

حَمْدُ اللَّهِ الْعَظِيمِ الْعَلِيمِ

قَالُوا سُبْحَانَكَ لَا عِلْمَ لَنَا

إِلَّا مَا عَلَّمْتَنَا

أَنْتَ أَنْتَ الْعَلِيمُ الْحَكِيمُ

صَدَقَ اللَّهُ الْعَظِيمُ

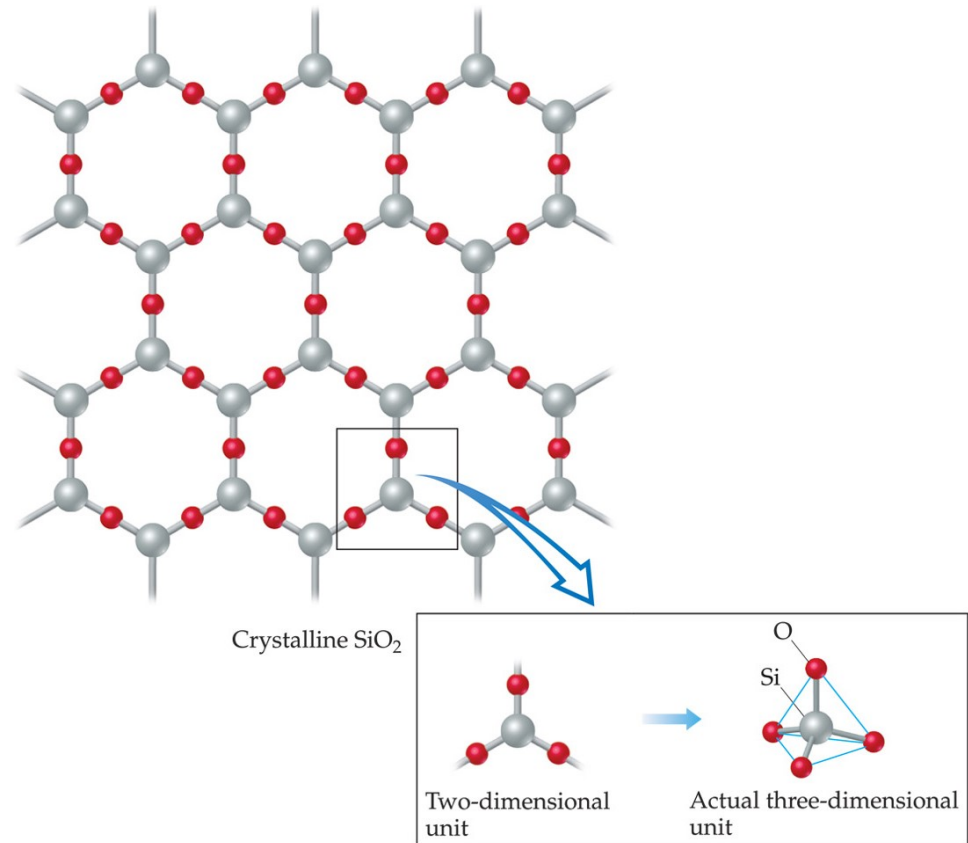
سورة البقرة الآية 32 *



Crystal structure and x-ray diffraction

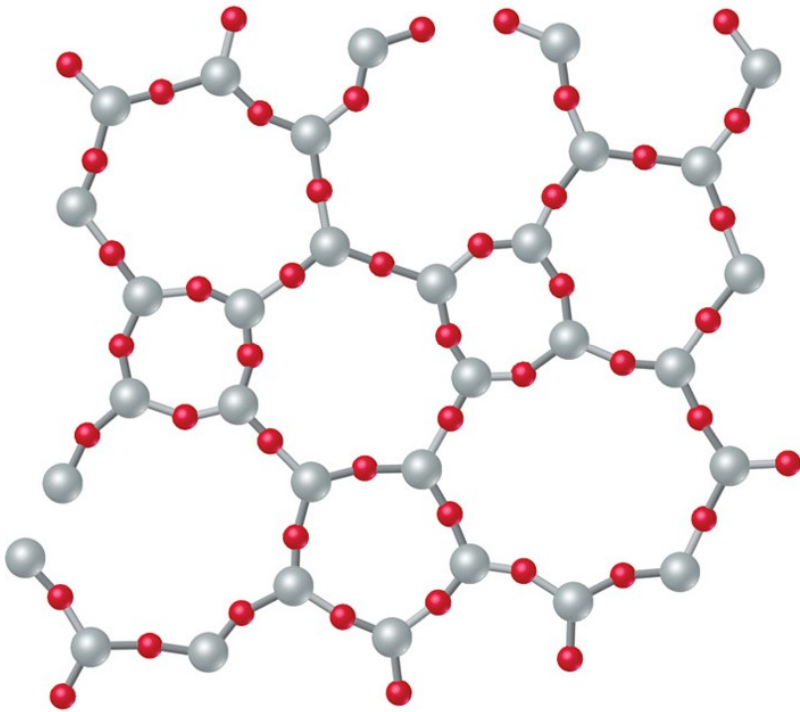
Solids

- We can think of solids as falling into two groups:
 - Crystalline—particles are in highly ordered arrangement.
 - pattern



Solids

- Amorphous—no particular order in the arrangement of particles.



Amorphous SiO₂

- **Review of Atomic Structure**

**Electrons, Protons, Neutrons, Quantum mechanics,
Electron states, The Periodic Table**

Interatomic bonding

First step in understanding material properties

- **Atomic Bonding in Solids**

Energies vs. Forces

Review of Atomic Structure

Atoms = nucleus (protons and neutrons) + electrons

Charges:

Electrons (-): protons(+) 1.6×10^{-19} Coulombs.

Neutrons are electrically neutral.

Masses:

Protons and Neutrons $\sim 1.67 \times 10^{-27}$ kg.

Electron 9.11×10^{-31} kg

Atomic mass = # protons + # neutrons

Atomic number (Z) = # protons
→ chemical identification of element

Isotope number → # neutrons

Atomic mass units. Atomic weight.

Atomic mass unit (amu)

