

CHEMICAL BONDING

Periodic Table of Elements

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
1	<div>1</div> <div>H</div> <div>Hydrogen</div> <div>1.00794</div>	<div>Atomic #</div> <div>Symbol</div> <div>Name</div> <div>Atomic Mass</div> <div><div>C Solid</div><div>Hg Liquid</div><div>H Gas</div><div>Rf Unknown</div></div> <div><div>Metals</div><div>Alkali metals</div><div>Alkaline earth metals</div><div>Lanthanoids</div><div>Actinoids</div><div>Transition metals</div><div>Poor metals</div><div>Other nonmetals</div><div>Noble gases</div></div>																	<div>2</div> <div>He</div> <div>Helium</div> <div>4.002602</div>
2	<div>3</div> <div>Li</div> <div>Lithium</div> <div>6.941</div>	<div>4</div> <div>Be</div> <div>Beryllium</div> <div>9.012182</div>																<div>10</div> <div>Ne</div> <div>Neon</div> <div>20.1797</div>	
3	<div>11</div> <div>Na</div> <div>Sodium</div> <div>22.98976928</div>	<div>12</div> <div>Mg</div> <div>Magnesium</div> <div>24.304</div>																<div>18</div> <div>Ar</div> <div>Argon</div> <div>39.948</div>	
4	<div>19</div> <div>K</div> <div>Potassium</div> <div>39.0983</div>	<div>20</div> <div>Ca</div> <div>Calcium</div> <div>40.078</div>	<div>21</div> <div>Sc</div> <div>Scandium</div> <div>44.955912</div>	<div>22</div> <div>Ti</div> <div>Titanium</div> <div>47.88</div>	<div>23</div> <div>V</div> <div>Vanadium</div> <div>50.9415</div>	<div>24</div> <div>Cr</div> <div>Chromium</div> <div>51.9961</div>	<div>25</div> <div>Mn</div> <div>Manganese</div> <div>54.938045</div>	<div>26</div> <div>Fe</div> <div>Iron</div> <div>55.845</div>	<div>27</div> <div>Co</div> <div>Cobalt</div> <div>58.933195</div>	<div>28</div> <div>Ni</div> <div>Nickel</div> <div>58.6934</div>	<div>29</div> <div>Cu</div> <div>Copper</div> <div>63.546</div>	<div>30</div> <div>Zn</div> <div>Zinc</div> <div>65.38</div>	<div>31</div> <div>Ga</div> <div>Gallium</div> <div>69.723</div>	<div>32</div> <div>Ge</div> <div>Germanium</div> <div>72.64</div>	<div>33</div> <div>As</div> <div>Arsenic</div> <div>74.9216</div>	<div>34</div> <div>Se</div> <div>Selenium</div> <div>78.96</div>	<div>35</div> <div>Br</div> <div>Bromine</div> <div>79.904</div>	<div>36</div> <div>Kr</div> <div>Krypton</div> <div>83.798</div>	
5	<div>37</div> <div>Rb</div> <div>Rubidium</div> <div>85.4678</div>	<div>38</div> <div>Sr</div> <div>Strontium</div> <div>87.62</div>	<div>39</div> <div>Y</div> <div>Yttrium</div> <div>88.90584</div>	<div>40</div> <div>Zr</div> <div>Zirconium</div> <div>91.224</div>	<div>41</div> <div>Nb</div> <div>Niobium</div> <div>92.90638</div>	<div>42</div> <div>Mo</div> <div>Molybdenum</div> <div>95.94</div>	<div>43</div> <div>Tc</div> <div>Technetium</div> <div>97.9072</div>	<div>44</div> <div>Ru</div> <div>Ruthenium</div> <div>101.07</div>	<div>45</div> <div>Rh</div> <div>Rhodium</div> <div>102.9055</div>	<div>46</div> <div>Pd</div> <div>Palladium</div> <div>106.42</div>	<div>47</div> <div>Ag</div> <div>Silver</div> <div>107.8682</div>	<div>48</div> <div>Cd</div> <div>Cadmium</div> <div>112.411</div>	<div>49</div> <div>In</div> <div>Indium</div> <div>114.818</div>	<div>50</div> <div>Sn</div> <div>Tin</div> <div>118.710</div>	<div>51</div> <div>Sb</div> <div>Antimony</div> <div>121.757</div>	<div>52</div> <div>Te</div> <div>Tellurium</div> <div>127.6</div>	<div>53</div> <div>I</div> <div>Iodine</div> <div>126.90549</div>	<div>54</div> <div>Xe</div> <div>Xenon</div> <div>131.29</div>	
6	<div>55</div> <div>Cs</div> <div>Cesium</div> <div>132.90545196</div>	<div>56</div> <div>Ba</div> <div>Barium</div> <div>137.327</div>	<div>57-71</div>		<div>72</div> <div>Hf</div> <div>Hafnium</div> <div>178.49</div>	<div>73</div> <div>Ta</div> <div>Tantalum</div> <div>180.94788</div>	<div>74</div> <div>W</div> <div>Tungsten</div> <div>183.84</div>	<div>75</div> <div>Re</div> <div>Rhenium</div> <div>186.207</div>	<div>76</div> <div>Os</div> <div>Osmium</div> <div>190.23</div>	<div>77</div> <div>Ir</div> <div>Iridium</div> <div>192.222</div>	<div>78</div> <div>Pt</div> <div>Platinum</div> <div>195.084</div>	<div>79</div> <div>Au</div> <div>Gold</div> <div>196.966569</div>	<div>80</div> <div>Hg</div> <div>Mercury</div> <div>200.59</div>	<div>81</div> <div>Tl</div> <div>Thallium</div> <div>204.3833</div>	<div>82</div> <div>Pb</div> <div>Lead</div> <div>207.2</div>	<div>83</div> <div>Bi</div> <div>Bismuth</div> <div>208.9804</div>	<div>84</div> <div>Po</div> <div>Polonium</div> <div>209</div>	<div>85</div> <div>At</div> <div>Astatine</div> <div>210</div>	<div>86</div> <div>Rn</div> <div>Radon</div> <div>222.2175</div>
7	<div>87</div> <div>Fr</div> <div>Francium</div> <div>223</div>	<div>88</div> <div>Ra</div> <div>Radium</div> <div>226</div>	<div>89-103</div>		<div>104</div> <div>Rf</div> <div>Rutherfordium</div> <div>261</div>	<div>105</div> <div>Db</div> <div>Dubnium</div> <div>262</div>	<div>106</div> <div>Sg</div> <div>Seaborgium</div> <div>266</div>	<div>107</div> <div>Bh</div> <div>Bohrium</div> <div>264</div>	<div>108</div> <div>Hs</div> <div>Hassium</div> <div>277</div>	<div>109</div> <div>Mt</div> <div>Meitnerium</div> <div>268</div>	<div>110</div> <div>Ds</div> <div>Darmstadtium</div> <div>271</div>	<div>111</div> <div>Rg</div> <div>Roentgenium</div> <div>272</div>	<div>112</div> <div>Uub</div> <div>Ununbium</div> <div>285</div>	<div>113</div> <div>Uut</div> <div>Ununtrium</div> <div>284</div>	<div>114</div> <div>Uuq</div> <div>Ununquadium</div> <div>289</div>	<div>115</div> <div>Uup</div> <div>Ununpentium</div> <div>288</div>	<div>116</div> <div>Uuh</div> <div>Ununhexium</div> <div>292</div>	<div>117</div> <div>Uus</div> <div>Ununseptium</div> <div>286</div>	<div>118</div> <div>Uuo</div> <div>Ununoctium</div> <div>294</div>

