

Welcome to Chemistry 154!

Chemistry for Engineering

On this sheep-scale, how do you feel today?



WOOL FOR EVERY DAY #IWOOLWOOLYOU



Reminders

- Worksheet: Unit 2
- Due September 18th at 11:59pm
- Achieve Assignment #2
- Due September 18th at 11:59pm
- Homework (optional)
- Review Chapter 2
- Watch Unit 2 Videos
- Preread the start of Unit 3 notes

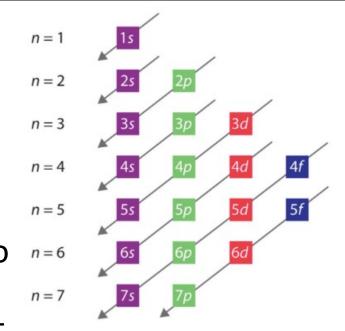
Instructor Office Hours

Monday and Friday 7-8pm via Zoom (All Lectures Site)

Worksheet →
All Lectures Canvas Site
Submission link →
Section 113 Canvas Site

Orbital Filling

- Aufbau Principle
- Fill orbitals with electrons from lowest energy first
- Pauli Exclusion Principle
- Each orbital holds no more than two electrons
- The two electrons in an orbital must have opposite spins
- Hund's Rule
- Electrons occupy orbitals of identical energy singly first (with parallel spins) before being paired up in an orbital



Electronic Structure

Electrons have negative charge but are also tiny magnets. Spin is our way of describing the orientation of the poles of these magnets ("spin up \uparrow " or "spin down \downarrow ").

The Pauli Principle states a maximum of 2 electrons can be assigned to any one orbital, and the electrons must have opposite spins $(\uparrow \downarrow)$.

Orbitals are arranged in shells, labelled by n, and sub-shells. Each shell contains only certain orbitals. Starting with the lowest shell, n=1, electrons are assigned to s, p, d orbitals until they are all accounted for. Note: orbitals get bigger as n increases (a 2s orbital is bigger than a 1s orbital) thus forming the shell structure of atoms.

Valence Electrons

For elements in the s- and p-blocks only

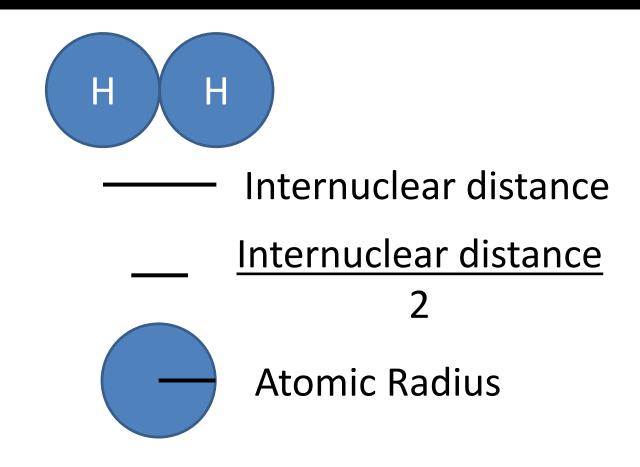
The electrons occupying the *s* and *p* subshells with the largest n (for the neutral element) are called valence electrons, and the collection of occupied subshells is called the valence shell.

Electrons which aren't valence electrons are called core electrons.

In solids, valence orbitals on atoms overlap to form valence bands extending throughout the material.

Valence electrons are fundamental to chemistry because they are involved in the formation of bonds. Core electrons are not involved in chemical bonding.