1 amu = 1/12 of mass of most common isotope of C
6 protons (Z=6) and six neutrons (N=6).

The atomic mass of ^{12}C atom is 12 amu.

Atomic weight: A

Weighted average of atomic masses of naturally
occurring isotopes.

Atomic weight of carbon is 12.011 amu.

Atomic weight is often in mass per mole.

A mole

Amount of matter with mass in grams equal to the
atomic mass in amu

(A mole of carbon has a mass of 12 grams).

One Mole contains **Avogadro's number of atoms**,

$$N_{\text{av}} = 6.023 \times 10^{23}.$$



Number density, n : (number of atoms per cm^3)

Mass density, ρ (g/cm^3)

Atomic mass, A (g/mol):

$$n = N_{\text{av}} \times \rho / A$$

Electrons form a cloud around the nucleus

Electrons “orbits” are ‘fuzzy‘

Can only discuss probability of finding it at some distance from the nucleus.

Only certain “orbits” or shells are allowed.

**Shells identified by principal quantum number n ,
 n related to size of radius (and energy)**

$n = 1$, smallest; $n = 2, 3 ..$ are larger.

Second quantum number l , defines subshells.

Two more quantum numbers characterize states within subshells.

Electrons in Atoms (II)

- Quantum Numbers came from solution of Schrodinger's equation
- Pauli Exclusion Principle: only one electron can have a given set of the four quantum numbers.