For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.

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57 La Lanthanum 138.90547	58 Ce Cerium 140.12	59 Pr Praseodymium 140.90766	60 Nd Neodymium 144.242	61 Pm Promethium (145)	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.92535	66 Dy Dysprosium 162.5001	67 Ho Holmium 164.93032	68 Er Erbium 167.259	69 Tm Thulium 168.93032	70 Yb Ytterbium 173.044	71 Lu Lutetium 174.967
89 Ac Actinium (227)	90 Th Thorium 232.0377	91 Pa Protactinium 231.036889	92 U Uranium 238.02891	93 Np Neptunium (237)	94 Pu Plutonium 244	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)	103 Lr Lawrencium (260)

Bonding

Primary bonding:

Ionic (transfer of valence electrons)

Covalent (sharing of valence electrons, directional)

Metallic (delocalization of valence electrons)

Secondary or van der Waals Bonding:

(Common, but weaker than primary bonding)

Dipole-dipole

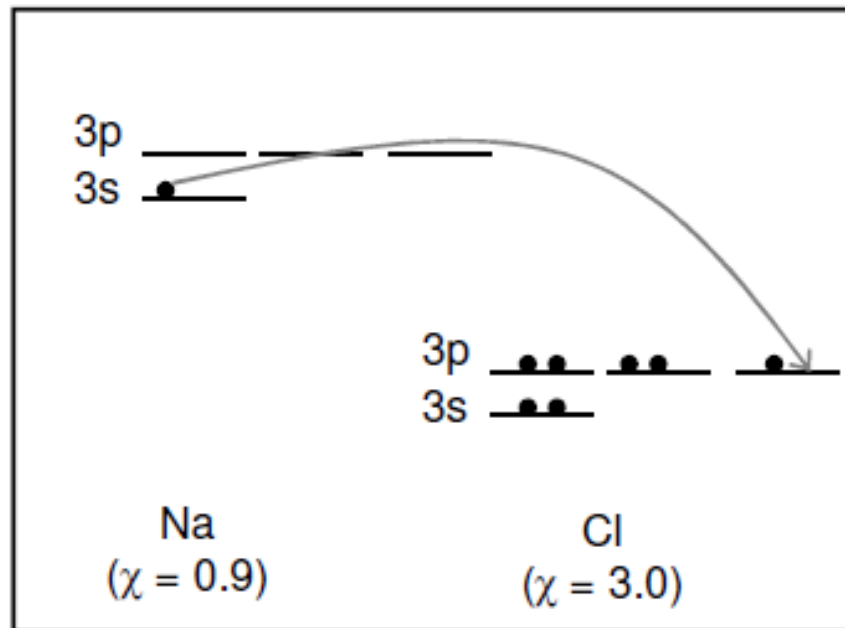
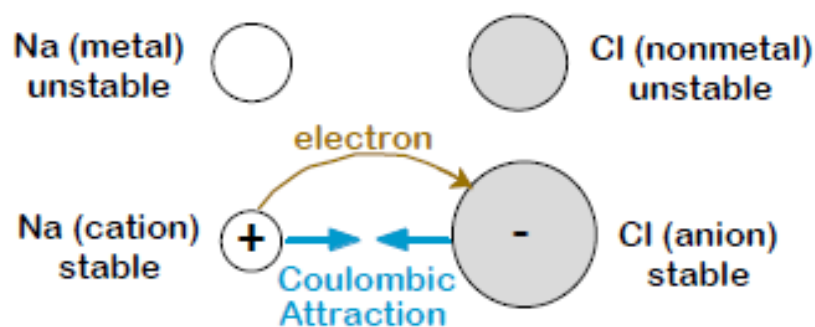
H-bonds

