CH101 - Multi-electron atoms handout

What we know about electron waves so far

(**Big idea #1**) More loops (n) = more energy (and bigger)

$E_n = -(2.18 \text{ aJ})(Z^2/n^2)$

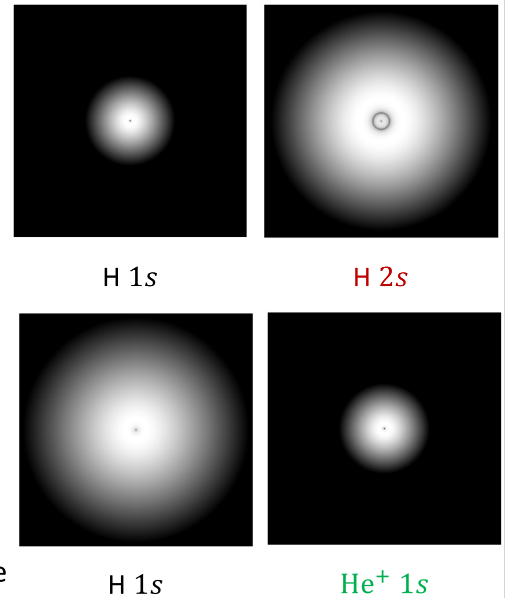
(**Big idea #2**) Bigger nuclear charge (Z) = lower energy (and smaller)

(**Big idea #3**) Electrons will always be the lowest possible energy (a.k.a., the Aufbau principle)

(**Big idea #4**) No two electrons can have the same set of 4 QN's (Pauli exclusion)

(**Little idea #5**) Electrons can shield each other from feeling the full nuclear charge

(**Little idea #6**) Hund's Rule: Electrons in different AOs are more stable when their spins are the same (parallel).