Maximum Number of Electrons in Shells and Subshells

Principal Q. N., n	Subshells	Number of States	Number of Electrons Per Subshell	Number of Electrons Per Shell
1 (l=0)	s	1	2	2
2 (l=0)	s	1	2	8
2 (l=1)	p	3	6	
3 (l=0)	s	1	2	18
3 (l=1)	p	3	6	
3 (l=2)	d	5	10	
4 (l=0)	s	1	2	32
4 (l=1)	p	3	6	
4 (l=2)	d	5	10	
4 (l=3)	f	7	14	

**Electronegativity - how willing atoms are to
accept electrons**

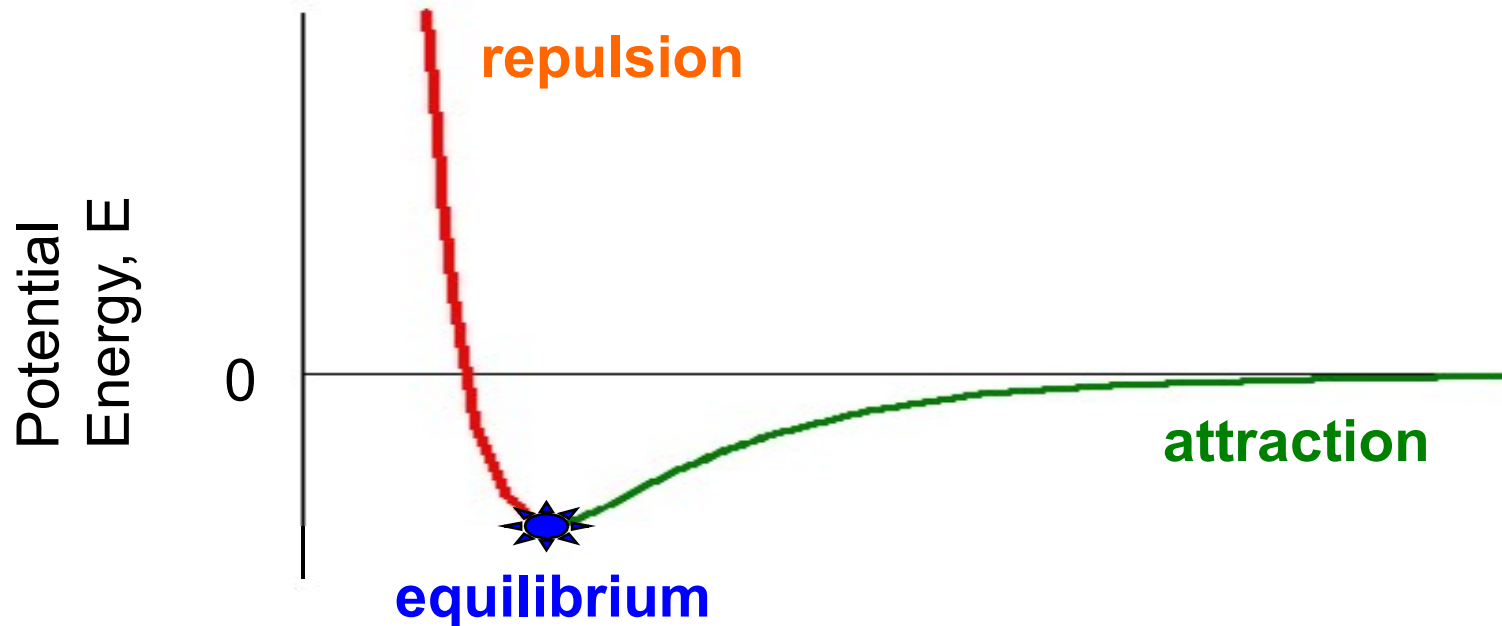
Subshells with one electron - low electronegativity

Subshells with one missing electron -high electronegativity

Electronegativity increases from left to right

**Metals are electropositive – can give up their few valence
electrons to become positively charged ions**

Bonding Energies and Forces



Typical potential between two atoms

Repulsion when they are brought close together
Related to Pauli principle
(As electron clouds overlap energy increases)

Attractive part: at large distances
12 (Depends on type of bonding)

The electron volt (eV)
Energy unit convenient for atomic bonding

Electron volt –

energy lost / gained when an electron is taken through a potential difference of one volt.

$$\mathbf{E = q \times V}$$

For $q = 1.6 \times 10^{-19}$ Coulombs

$V = 1$ volt

$$\mathbf{1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}}$$



Types of Bonds

Ionic Bonding (I)

Mutual ionization by electron transfer

(remember electronegativity table)

