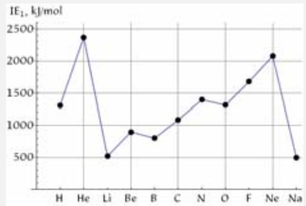


[TP] The decrease in IE_1 from Be to B primarily is due to ...



20% 1. increase in atom size
20% 2. increase in the number of loops in the atomic orbitals
20% 3. increase in electrical shielding
20% 4. increase in effective nuclear charge
20% 5. some other reason

Lecture 34 CH101 A1 (MWF 9 am)

Monday, December 5, 2016

- Complete: Electrical shielding of one electron by others http://goo.gl/hMNPLA
- Building electron configurations

Next lecture: Begin ch 10: Modelling bonding in molecules. Bonding in diatomic molecules http://goo.gl/1h0S9C

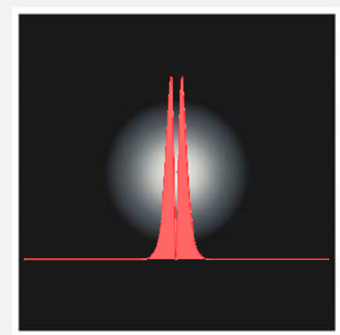
The goal: Why $1s^22s$ and not $1s^22p$

The Li atom electron configuration $1s^22s$ is more stable than $1s^22p$.

The reason is, the 2s electron feels a greater nuclear charge, Z_{eff}, than does the 2p electron.

The following illustrations (http://goo.gl/hMNPLA) show qualitatively why this is so.

$1s^2$ portion of Li electron cloud



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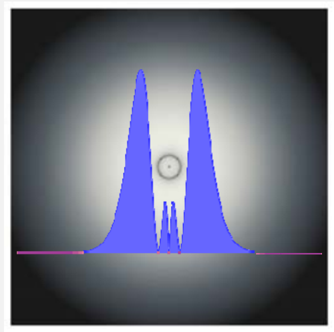
2s portion of Li $1s^22s$ electron cloud



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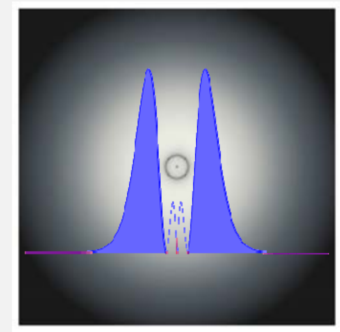
2s **outer loop** of Li $1s^22s$ electron cloud



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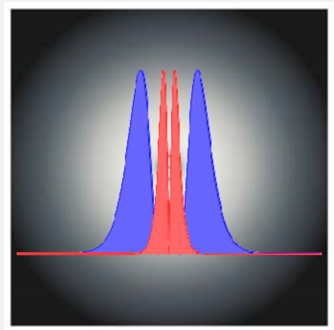
2s **outer loop is shielded** by $1s^2$ cloud



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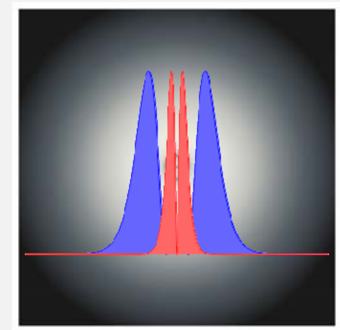
For ~90% of 2s, $Z_{\text{eff,outer}} \approx 0.90 \times (3 - 2) = 0.9$



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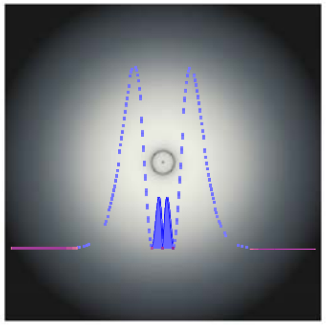
2s inner loop of Li $1s^2 2s$ electron cloud