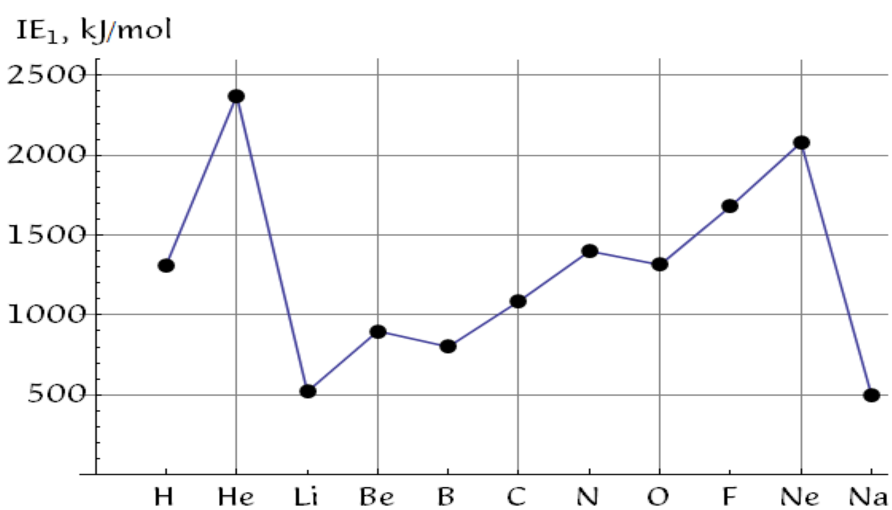


BOSTON UNIVERSITY

1

CH101 - Multi-electron atoms handout

First ionization energy of first two periods

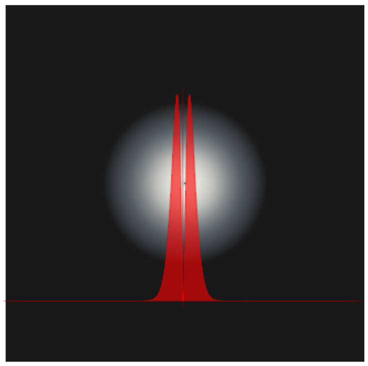


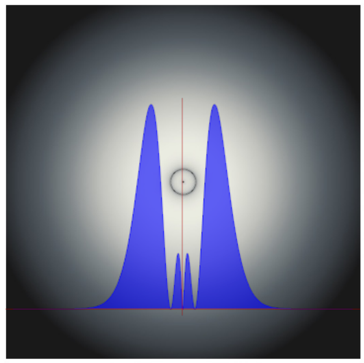
BOSTON UNIVERSITY

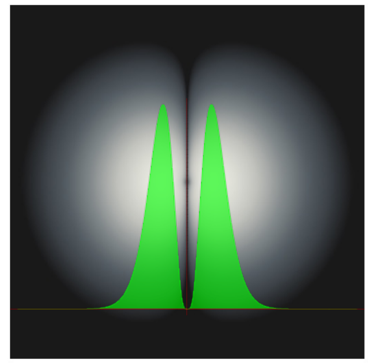
2

CH101 - Multi-electron atoms handout

Two of lithium's electrons are 1s



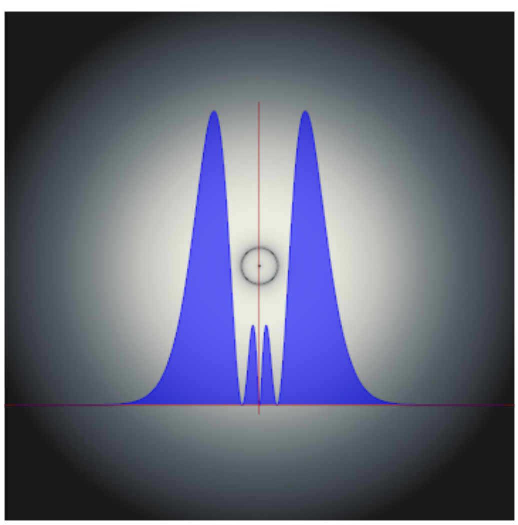




3

CH101 - Multi-electron atoms handout

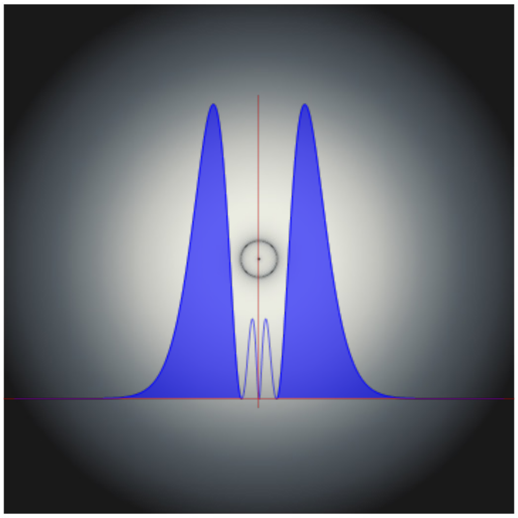
2s portion of Li $1s^22s$ electron cloud



