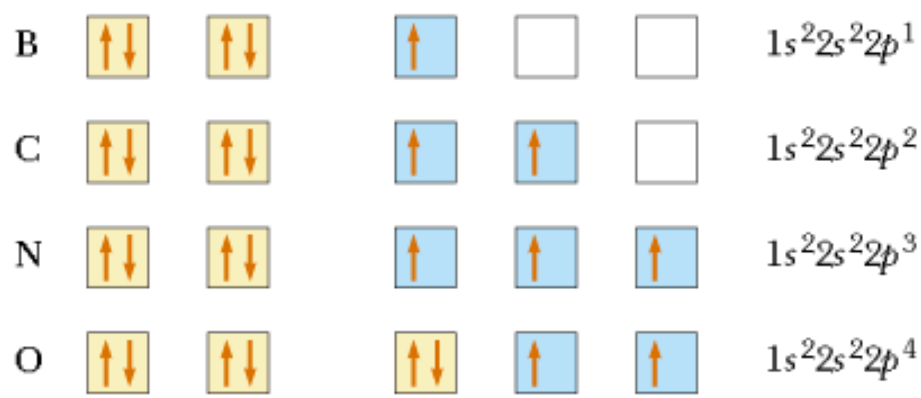


Hund's Rules

I. The configuration with the highest total spin S has the lowest energy
II. For a given total spin S, the configuration with the highest total angular momentum L has the lowest energy
III. For a a subshell less (more) than half filled, the configuration with lowest (highest) total angular momentum J = L + S has the lowest energy

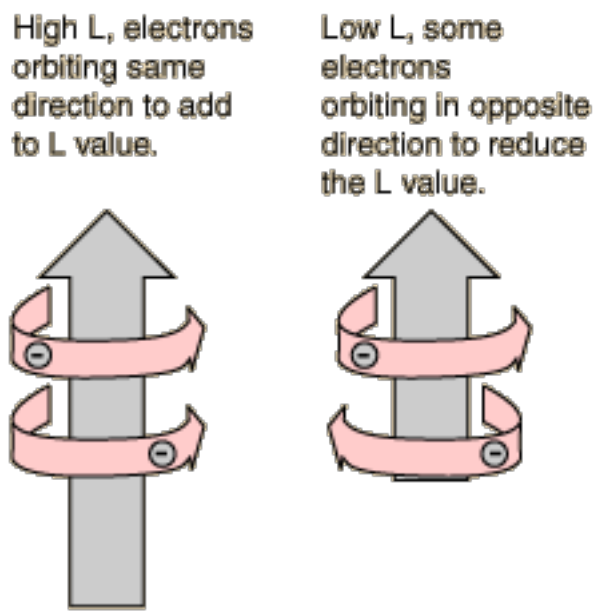
Hund’s Rule I

- Electrons in different orbitals are less well screened, so it is energetically favorable to put one electron in every available orbital before putting two in any given orbital



Hund's Rule II

- Semi-classical explanation: If all electrons orbit in a common direction they meet less often and thus have less mutual repulsion



Concept Check

- Which set of quantum numbers for two electrons in a 3p subshell is the ground state?

A. $m_l = 1, m_s = 1/2$ and $m_l = 0, m_s = -1/2$
B. $m_l = 1, m_s = 1/2$ and $m_l = -1, m_s = 1/2$
C. $m_l = 1, m_s = 1/2$ and $m_l = 0, m_s = 1/2$
D. $m_l = 1, m_s = 1/2$ and $m_l = 1, m_s = -1/2$

