Review

Quantization of Energy = e^- are confined to very specific energies as they interact with the nucleus of an atom

- these energies can be calculated for 1 e^- atoms (can also be done for multi-e- atoms, but it's much more difficult!)

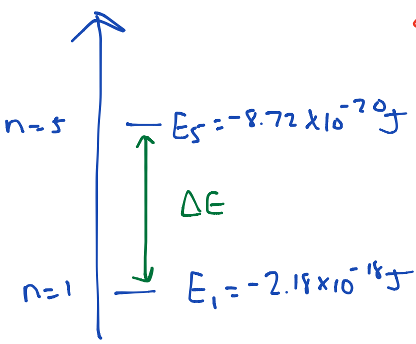
$$E_n = \frac{-2.18\times10^{-18}J}{n^2}(z)^2$$

only for an atom with 1 e^-! (H, He^+, Li^{2+}, Be^{3+}, etc)

Hydrogen ($z=1$)

$$E_1 = \frac{-2.18\times10^{-18}J}{1^2}(1)^2 = -2.18\times10^{-18}J$$

$$E_5 = \frac{-2.18\times10^{-18}J}{5^2}(1)^2 = -8.72\times10^{-20}J$$



So, in the 1st shell, the e^- is attracted to the nucleus with $-2.18\times10^{-18}J$ of potential (negative is good)

In the 5th shell, only $-8.72\times10^{-20}J$

-An e^- in the 5th shell does NOT interact with a nucleus as strongly as the 1st shell (this is consistent with Coulomb's law)

The difference in energy between these levels (ΔE) is the amount of energy that is required to move the e^- from n=1 to n=5 (this takes energy) or the energy that is released when the e^- relaxes back to n=1

Calculate Ephoton that is required to excite an e^- from the groundstate (n=1) to the 4th excited state (n=5)

$$\Delta E = E_5 - E_1 = -8.72\times10^{-20}J - (-2.18\times10^{-18}J) = 2.09\times10^{-18}J$$

Is this in the UV, vis or IR?

for H atom $E_n \rightarrow E_1$ is always UV (Lyman series)

$$E_{photon} = \frac{hc}{\lambda} \qquad \lambda = \frac{hc}{E} = \frac{6.626\times10^{-34}Js\,(2.998\times10^{8}\frac{m}{s})}{2.09\times10^{-18}J}$$

$$\lambda = 9.49\times10^{-8}m \cdot \frac{1nm}{10^{-9}m} = \boxed{94.9nm} \text{ UV}$$

These same ideas can be extended to multi-e^- atoms, but the math to calculate e^- levels is not as simple.

- Important points for Energy diagrams:

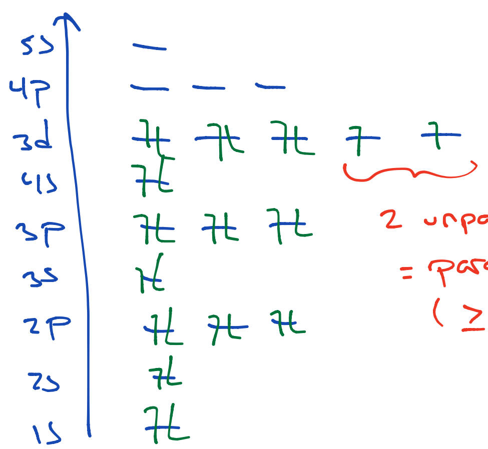
  s = — 1 orbital

  p = — — — 3 orbitals

  d = — — — — — 5 orbitals

  f = — — — — — — — 7 orbitals

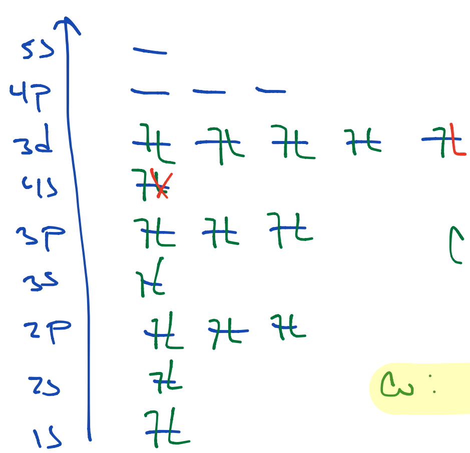
- order follows the e^- config: 1s 2s 2p 3s 3p 4s 3d 4p etc



2 unpaired e^-
= paramagnetic
(≥ 1 unpaired)

- fill lowest energy 1st
- 1 e^- per orbital for degenerate orbitals
- filled shell = super stable
- filled subshell = very stable
- ½ filled subshell = stable

Ni: $1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,4s^2\,3d^8$



Cu: $1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,\cancel{4s^2\,3d^9}$

more stable to fill d^{10}!