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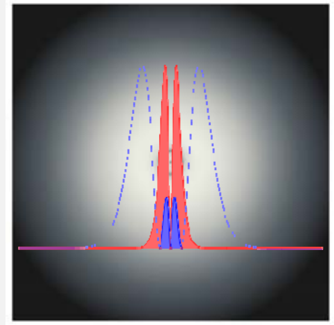
2s inner loop is not shielded by $1s^2$ cloud



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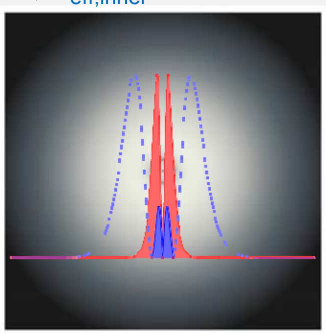
For ~10% of 2s, $Z_{eff,inner} \approx 0.10 \times 3 = 0.3$



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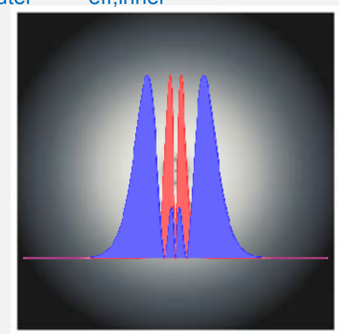
$Z_{eff,2s} = Z_{eff,outer} + Z_{eff,inner} = 0.9 + 0.3 = 1.2$



Li $1s^2 2s$ valence electron energy

$E_{2s} = -13.6 \text{ eV } Z_{\text{eff},2s}{}^2/4$

$= -13.6\text{eV x } 1.2^2/4 = -4.90 \text{ eV}$

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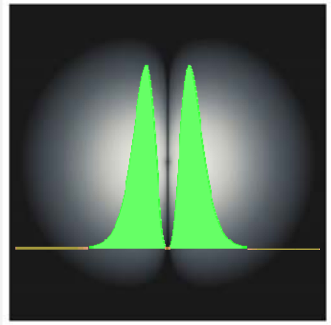
2p portion of Li $1s^2 2p$ electron cloud



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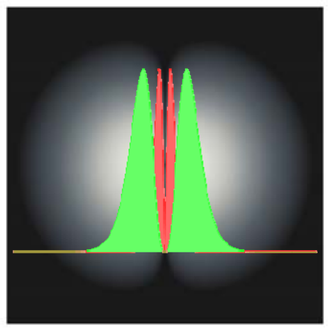
2p is shielded by $1s^2$ cloud



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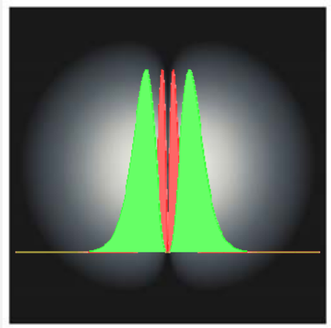
For ~100% of 2p, $Z_{\text{eff},2p} \approx 1 \text{ x } (3 - 2) = 1$



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Li 1s²2p valence electron energy

$E_{2p} = -13.6 \text{ eV } Z_{eff,2p}^2/4$

$= -13.6 \text{ eV x } 1^2/4 = -3.40 \text{ eV}$

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Li 1s²2s more stable than Li 1s²2p

$E_{2s} = -13.6 \text{ eV } Z_{eff,2s}^2/4$

$= -13.6\text{eV x } 1.2^2/4 = -4.90 \text{ eV}$

$E_{2p} = -13.6 \text{ eV } Z_{eff,2p}^2/4$

$= -13.6 \text{ eV x } 1^2/4 = -3.40 \text{ eV}$

The reason is, the 2s electron feels a greater nuclear charge, Z_{eff}, than does the 2p electron.

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Building electron configurations

Make a sketch of IE versus atom, for H through Na.

The goal: Understand the pattern of stability across the periodic table.