Atomic Radius



Atomic radius is calculated by measuring the internuclear distance and dividing by 2

Atomic Radius (across a period)

Element	Radius (Å)
Be	0.96
В	0.84
С	0.76
N	0.71
0	0.66
F	0.57
Ne	n/a

Atomic radius (down a group)

Element	Radius (Å)
Li	1.28
Na	1.66
K	2.03
Rb	2.20
Cs	2.44
Fr	n/a

Effective nuclear charge (Z_{eff})

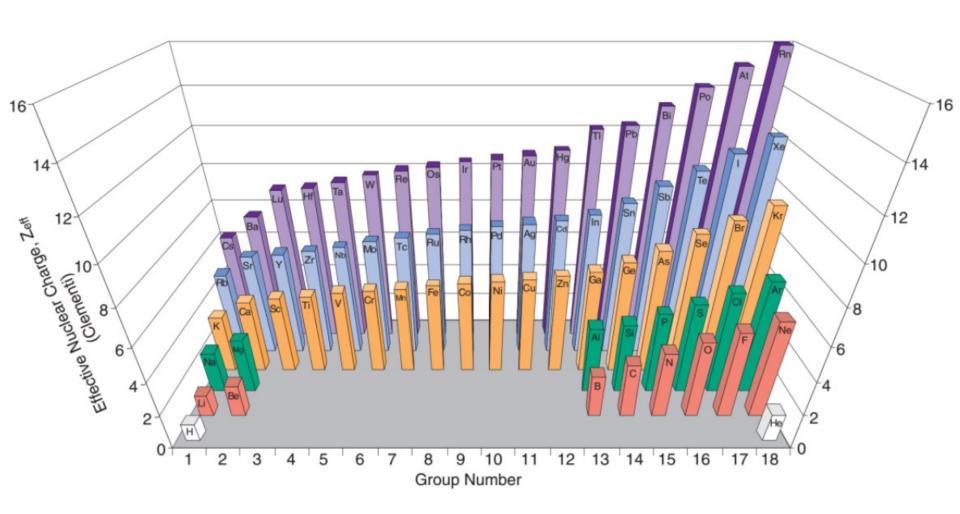
Coulomb's Law

$$E \propto \frac{q^{(+)}q^{(-)}}{r}$$

Core electrons are close to the nucleus and effectively screen some of its positive charge from valence electrons further away. Valence electrons also partially screen each other from the nuclear charge. Thus, a valence electron "feels" an effective nuclear charge ($Z_{\rm eff}$) that is less than the actual nuclear charge Z.

Note: Z_{eff} is a theoretically calculated property.

Effective nuclear charge (Z_{eff})



Ionization Energy (IE)

For atoms, molecules or ions: the minimum energy required to remove a single electron from an atom, molecule or ion in its gaseous state.

$$X(g) \rightarrow X^{+}(g) + e^{-}$$

<u>For solids</u>: the minimum energy required to remove an electron from the valence band of the solid.

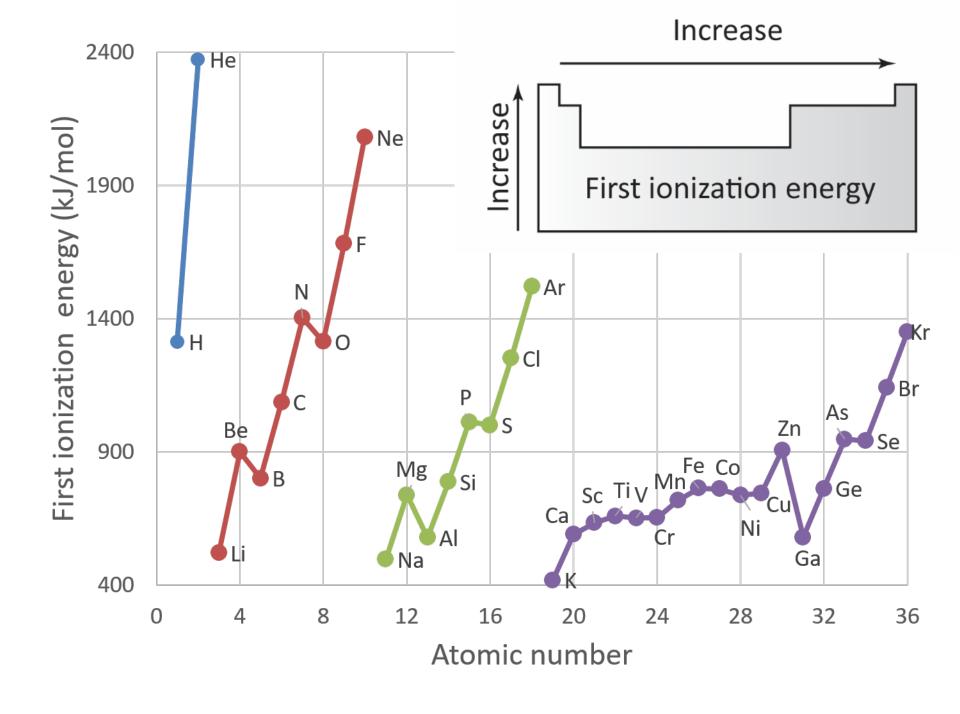
As many elements are solids, values may be available for both, and differ due to the nature of bonding in solids. The elemental values always refer to the gas phase.