Polar molecule-induced dipole

Fluctuating dipole (weakest)

Ionic Bonding

- Occurs between + and - ions.
- Requires **electron transfer**.
- Large difference in electronegativity required.
- Example: NaCl
- Nondirectional



Example: table salt (NaCl)

Na has 11 electrons, 1 more than needed for a full outer shell (Neon)

11 Protons Na $1s^2 2s^2 2p^6 3s^1$
11 Protons Na⁺ $1s^2 2s^2 2p^6$



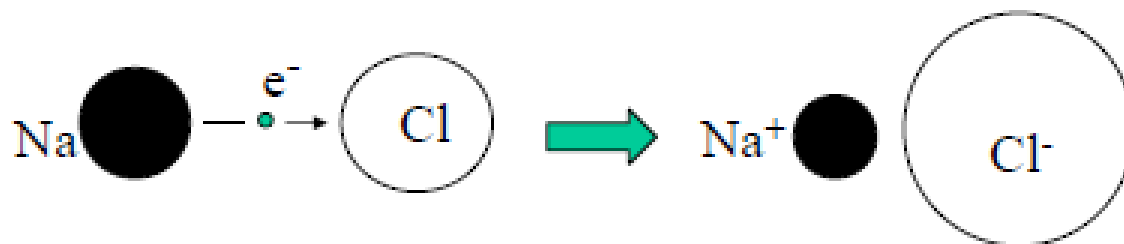
donates e^-
10 e^- left

Cl has 17 electron, 1 less than needed for a full outer shell (Argon)

17 Protons Cl $1s^2 2s^2 2p^6 3s^2 3p^5$
17 Protons Cl⁻ $1s^2 2s^2 2p^6 3s^2 3p^6$

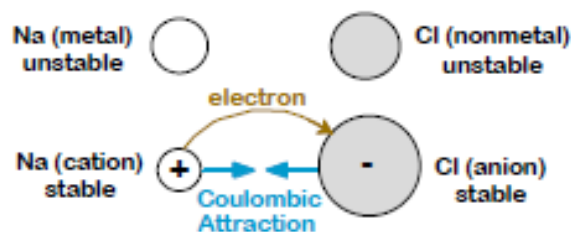


receives e^-
18 e^-



- Electron transfer reduces the energy of the system of atoms, that is, electron transfer is energetically favorable
- Note relative sizes of ions: Na shrinks and Cl expands

Ionic Bonding



$$E_A = \frac{z_1 z_2 e^2}{4\pi\epsilon_o r}$$

Since $z_1 = +1$ for Na^+ and $z_2 = -1$ for Cl^- $\epsilon_o = 8.854 \times 10^{-12} \frac{\text{C}^2}{\text{N}\cdot\text{m}^2}$

$$E_A = -\frac{e^2}{4\pi\epsilon_o r} = -\frac{A}{r}$$

Negative energy means attraction only.
Will the atoms collapse on themselves?

No, there is also repulsive energy (e.g. steric repulsion, e-e repulsion)

$$E_R = \frac{B}{r^n}$$

B and n depend on atoms involved.
In many cases $n \sim 8$.

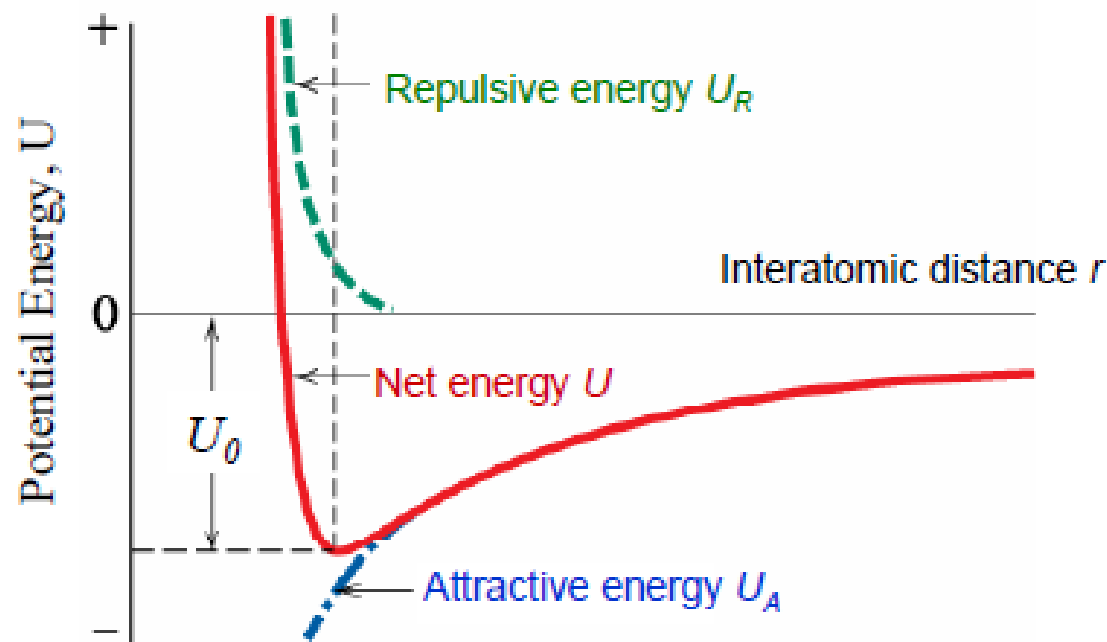
Attractive coulomb interaction between charges of opposite sign:

$$U_A = \frac{1}{4\pi\epsilon_0} \frac{q_1 q_2}{r} = -\frac{A}{r}$$

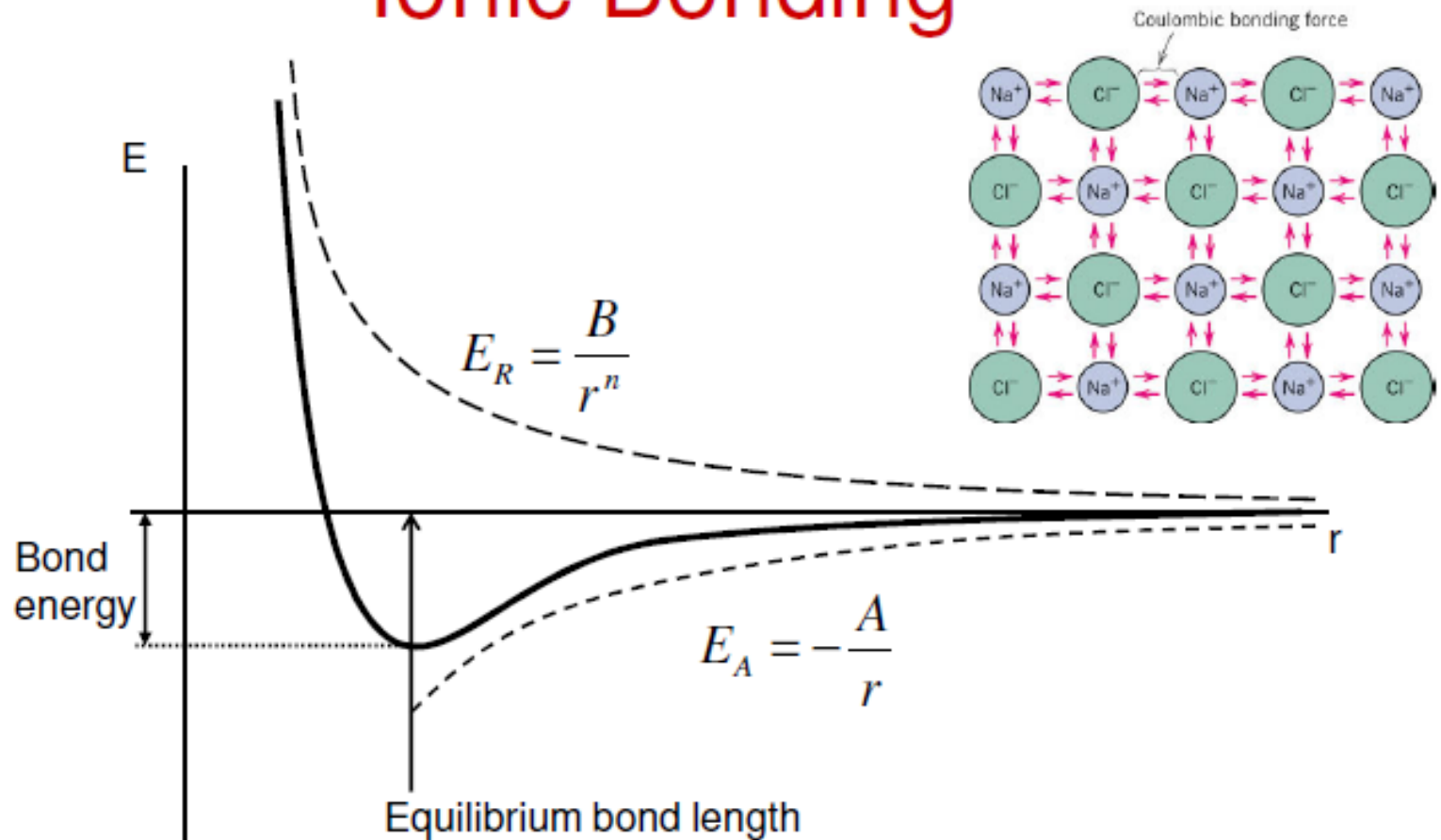
Repulsion due to the overlap of electron clouds at close distances (Pauli principle of QM):