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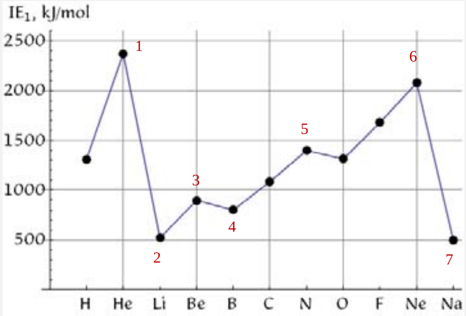
$IE_1 = 13.6 \text{ eV } Z_{eff}^2/n^2$



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Li $1s^3$?

Not possible, since at least two electrons would have the same spin in the same orbital.

Such an electron wave vanishes everywhere and so there can be no atom with this configuration.

Energy order of relative spins (Pauli)

Key point: “spin” = magnetic moment, either up or down

↑↑ impossible; ↑↓ (worst) > ↑ ... ↓ > ↑ ... ↑ (best)

Li $1s^2 2s$ or $1s^2 2p$?

The 2s inner loop escapes the shielding of the $1s^2$ part of the electron cloud.

The 2p has no inner loop and so would be more shielded by the $1s^2$ part of the electron cloud.

Hence, the 2s electron experiences slightly greater nuclear charge (Z_{eff}) and so it is more tightly held than the 2p electron would be.

So, $1s^2 2s$ is more stable than $1s^2 2p$

Be $2s^2$ or $2s2p$?

$2s^2$ are in same orbital and so must have greater electron-electron repulsion

But, the 2s inner loops result in greater nuclear attraction than the 2p.

Nuclear attraction trumps electron repulsion, and so $2s^2$ is more stable.

B $2s^3$ or $2s^22p_x$ or $2s^22p_y$ or $2s^22p_z$?

$2s^3$ is not possible for the same reason as $1s^3$ is not.

Either $2s^22p_x$ or $2s^22p_y$ or $2s^22p_z$ are possible and equivalent.

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C $2p_x^2$ or $2p_x2p_y$?

$2p_x^2$ are in same orbital and so must have greater electron-electron repulsion

What about electrons in different 2p orbitals?

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Energy order of relative spins (Pauli)

Key point: "spin" = magnetic moment, either up or down

↑↑ impossible; ↑↓ (worst) > ↑ ... ↓ > ↑ ... ↑ (best)

↑↓ (worst): Electrons in same spatial region (orbital) and so repel one another the most

↑ ... ↓: Electrons clump together (Fermi clump) in different spatial regions (orbitals) and so repel somewhat less

↑ ... ↑ (best): Electrons "avoid" one another (Fermi hole) and are in different spatial regions (orbitals) and so repel one another the least

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C $2p_x^2$ or $2p_x2p_y$?

$2p_x^2$ are in same orbital and so must have greater electron-electron repulsion

What about electrons in different 2p orbitals?

$2p_x2p_y$ can have spins parallel and so decreased repulsion (Fermi hole).

Both configurations have the same nuclear attraction (Z_{eff} and no inner loops).

Hence $2p_x2p_y$ (or $2p_x2p_z$ or $2p_y2p_z$) more stable.

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N $2p_x^2 2p_y$ or $2p_x 2p_y 2p_z$?

In $2p_x^2 2p_y$ the $2p_x$ is in same orbital and so must have greater electron-electron repulsion

In $2p_x 2p_y 2p_z$ all spins are parallel and so there are only Fermi holes and so reduced repulsion.

Hence $2p_x 2p_y 2p_z$ is more stable.

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O $2p_x 2p_y^2 2p_z$ or $2p_x 2p_y 2p_z 3s$?

$2p_x 2p_y^2 2p_z$ has increased electron repulsion (Fermi clump).

$2p_x 2p_y 2p_z 3s$ has decreased electron repulsion (Fermi hole).

$2p_x 2p_y^2 2p_z$ has greater nuclear attraction since the n = 2 orbitals are more bound than n = 3 orbitals.

Nuclear attraction trumps electron repulsion, and so $2p_x 2p_y^2 2p_z$ is more stable.

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