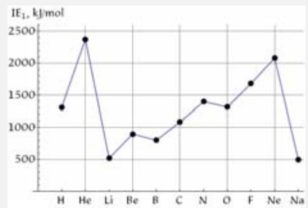


[TP] The steady increase in IE_1 from Li to Ne primarily is due to …

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



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Lecture 35 CH101 A2 (MWF 11:15 am)
Wednesday, December 6, 2017

For today …
- Electron shielding of one electron by others: http://goo.gl/hMNPLA
- Building electron configurations

Next lecture: Complete: Building electron configurations; Modeling bonding in molecules: http://goo.gl/1h0S9C

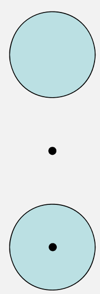
Note: We will not use Slater's rules for Z_{eff}, so please ignore Mahaffy et al., section 8.6, pages 289 to 291.

Lesson of shielding demonstration

Graduate cylinder, charge seen is "–"

Bakelite rod, charge seen is "+"

Rod inside cylinder, charge seen is 0



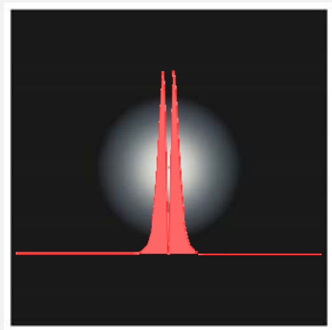
The goal: Why Li is $1s^22s$ and not $1s^22p$

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

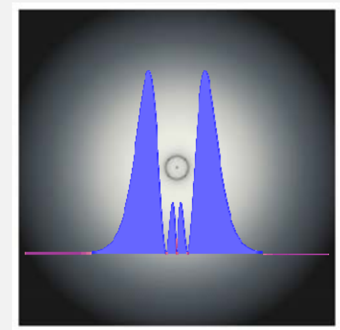
The reason is, the 2s electron feels a greater nuclear charge, Z_{eff}, than does the 2p electron.

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

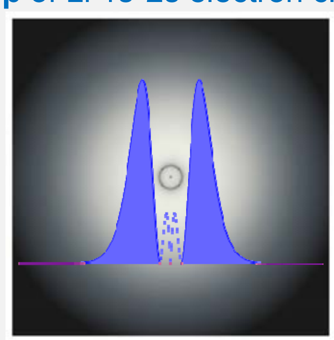
$1s^2$ portion of Li electron cloud



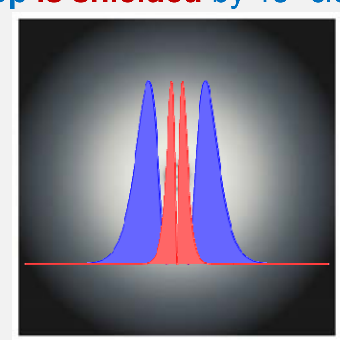
2s portion of Li $1s^22s$ electron cloud



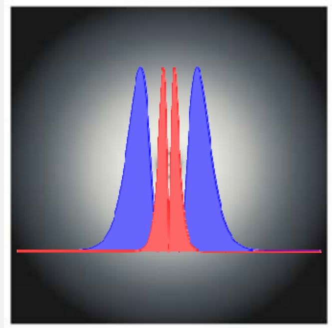
2s **outer loop** of Li $1s^22s$ electron cloud



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



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



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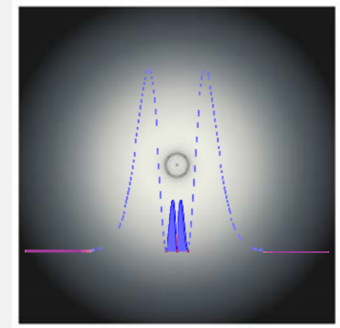
2s inner loop of Li $1s^22s$ electron cloud



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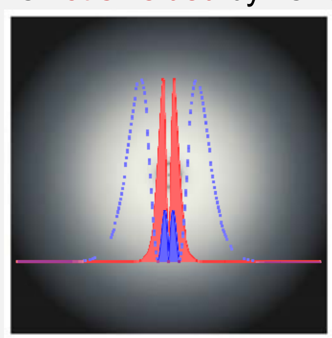
2s inner loop is not shielded by $1s^2$ cloud