$$U_R = \frac{B}{r^n}$$

$$U = U_A + U_R = -\frac{A}{r} + \frac{B}{r^n}$$



Ionic Bonding



Note: Other types of bonds can also be described in a similar manner

Ionic Bonding: examples

- Predominant bonding in **Ceramics**

dominant bonding in Ceramics

NaCl

MgO

CaF₂

CsCl

IA																	0				
H 2.1																	He -				
Li 1.0	Be 1.5															B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	Ne -
Na 0.9	Mg 1.2															Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	Ar -
K 0.8	Ca 1.0	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Cobalt 1.8	Ni 1.8	Cu 1.9	Zn 1.8	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	Kr -					
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.6	Tc 1.9	Ru 2.2	Rh 2.2	Pt 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.9	Sb 1.9	Te 2.1	Xe -					
Cs 0.7	Ba 0.9	La-Lu 1.1-1.3	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.6	Rn -					
Fr 0.7	Ra 0.9	Ac-No 1.1-1.7																			

Give up electrons

Acquire electrons

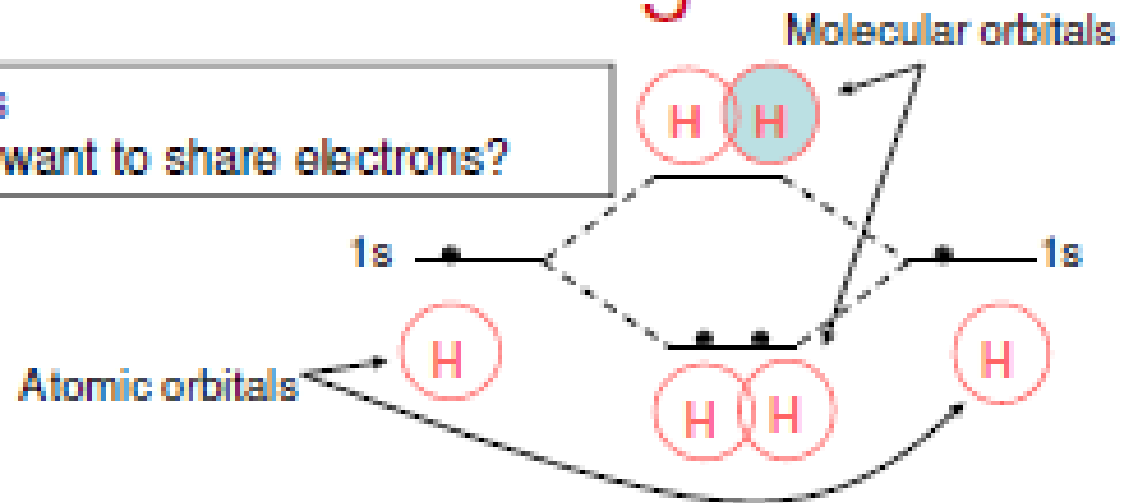
Adapted from Fig. 2.7, *Callister 6e*. (Fig. 2.7 is adapted from Linus Pauling, *The Nature of the Chemical Bond*, 3rd edition, Copyright 1939 and 1940, 3rd edition. Copyright 1960 by Cornell University.

From Callister 6e resource CD.

Covalent Bonding

- “Sharing” of electrons
- Why do some atoms want to share electrons?