Ionization Energy

Element	IE ₁ (kJ/mol)
Li	520.2
Be	899.4
В	800.6
С	1086.1
N	1402
О	1314
F	1681
Ne	2081

Ionization Energy

Element	IE ₁ (kJ/mol)
Li	520.2
Na	495.8
K	418.8
Rb	403.0
Cs	375.7
Fr	~375



DEMO TIME

$$2M(s) + 2H_2O(I) \rightarrow 2M^+(aq) + 2OH^-(aq) + H_2(g)$$

or
 $2M(s) + 2H_2O(I) \rightarrow 2MOH(aq) + H_2(g)$

where M = Li, Na, K.

Electron Affinity (EA)

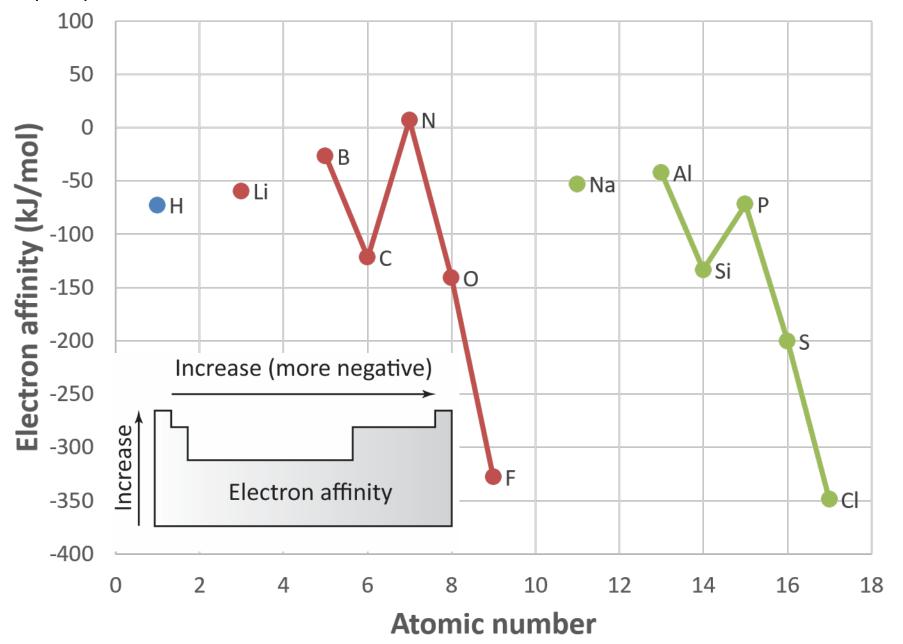
<u>For atoms or molecules</u>: the energy change resulting from the addition of a single electron to an atom or molecule in its gaseous state.

$$X(g) + e^{-} \rightarrow X^{-}(g)$$

<u>For solids</u>: the minimum energy change resulting from adding an electron to the lowest lying electronic states (of the conduction band) of the solid.