- **Anion** = negatively charged atom
- **Cation** = positively charged atom

Ions are attracted by strong coulombic interaction

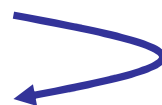
- **Oppositely charged atoms attract**
- **An ionic bond is non-directional**

Example: 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)

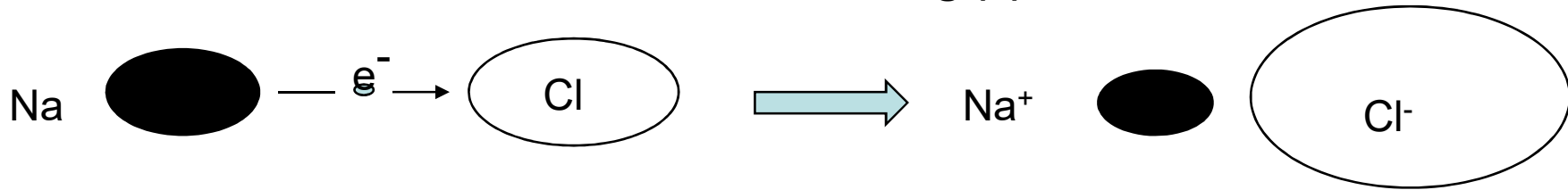
17 Protons Cl $1S^2 2S^2 2P^6 3S^2 3P^5$

17 Protons Cl⁻ $1S^2 2S^2 2P^6 3S^2 3P^6$

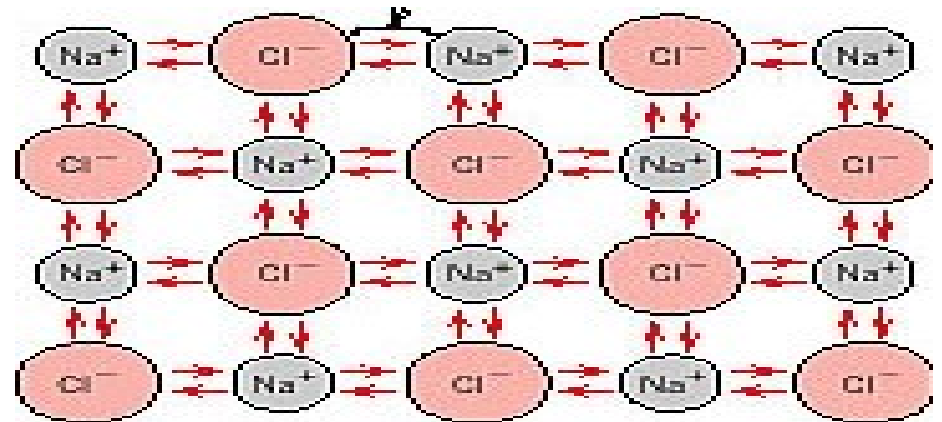
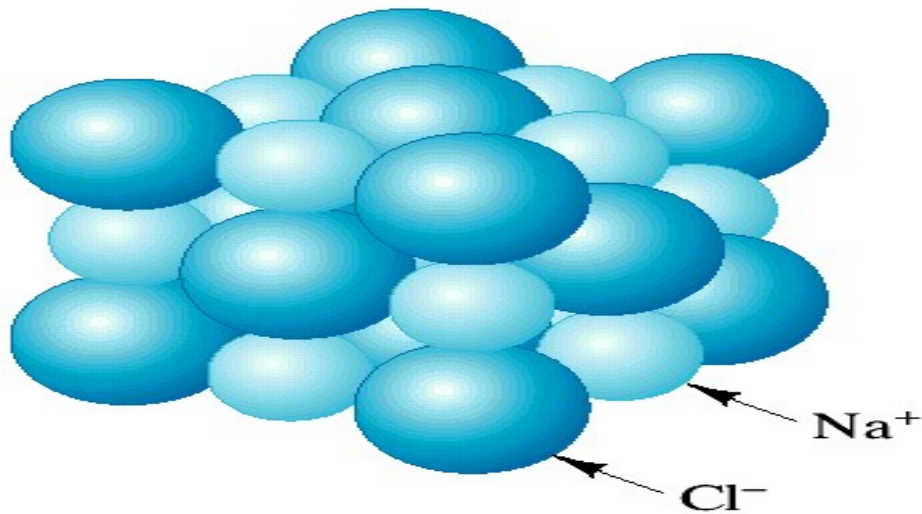


receives e⁻
18 e⁻

Ionic Bonding (II)



