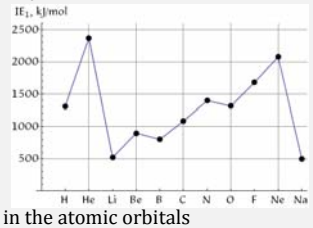
[TP] The decrease in IE_1 from Be to B primarily is due to ...



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

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Lecture 35 CH101 A1 (MWF 9 am)

Wednesday, December 7, 2016

- Complete: Building electron configurations

Begin ch 10: Modeling bonding in molecules
- Mixing AO's makes MO's https://goo.gl/eliM2a

Next lecture: AO-MO correlation diagrams; 2p MO's https://goo.gl/2MEiRA; B2 to Ne2 (!); When atoms are different, which AO's make MO's: Symmetry, overlap, energy (SOE)

Bonding in diatomic molecules http://goo.gl/1h0S9C
Questions on Symmetry, Overlap, Energy (SOE) http://goo.gl/oYEf3b

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

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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 $2p_x2p_y^2 2p_z$ or $2p_x2p_y2p_z3s$?

O $2p_x2p_y^2 2p_z$ or $2p_x2p_y2p_z3s$?

$2p_x2p_y^2 2p_z$ has increased electron repulsion (Fermi clump).

$2p_x2p_y2p_z3s$ has decreased electron repulsion (Fermi hole).

$2p_x2p_y^2 2p_z$ has greater nuclear attraction since the n = 2 orbitals are more bound than n = 3 orbitals.

Nuclear attraction trumps electron repulsion, and so $2p_x2p_y^2 2p_z$ is more stable.

F $2p_x^2 2p_y^2 2p_z$ or $2p_x2p_y^2 2p_z3s$?

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

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

$2p_x^2 2p_y^2 2p_z^2$ has larger Z_{eff}, since 2p electrons do not shield

$2p_x^2 2p_y^2 2p_z 3s$ has less electron repulsion but much smaller Z_{eff}, since $n = 2$ electron shield nearly completely.

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Na $2p_x^2 2p_y^2 2p_z^2$ 3s or $2p_x^2 2p_y^2 2p_z^2$ 3p?

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Na $2p_x^2 2p_y^2 2p_z^2$ 3s or $2p_x^2 2p_y^2 2p_z^2$ 3p?

3s inner loop means 3s has more attraction than 3p.

Hence $2p_x^2 2p_y^2 2p_z^2$ 3s more stable (analogous to $1s^2 2s$ being more stable than $1s^2 2p$.

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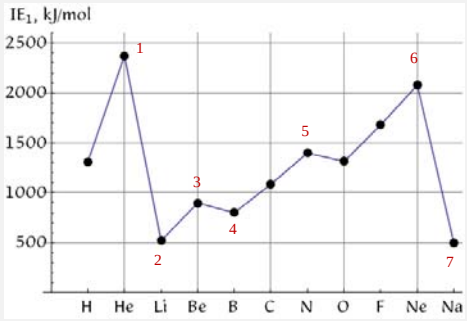
First ionization energy, IE_1



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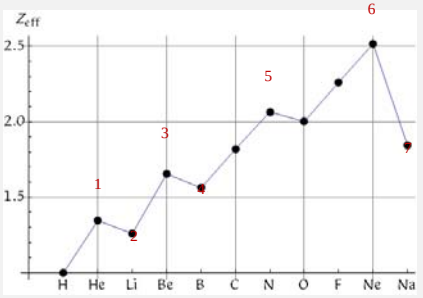
Effective nuclear charge, Z_{eff}

Z_{eff} is the value for which IE_1 is equal to the one-electron energy formula, $IE_1 = 13.6 \text{ eV } Z_{eff}^2/n^2$



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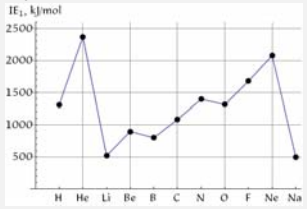

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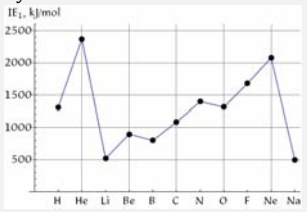
[TP] The decrease in IE_1 from N to O primarily is due to ...



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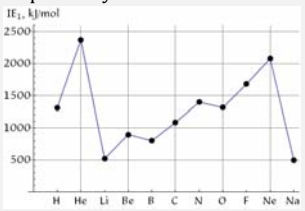
[Quiz] The steady increase in IE_1 from Li to Ne primarily is due to ...



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Bonding in diatomic molecules
http://goo.gl/1h0S9C

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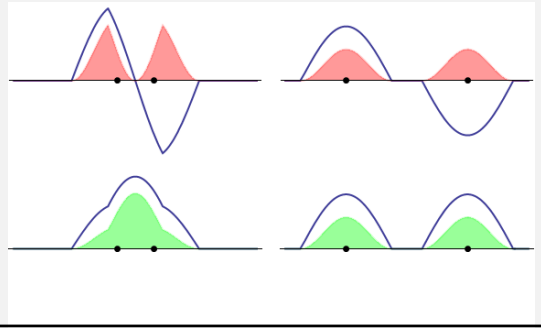
1s molecular orbitals:
http://quantum.bu.edu/CDF/101/1sMolecularOrbitals.cdf



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