As many elements are solids, values may be available for both, and differ due to the nature of bonding in solids. The elemental values always refer to the gas phase.

He, Be, Ne and Ar do NOT form stable anions.



Clicker Question

Which equation describes the first ionization energy of Al?

- a) $Al_{(g)} + e^{-} \rightarrow Al_{(g)}^{-} + energy$
- b) $Al_{(g)}$ + energy $\rightarrow Al_{(g)}^+ + e^$
 - c) $Al^{+}_{(g)}$ + energy $\rightarrow Al^{2+}_{(g)}$ + e^{-}
 - d) $AI_{(g)}^{-}$ + energy $\rightarrow AI_{(g)}$ + e^{-}
 - e) $AI_{(s)}$ + energy $\rightarrow AI^{+}_{(aq)}$ + e^{-}

Clicker Question

Which equation describes the electron affinity of Al?

- (a) $Al_{(g)} + e^{-} \rightarrow Al_{(g)}^{-} + energy$
 - b) $Al_{(g)}$ + energy $\rightarrow Al_{(g)}^+ + e^-$
 - c) $AI^{+}_{(g)}$ + energy $\rightarrow AI^{2+}_{(g)}$ + e^{-}
 - d) $AI_{(g)}^{-}$ + energy $\rightarrow AI_{(g)}$ + e^{-}
 - e) $AI_{(s)}$ + energy $\rightarrow AI^{+}_{(aq)}$ + e^{-}

Worksheet Question #7 – GOOD QUESTION

Explain why elements with very large ionization energies also tend to have highly exothermic electron affinities.

Electronegativity (EN or χ)

- The ability of an atom to attract shared electrons to itself in a chemical bond.
- greater EN = greater affinity for e⁻
- not an atomic property because it refers to atoms in a bond
- is a calculated value, not measured
- correlates with IE and EA
- The greater the electronegativity difference, $\Delta(EN)$, the more polarized a chemical bond.

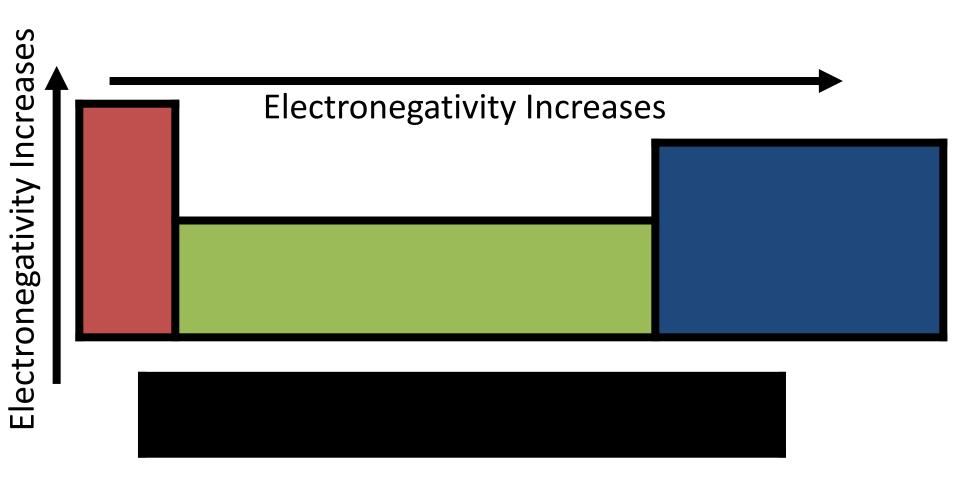
You do NOT need to know electronegativity values for exams but you MUST know the overall trend (mnemonic: FOCIN BrISCH)