- Example 1: H_2

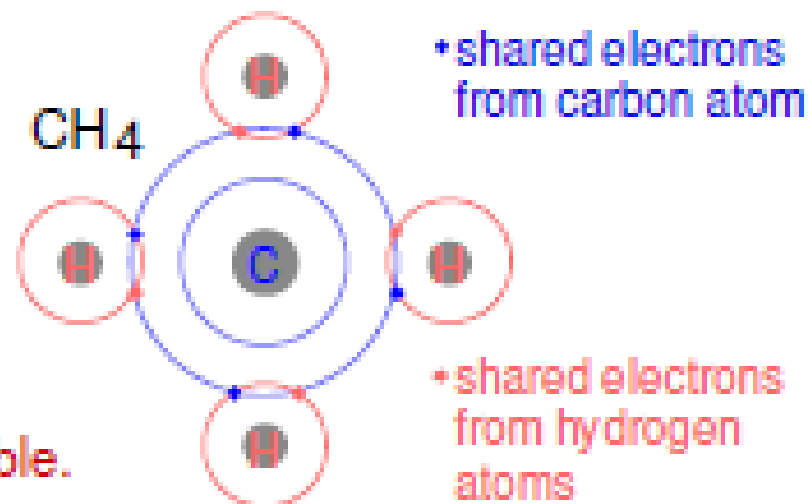


- Example 2: CH_4

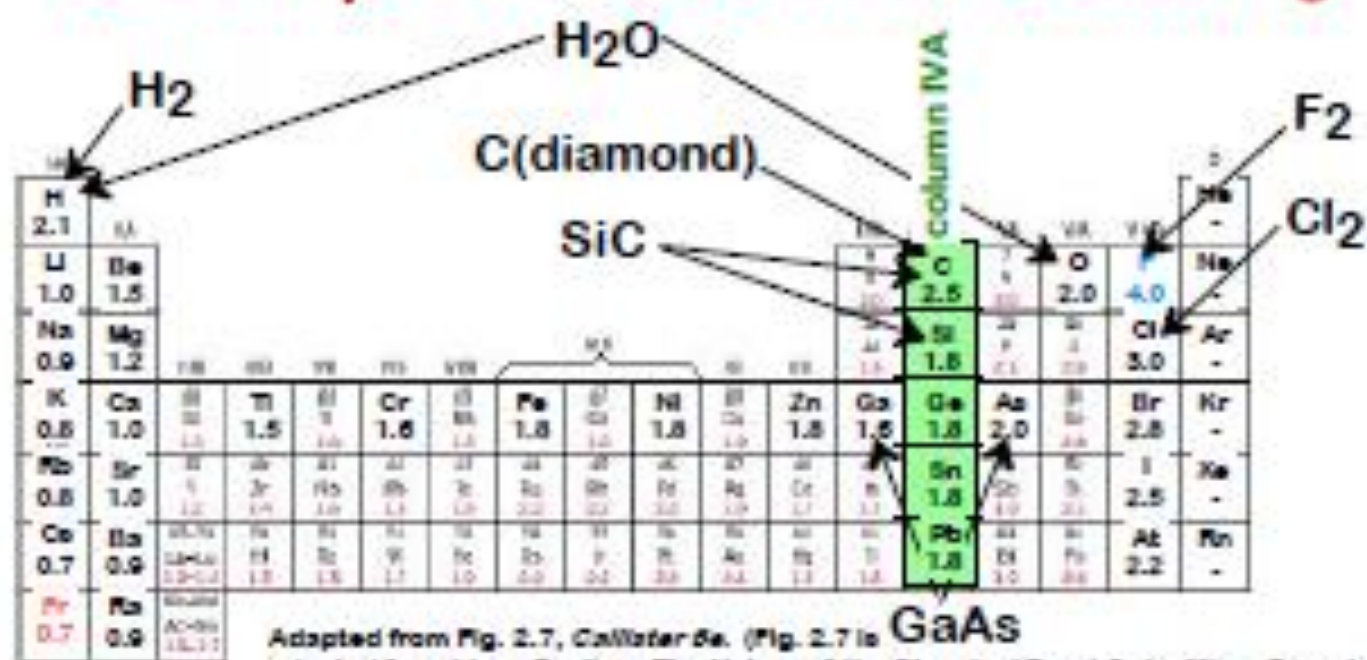
C: has 4 valence e,
needs 4 more

H: has 1 valence e,
needs 1 more

Electronegativities
are same or comparable.



Examples: Covalent Bonding



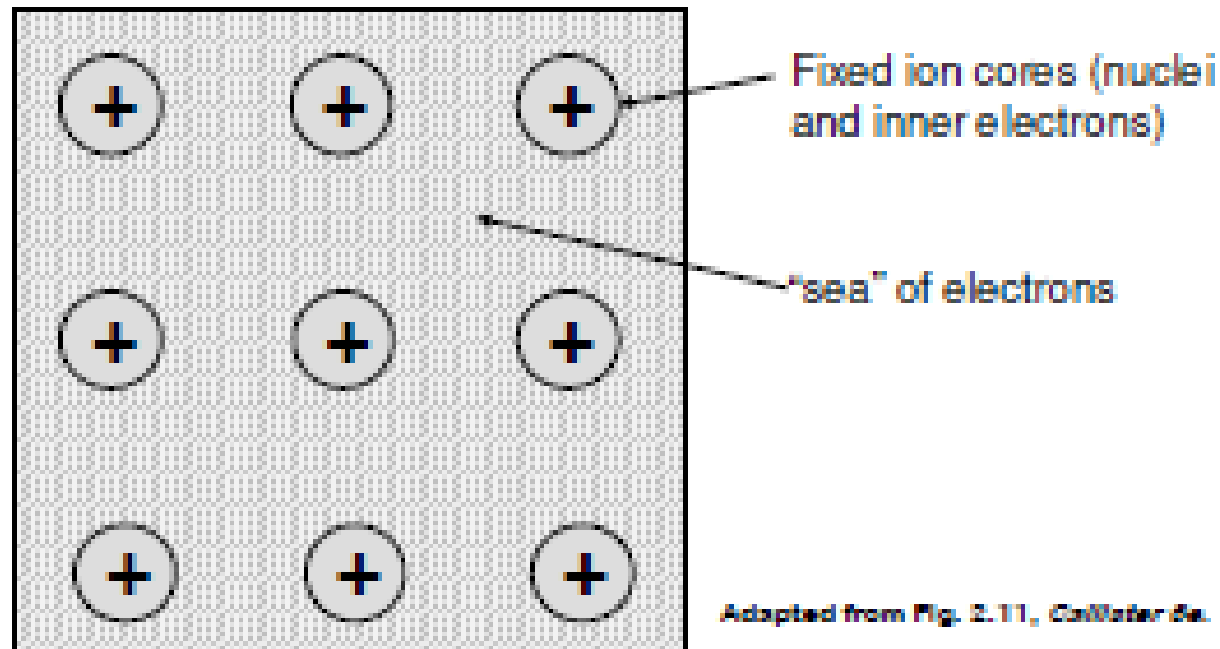
Adapted from Fig. 2.7, Callister 8e. (Fig. 2.7 is adapted from Linus Pauling, *The Nature of the Chemical Bond*, 3rd edition, Copyright 1939 and 1940, 3rd edition. Copyright 1960 by Cornell University.

From Callister 8e resource CD.