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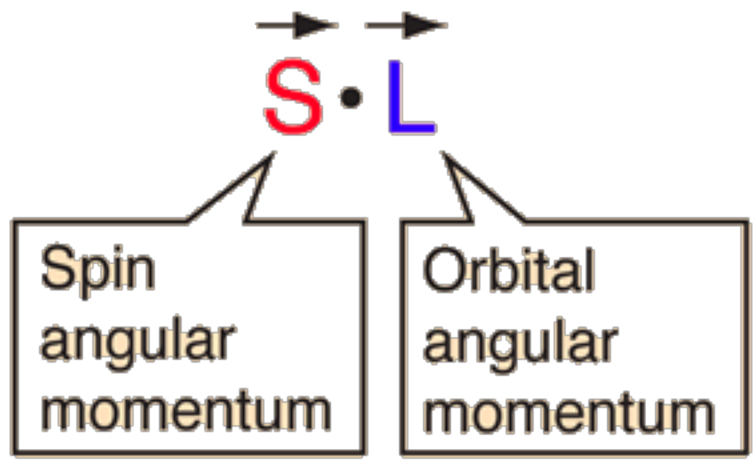
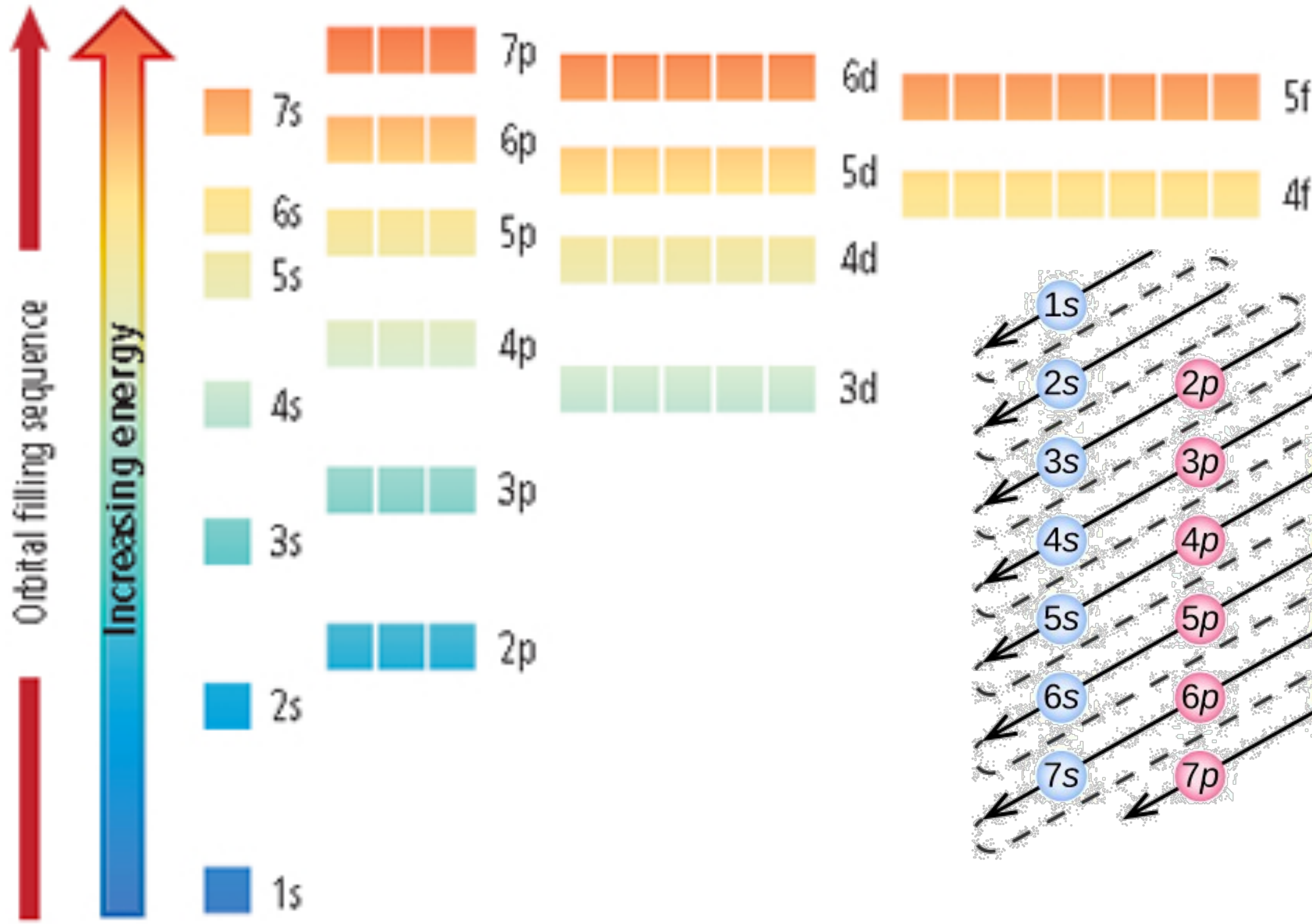
D. $m_l = 1$, $m_s = 1/2$ and $m_l = 1$, $m_s = -1/2$