H 2.20	Pauling Electronegativities											Не					
Li 0.98	Be 1.57												Ne				
Na 0.93	Mg 1.31	AI 1.61									Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar		
K 0.82	Ca 1.00	Sc 1.36	Ti 1.54	V 1.63	Cr 1.66	Mn 1.55	Fe 1.83	Co 1.88	Ni 1.91	Cu 1.90	Zn 1.65	Ga	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr 3.00
Rb 0.82	Sr 0.95	Y 1.22									In 1.78	Sn 1.96	Sb 2.05	Te 2.1] 2.66	Xe 2.60	
Cs 0.79	Ba 0.89	La	Hf 1.3	Ta	W 2.36	Re 1.9	Os 2.2	lr 2.20	Pt 2.28	Au 2.54	Hg 2.00	TI 1.62	Pb 1.87	Bi 2.02	Po 2.0	At 2.2	Rn 2.2
Fr 0.7	Ra 0.9	Ac 1.1															

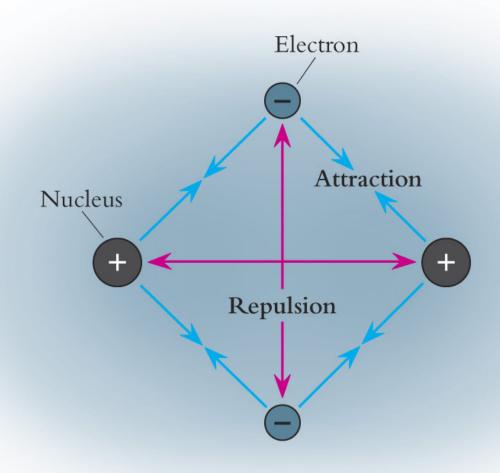
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Но	Er	Tm	Yb	Lu
1.12	1.13	1.14	1.13	1.17	1.2	1.2	1.1	1.22	1.23	1.24	1.25	1.1	1.27
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Electronegativity and the Periodic Table

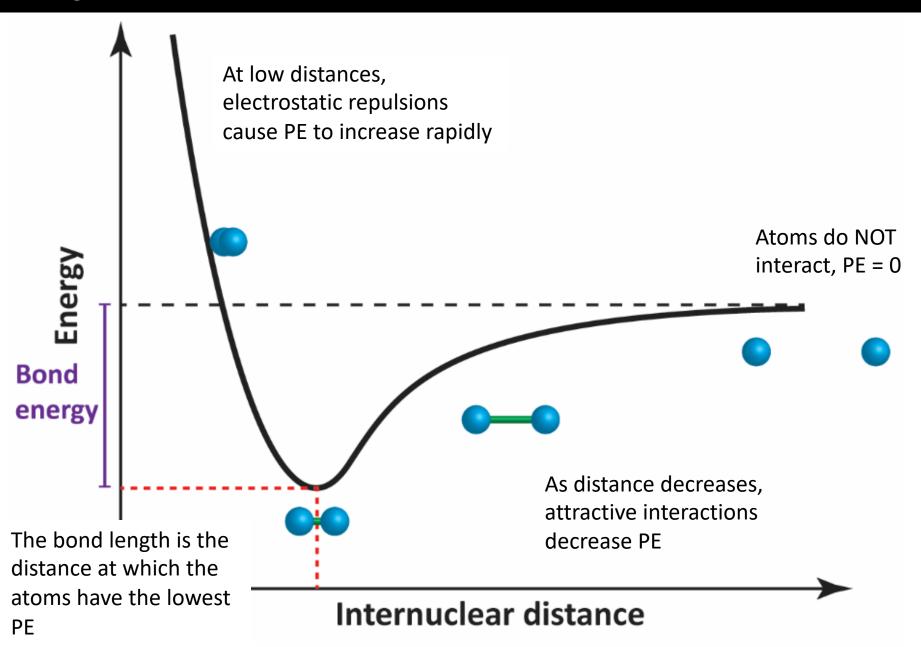
Electronegativity generally increases from left to right of the periodic table and from bottom to top.



Bonding Context



Why do bonds form?