- Molecules with **nonmetals**
- Molecules with **metals** and **nonmetals**
- Elemental solids (RHS of Periodic Table)
- Compound solids (about **column IVA**)

Metallic Bonding

- Arises from a sea of donated valence electrons



- Primary bond for metals and their alloys.
- Large atomic radius and small IP will more likely lead to metallic bonding.

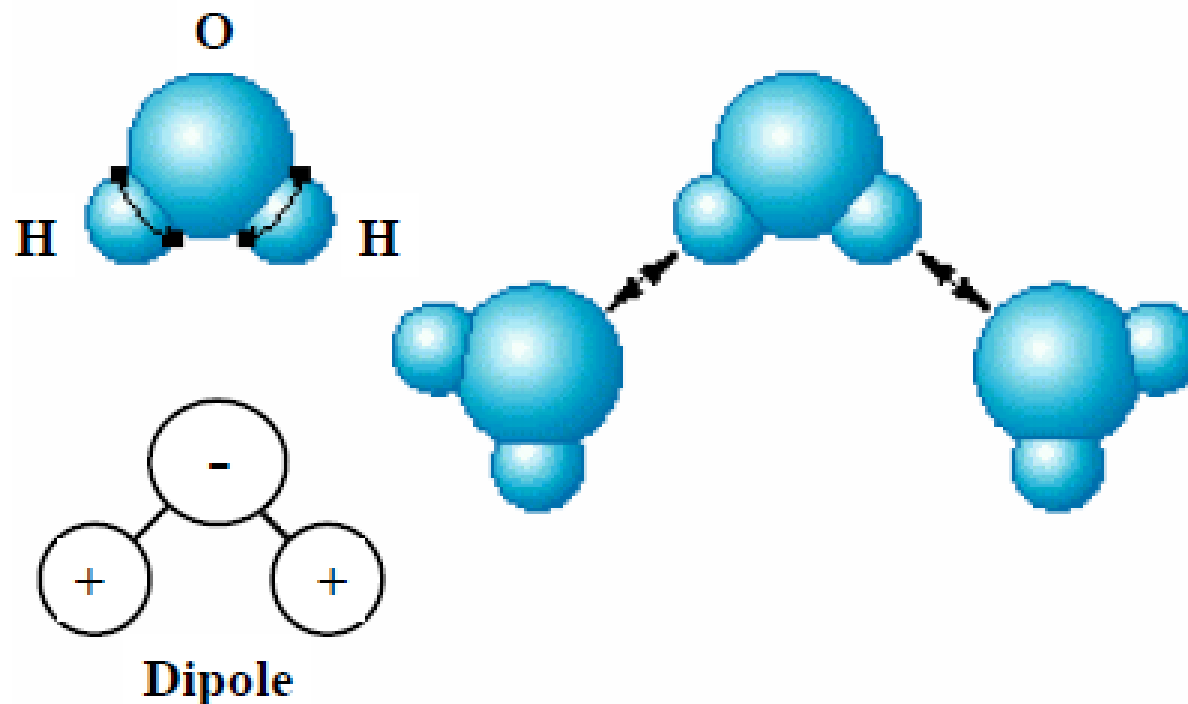
Metallic Bonding

- **Valence** electrons are completely delocalized to form an electron cloud, in which positive ionic cores are embedded.
- The remaining nonvalence electrons and atomic nuclei form "ion cores", which possess a net positive charge equal in magnitude to the total valence electron charge per atom.
- The metallic bond is nondirectional.
- Metallic bonding is found in the periodic table for Group IA and IIA elements.
- Electron delocalization is the origin of good electrical and thermal conductivities in metals. (Ionically and covalently bonded materials are typically electrical and thermal insulators, due to the absence of large numbers of free electrons) .

Secondary Bonds: Intermolecular Forces

- Secondary, Van der Waals, or physical bonds are weak in comparison to the primary bonds.
- Secondary bonding exists between virtually all atoms or molecules, but its presence may be obscured if any of the three primary bonding types is present.
- Secondary bonding forces arise from atomic or molecular dipoles. An electric dipole exists whenever there is some separation of positive and negative portions of an atom or molecule.
- Dipole interactions occur between induced dipoles, between induced dipoles and polar molecules (which have permanent dipoles), and between polar molecules.
- Hydrogen bonding, a special type of secondary bonding, is found to exist between some molecules that have hydrogen as one of the constituents.

Example: hydrogen bond in water. The H end of the molecule is positively charged and can bond to the negative side of another H_2O molecule (the O side of the H_2O dipole)



“Hydrogen bond” – secondary bond formed between two permanent dipoles in adjacent water molecules.

Secondary Bonds: Intermolecular Forces

- **Dipole-dipole interaction:** secondary bond between molecules with permanent dipole moments



Adapted from Fig. 2.14,
Callister 8e.

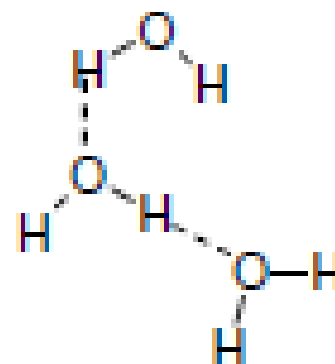


Adapted from Fig. 2.14,
Callister 8e.