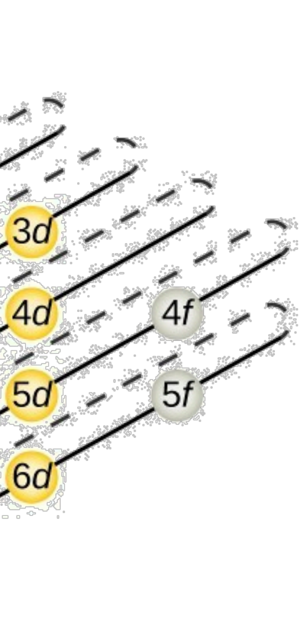
Hund's Rule III

- Spin-Orbit coupling lowers energy levels where L and S are anti-aligned and raises those where they are aligned



Energy Levels





Concept Check

- Lithium has three protons (and four neutrons) in the nucleus, surrounded by three electrons. For the outermost electron (well outside of the inner two), what does the nuclear charge appear to be?

- 0
- ~ +e
- ~ +2e
- ~ +3e

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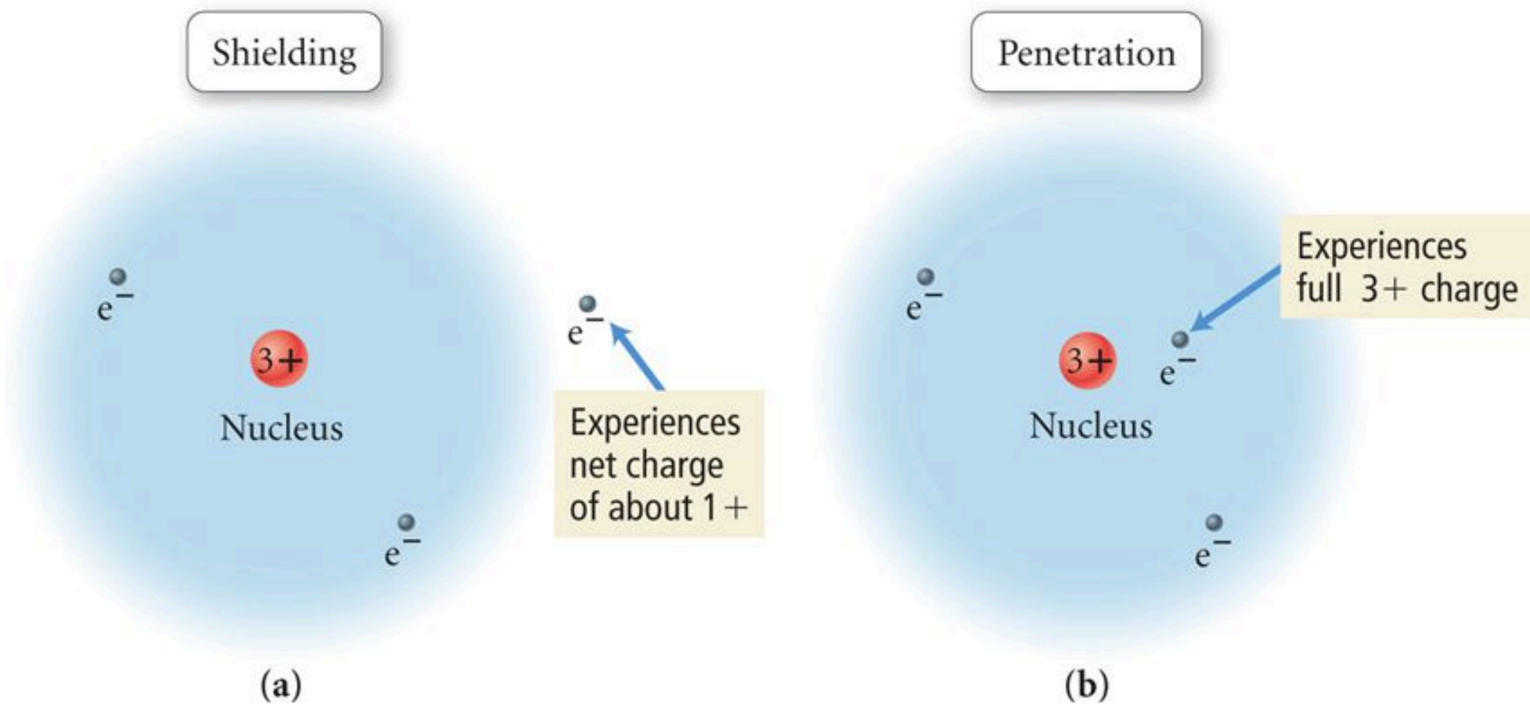
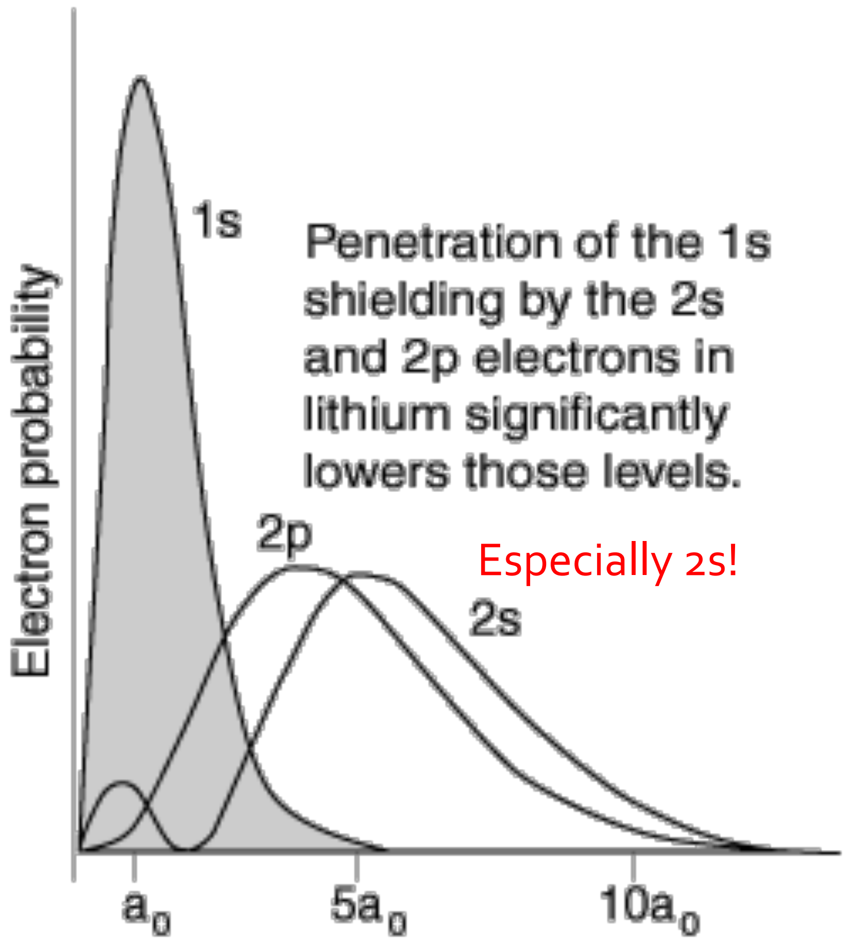
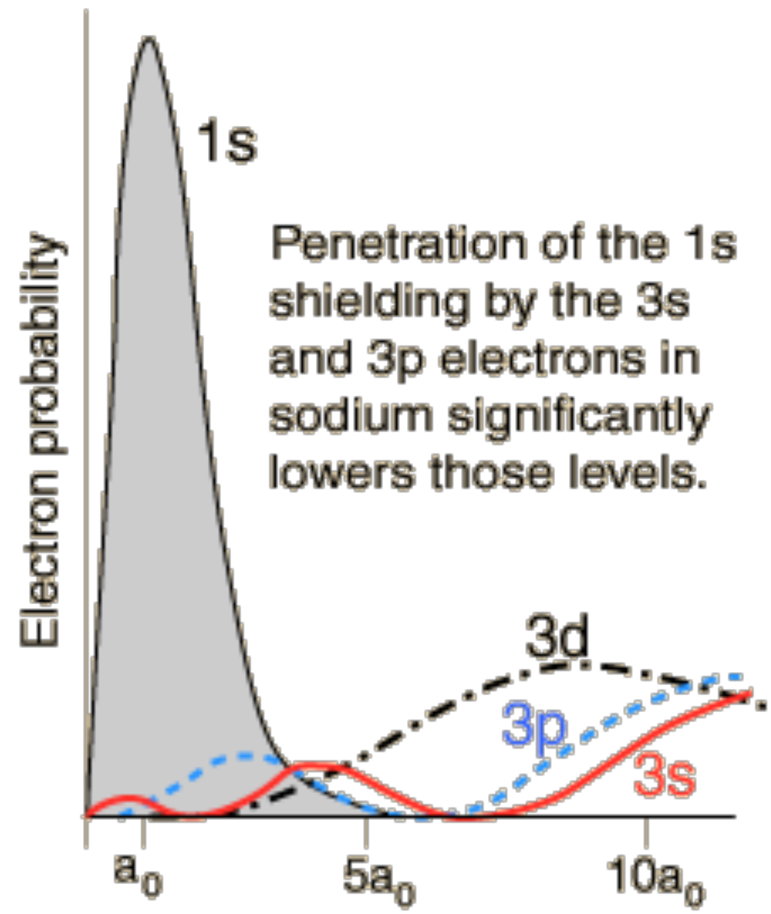
Penetration and Shielding