Bond energies and bond orders

When a bond is formed, energy is released (exothermic process).

The bond energy is the energy required to break a covalent bond, and the bond order is the number of electron pairs shared by two atoms in a covalent bond.

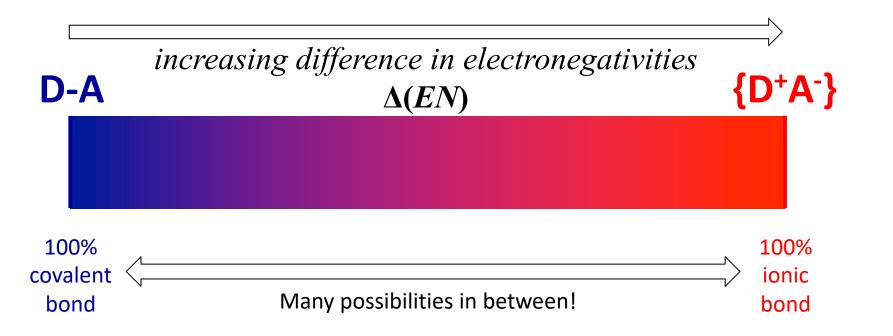
The lattice energy is the energy required to dissociate an ionic solid into its separate ions, and increases with the charges on the ions or as the distance between charges decreases.

Bond energies and bond orders

Bond	Bond energy (kJ/mol)	Bond order
C-F	485	1
C-H	415	1
O-F	190	1
О-Н	460	1
C – C	346	1
C = C	602	2
C≡C	835	3

What type of bond will form?

Can range from <u>covalent</u> (where a pair of electrons are <u>shared</u> between two atoms with no net charge) to <u>ionic</u> (where an electron is transferred from a donor to acceptor) $\triangle \triangle \triangle$



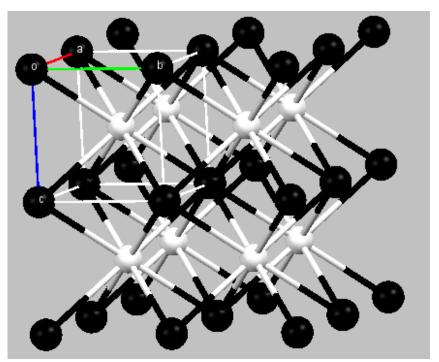
Ionic Bonding

Cesium cations (white) are electrostatically attracted to chloride anions (black). In a crystalline state, the ions form an "infinite", 3D array or lattice.

Rule of Thumb:

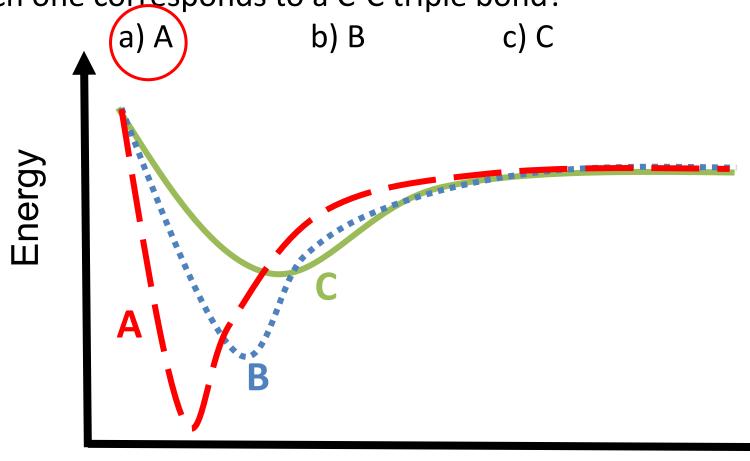
 $\Delta(EN) \gtrsim 1.7$

for ionic bonding



Clicker Question

The following potential energy plots correspond to a C-C single bond, a C-C double bond and a C-C triple bond. Which one corresponds to a C-C triple bond?



Internuclear distance