Cu: $1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,4s^1\,3d^{10}$

Periodic Trends

All trends we talk about deal with how an electron interacts with the nucleus

Important players:

- Coulombs Law → how strongly is the e⁻ attracted to the nucleus

$$E_p \propto \frac{q_1 q_2}{r}$$

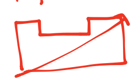
$q_1 = -1 =$ charge of e⁻

$q_2 = Z =$ charge of nucleus

- Extra stable e⁻ configurations. → Filling a shell is REALLY favorable
  - filling any subshell is favorable → s^2, p^6, d^{10} ← super good!
  - A half full subshell is more favorable than not half full → d^5 = good, d^4 = not as good
- Shielding → inner e⁻ shield outer e⁻ from feeling the full "pull" of the nucleus

Ionization Energy: $X \rightarrow X + e^-$

general trend



predicted by

① Coulomb's Law

② Exception to trend explained by considering stable e^- configs (see above for examples)

Ok, so we have an Lithium atom that undergoes this reaction:

$Li \longrightarrow Li^+ + e^-$ — we are forming an ion $\rightarrow$ this is an ionization process

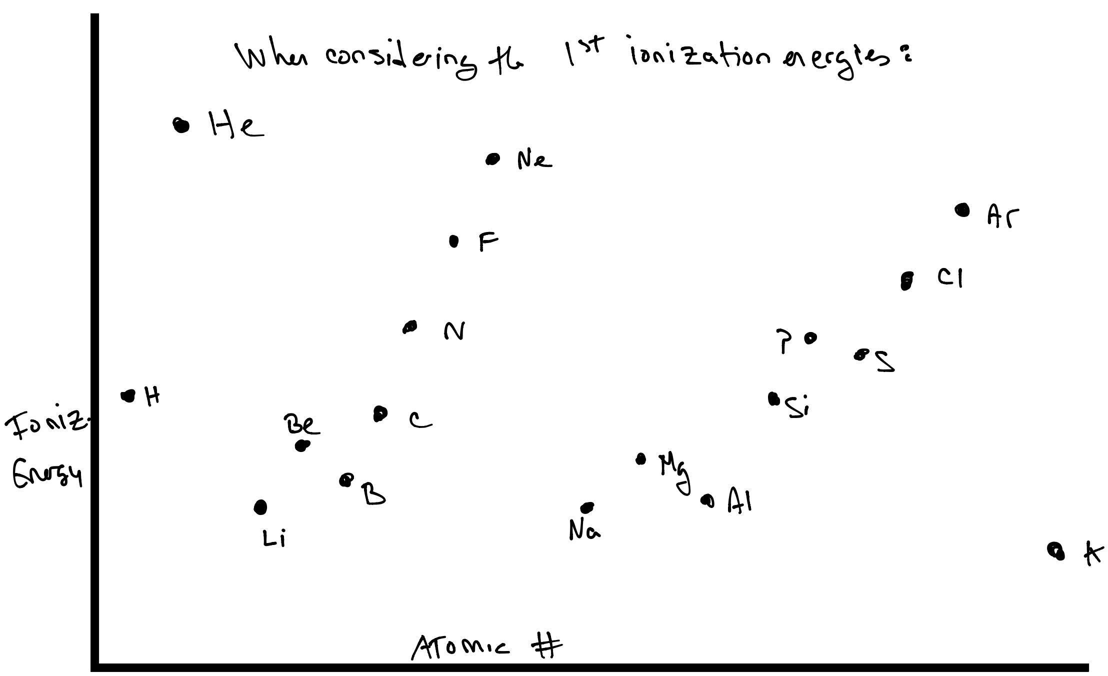
because that electron is attracted to the (+) nucleus (Potential energy < ⊖)
It takes energy to get the electron to separate; It takes energy to make this ionization reaction happen.