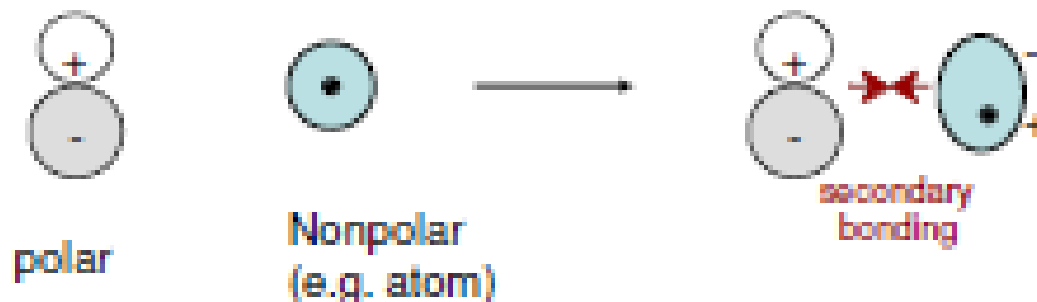
from callister 8e resource co.

- **Hydrogen bonding**



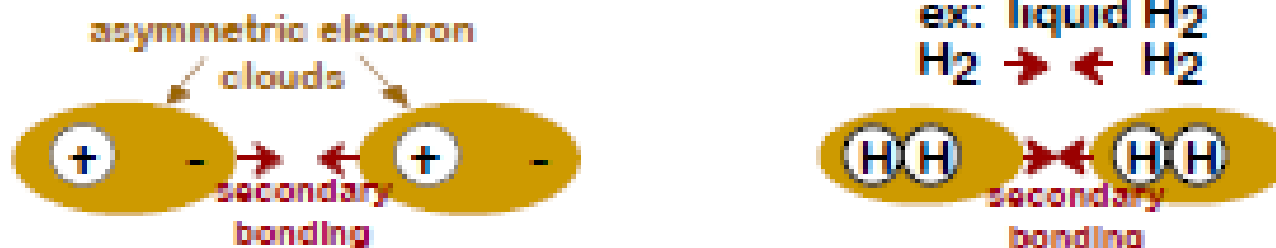
- **Polar molecule-induced dipole interaction:**

Polar molecules (with asymmetric arrangement of positively and negatively charged regions) can induce dipoles in adjacent nonpolar molecules



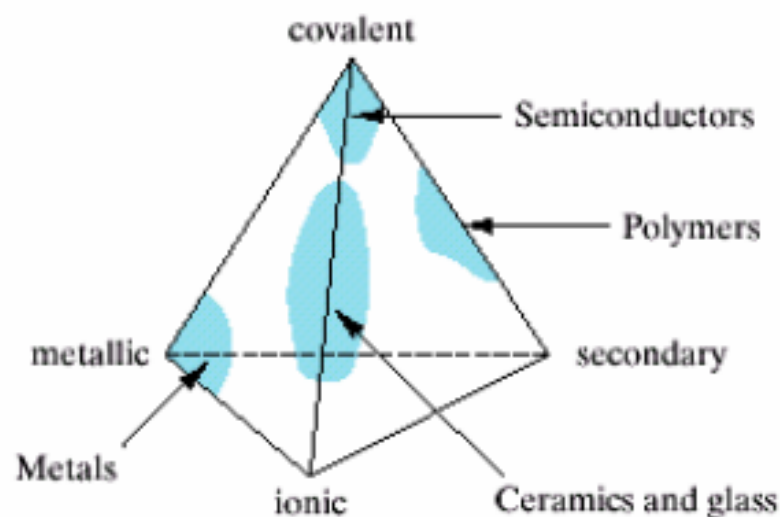
- **Fluctuating dipoles**

Constant vibrational motion can cause distortions of electrical symmetry



Adapted from Fig. 2.13, Callister 6e.

In many materials more than one type of bonding is involved (ionic and covalent in ceramics, covalent and secondary in polymers, covalent and ionic in semiconductors).



Examples of bonding in Materials:

Metals: Metallic

Ceramics: Ionic / Covalent

Polymers: Covalent and Secondary

Semiconductors: Covalent or Covalent / Ionic

Bonding Energies and Melting Temperatures for Various Substances

<i>Bonding Type</i>	<i>Substance</i>	<i>Bonding Energy</i>		<i>Melting Temperature (°C)</i>
		<i>kJ/mol</i>	<i>eV/Atom, Ion, Molecule</i>	
Ionic	NaCl	640	3.3	801
	MgO	1000	5.2	2800
Covalent	Si	450	4.7	1410
	C (diamond)	713	7.4	>3550
Metallic	Hg	68	0.7	-39
	Al	324	3.4	660
	Fe	406	4.2	1538
	W	849	8.8	3410
van der Waals	Ar	7.7	0.08	-189
	Cl ₂	31	0.32	-101
Hydrogen	NH ₃	35	0.36	-78
	H ₂ O	51	0.52	0

SUMMARY: BONDING

Type	Bond Energy	Comments
Ionic	Large!	Nondirectional (ceramics)
Covalent	Variable large-Diamond small-Bismuth	Directional (semiconductors, ceramics polymer chains)
Metallic	Variable large-Tungsten small-Mercury	Nondirectional (metals)
Secondary	smallest	Directional inter-chain (polymer) inter-molecular