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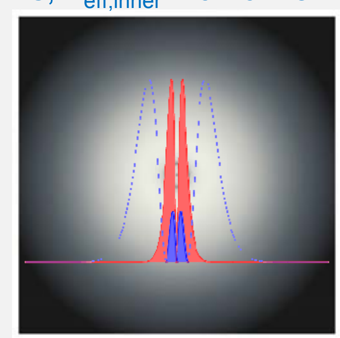
For ~10% of 2s, $Z_{eff,inner} \approx 0.10 \times 3 = 0.3$



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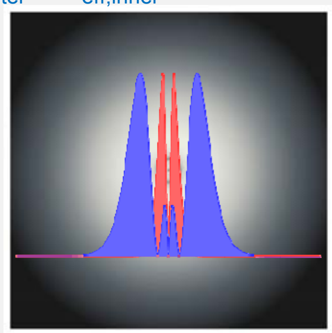
$Z_{\text{eff},2s} = Z_{\text{eff,outer}} + Z_{\text{eff,inner}} = 0.9 + 0.3 = 1.2$

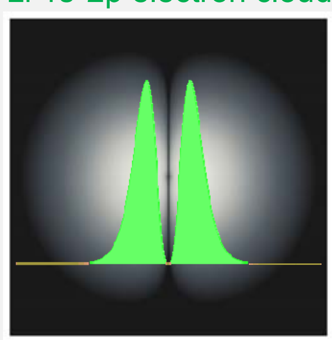


Li $1s^2 2s$ valence electron energy

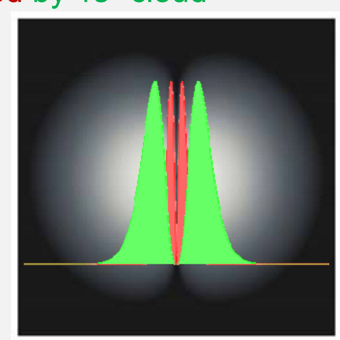
$$E_{2s} = -13.6\ \text{eV} \times \frac{Z_{\text{eff},2s}^2}{2^2}$$

$$= -13.6\text{eV} \times \frac{1.2^2}{4} = -4.90\ \text{eV}$$

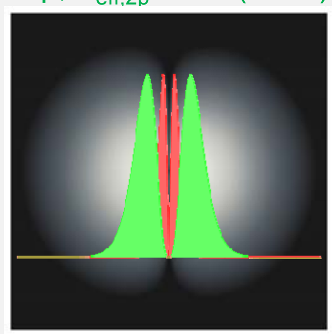
2p portion of Li $1s^2 2p$ electron cloud



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



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



Li 1s²2p valence electron energy

$$E_{2p} = -13.6\text{ eV} \times \frac{Z^2_{eff,2p}}{2^2}$$

$$= -13.6\text{ eV} \times \frac{1^2}{4} = -3.40\text{ eV}$$

Li 1s²2s more stable than Li 1s²2p

$$E_{2s} = -13.6\text{ eV} \times \frac{Z^2_{eff,2s}}{2^2} = -13.6\text{eV} \times \frac{1.2^2}{4} = -4.90\text{ eV}$$

$$E_{2p} = -13.6\text{ eV} \times \frac{Z^2_{eff,2p}}{2^2} = -13.6\text{ eV} \times \frac{1^2}{4} = -3.40\text{ eV}$$

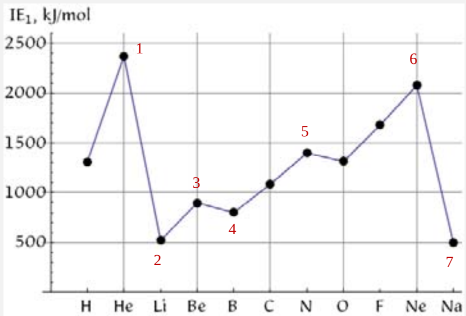
The reason is, the 2s electron feels a greater nuclear charge, Z_{eff}, than does the 2p electron.

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.

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



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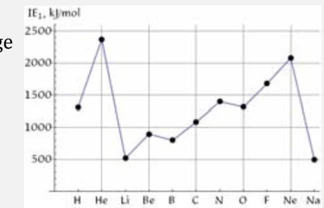

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Li $1s^3$?

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

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

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Energy order of relative spins (Pauli)

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

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

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Li $1s^22s$ or $1s^22p$?

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, $1s^22s$ is more stable than $1s^22p$

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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 more important than electron repulsion, and so $2s^2$ is more stable.

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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.