4

CH101 - Multi-electron atoms handout

2s **outer loop** of Li $1s^2 2s$ electron cloud

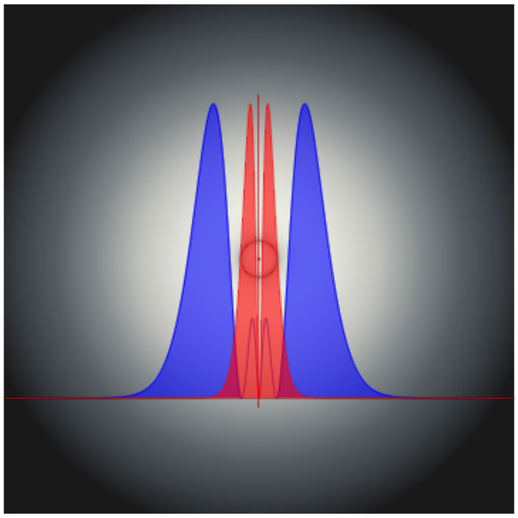


BOSTON UNIVERSITY

5

CH101 - Multi-electron atoms handout

2s **outer loop is shielded** by $1s^2$ cloud

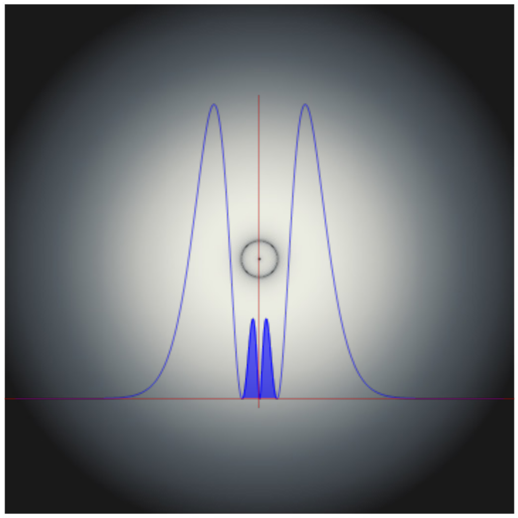


BOSTON UNIVERSITY

6

CH101 - Multi-electron atoms handout

2s inner loop of Li $1s^2 2s$ electron cloud

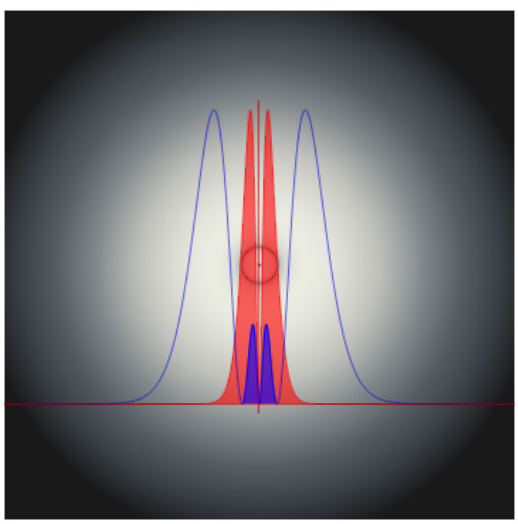


BOSTON UNIVERSITY

7

CH101 - Multi-electron atoms handout

2s inner loop is not shielded by $1s^2$ cloud

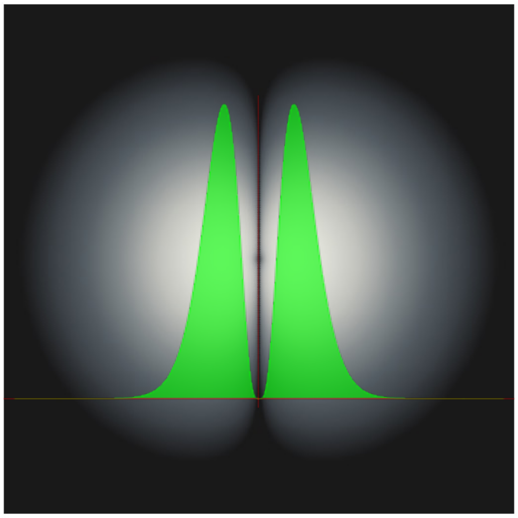


BOSTON UNIVERSITY

8

CH101 - Multi-electron atoms handout

2p portion of Li $1s^2 2p$ electron cloud

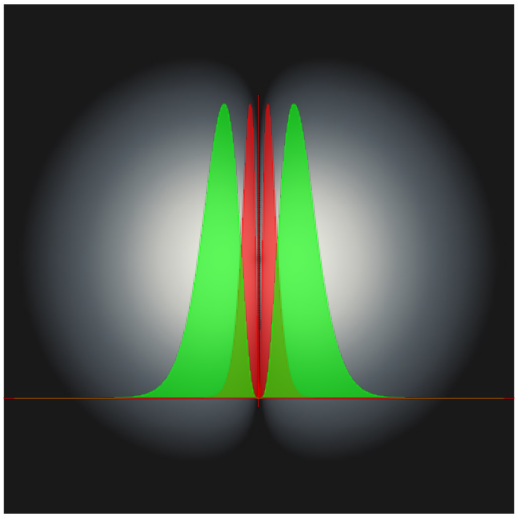


BOSTON UNIVERSITY

9

CH101 - Multi-electron atoms handout

2p is shielded by $1s^2$ cloud

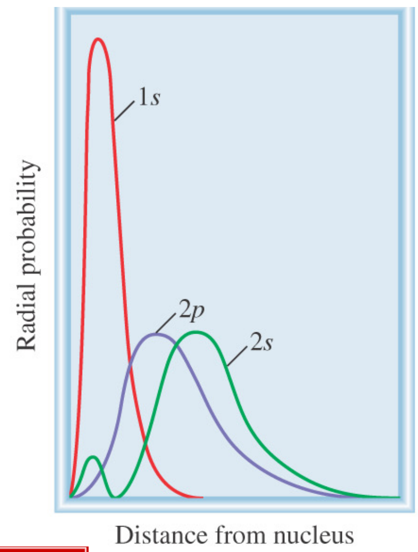


BOSTON UNIVERSITY

10

CH101 - Multi-electron atoms handout

Shielding of 2p

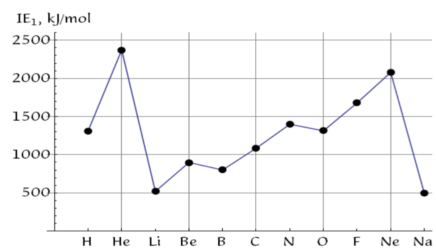


BOSTON UNIVERSITY

11

CH101 - Multi-electron atoms handout

First ionization energy, I_1



Big take-away messages:

- **Biggest effect** is number of loops (n)
- Then we look at the nuclear charge
  In general, increasing Z leads to larger Z_{eff} and higher ionization energy

Small things:

- First new shielding (i.e., new subshell) decreases IE
- First electron/electron repulsion decreases IE

TRENDS: (a) Size and (b) Ionization energy→ ALL FOLLOW ABOVE RULES!

$E_n = -(2.18 \text{ aJ}) Z_{eff}^2/n^2$

radius = 52.9 pm n^2/Z_{eff}^2

BOSTON UNIVERSITY

12

CH101 - Multi-electron atoms handout

Periodic Trends summary

Valence electrons are the ones with the largest value of "*n*" (number of loops) → easiest to ionize and largest in size

Trends:

(1) Down family → increase *n*, so decrease in ionization energy (also explains why alkali metals are the lowest ionization energy)

(2) Across period → increase Z leads to increase Z_{eff} and so increase in ionization energy (explains why the noble gases are the highest ionization energies)

(3) Small "blips" across period → shielding and e^-/e^- repulsion

BOSTON UNIVERSITY

13