Penetrating Orbits





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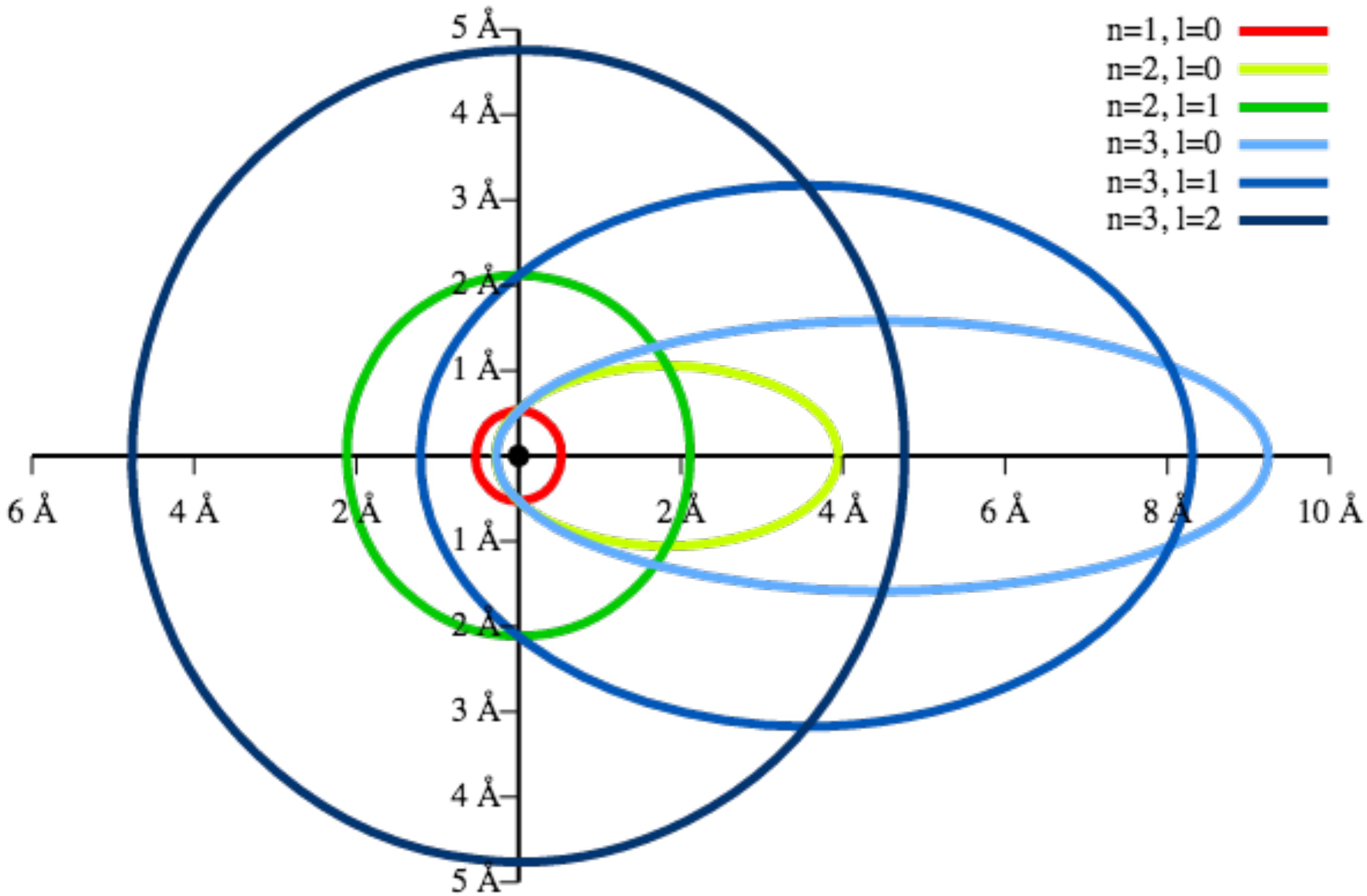
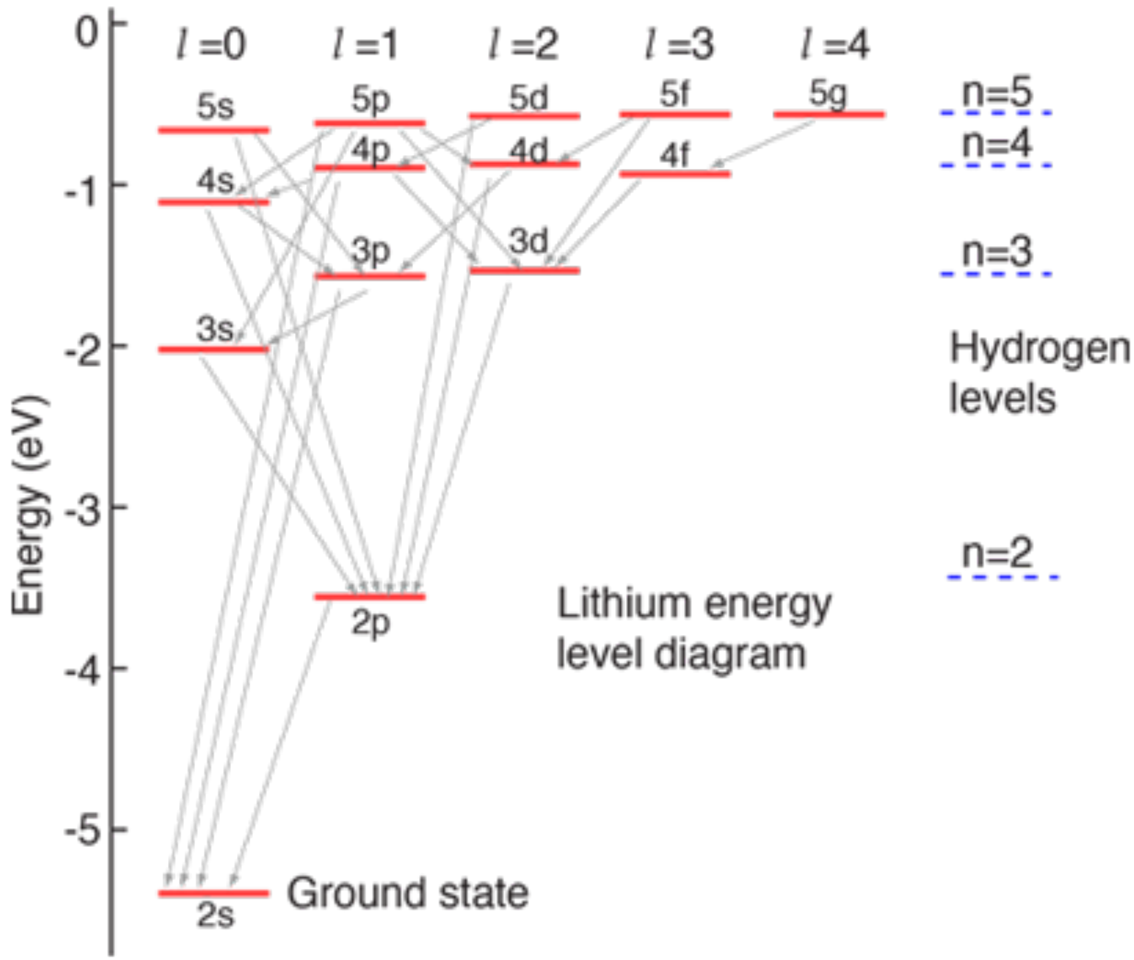