This is called an ionization energy → actually the 1st ionization energy

$Li^+ \rightarrow Li^{2+} + e^-$ ⟹ 2^{nd} ionization

$Li^{2+} \rightarrow Li^{3+} + e^-$ ⟹ 3^{rd} ionization

When considering the 1st ionization energies:



H vs He

$Z=1$ $\quad$ $Z=2$

$1e^-$ $\quad$ $2e^-$

He

(+2) $\quad e^-$

$$E = \frac{+2(-1)}{r} = \frac{-2}{r}$$

H

$$E = \frac{(+1)(-1)}{r} = -\frac{1}{r}$$

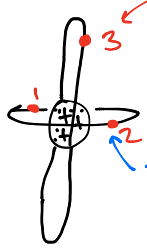
So He is more negative ∴ the e^- is more attracted to the nucleus

But Li has +3, so shouldn't $E = -3/r$ be more stable than He (and therefore take more energy to ionize)?

No, because the 3rd electron in Li occupies a new shell!

Roughly speaking, as we move to a new period, an atom gets a new shell!

So Z, still $= +3$, but now r is <u>much</u> bigger for Li than He or H



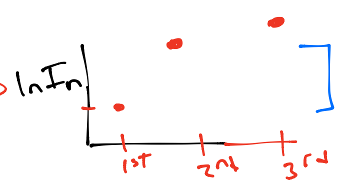
this e^- is weakly bound because its farther away from the nucleus

$Li \rightarrow Li^+ + e^-$ $\quad I_1$

$Li^+ \rightarrow Li^{2+} + e^-$

this e^- is much closer to the nucleus because its in the 1st shell

In is used b/c the difference in energies is <u>VERY</u> big



big difference b/c going down a shell

So why is the 1st Ionization energy for Be > Li?

Now we're back to the charge of the nucleus:

(radii are about equal b/c in the same shell)

Be

$$\frac{+4(-1)}{r} > \frac{+3(-1)}{r}$$

more energy is needed for Be b/c more protons

The 1st two ionization energies for Carbon are 1.81 & 3.90 aJ

How much energy is required to create C^{+2}?

atto = 10^{-18}

$C \rightarrow C^{+} + e^{-}$ 1.81 aJ
$C^{+} \rightarrow C^{2+} + e^{-}$ 3.90 aJ
} added up = 5.71 aJ

Carbon Ionization energies: 1.81 → 3.90 → 7.67 → 10.3 → 62.8 → 78.5

Huge jump b/c going from 2nd shell to 1st shell

It's always the electrons in the outer-most shell that are easiest to ionize

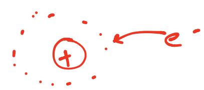
- we give these a special name ⟹ Valence electrons

Core electrons are those in the inner shells

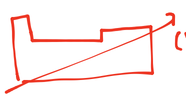
Electron Affinity : $X + e^- \rightarrow X^-$

How likely is it for an atom to GAIN an e^- to become an anion.

Think about this in the same way as Ionization Energy



e^- gets added to the atom... so it is attracted by the nucleus.

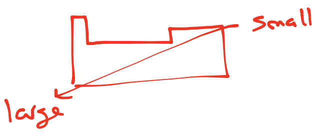


high E.A. (likely to make anion)

1. small shell (small radius) gives strong pull = ↑ E.A.
2. More protons attract e^- more
3. Creating or destroying a stable e^- config will explain deviations

Atomic Radius :

1. going to a higher shell makes a larger atom
2. within a shell, the more protons, the smaller the atom



Ionic Radius : adding or removing e^- will have a large influence on size

Na vs. Na^+

$1s^2 2s^2 2p^6 3s^1$ ← Na

$1s^2 2s^2 2p^6$ ← Na^+

atom has 3^{rd} shell e^- while the cation does not

think about the # of repulsions vs. attraction (repulsion makes the size larger)

$e^- \leftrightarrow e^-$ repel

$\oplus \leftrightarrow e^-$ attract

F^- : 9 protons + 10 e^-

F : 9 protons + 9 e^-

	attraction		repulsion	
F	9	−	9	= ∅
F^-	9	−	10	= −1

F^- has more repulsion ... bigger