Lithium (Z=3) Transitions



Concept Check

- The binding energy of hydrogen (one electron in 1s orbital) is 13.6 eV. Helium has two 1s electrons. Would you expect the binding energy of each electron to be…

- Less than for hydrogen?
- Equal to hydrogen?
- Greater than for hydrogen?

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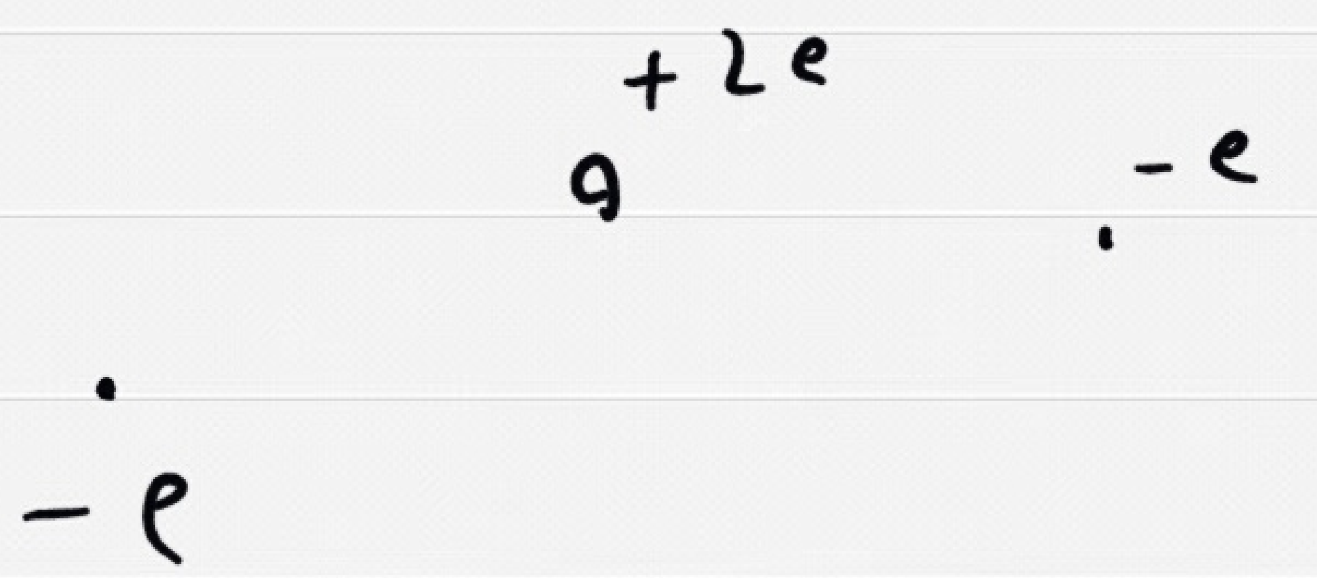
Helium



E_n for $Z = 2$
w/ no screening

$$E_n = -13.6\, Z^2/n^2$$
$$= -54.4/n^2$$

E_n w/ perfect screening
$Z_{eff} = 1 \qquad E_n = -13.6/n^2$

Actual $E_1 = -25.4$

Characterize as $E_1 = -13.6\, Z_{eff}^2$

$\Rightarrow Z_{eff} \sim 1.37$

2nd electron screens
~ 31 % of nuclear charge

Helium (Z=2) Transitions