- Electron transfer reduces energy of the system
- Na shrinks and Cl expands



Ionic bonds: very strong, nondirectional bonds

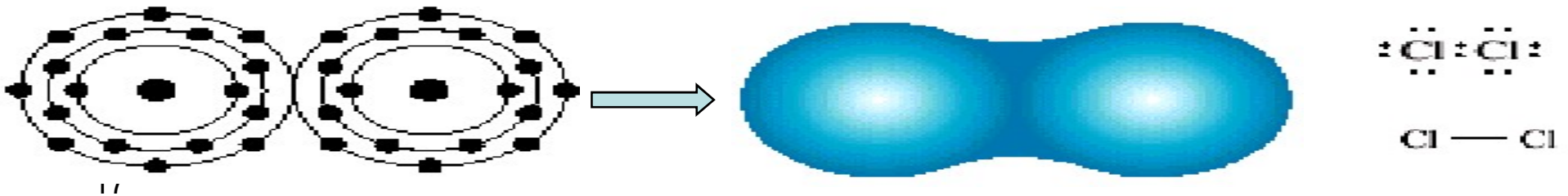
Covalent Bonding (I)

Electrons shared between the atoms.

Valence electrons spend more time between nuclei than outside → bonding.

Covalent bonds - HIGHLY directional in direction of greatest orbital overlap

Example: Cl₂ molecule. $Z_{\text{Cl}} = 17$ ($1s^2 2s^2 2p^6 3s^2 3p^5$)
 $N' = 7$, $8 - N' = 1$ → can form only one covalent bond

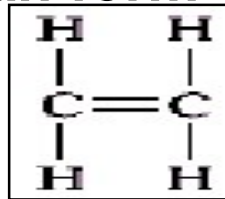


Covalent Bonding (II)

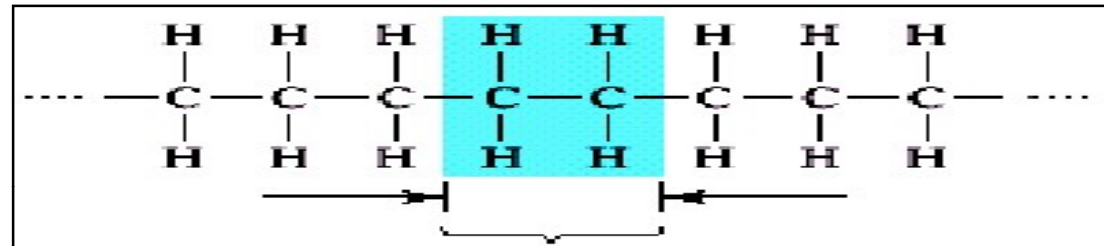
Example: Carbon $Z_c = 6$ ($1S^2 2S^2 2P^2$)

$N' = 4$, $8 - N' = 4 \rightarrow$ can form up to four covalent bonds

ethylene molecule:



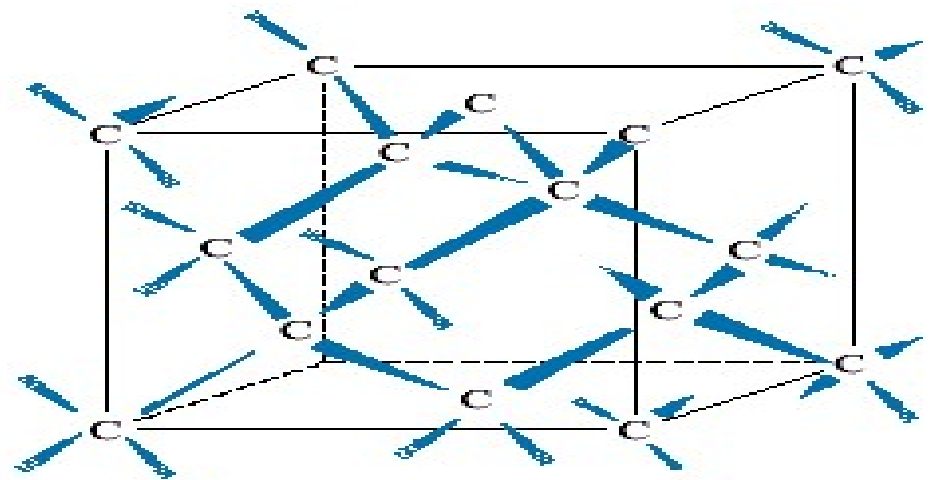
polyethylene molecule:



ethylene mer

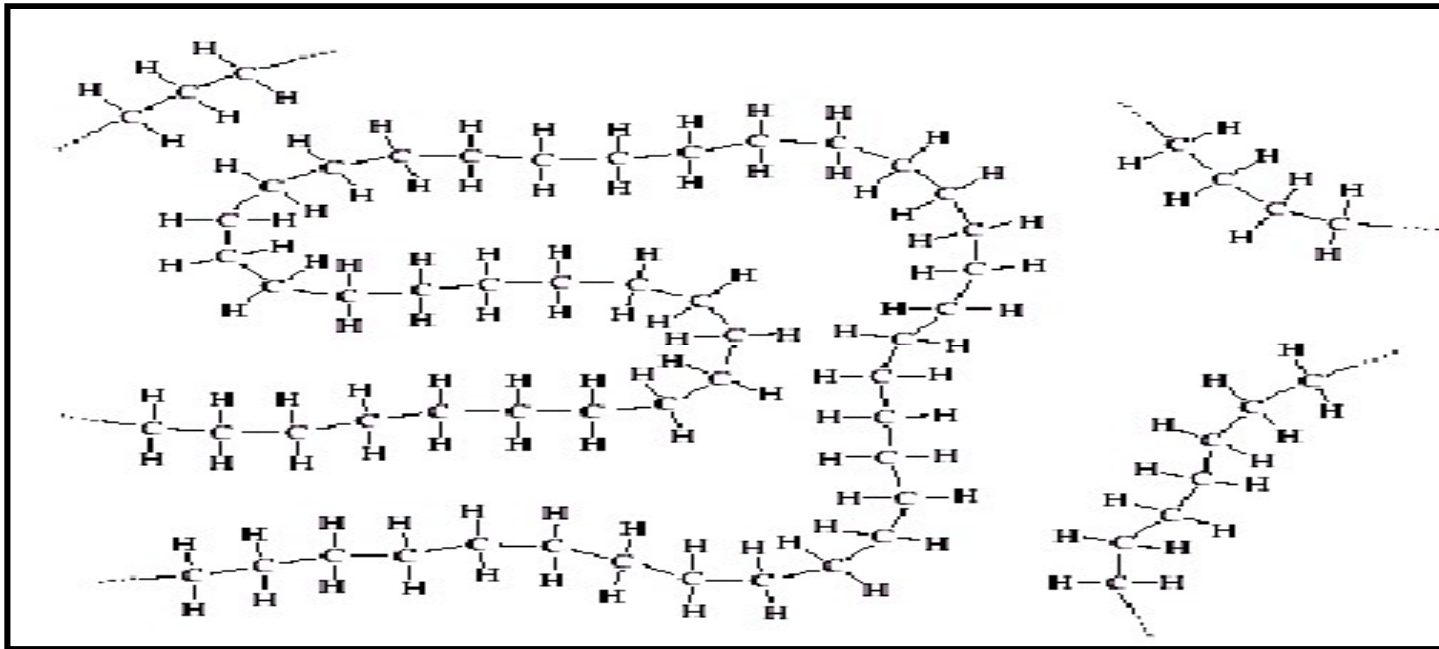
diamond:

(each C atom has four covalent bonds with four other carbon atoms)



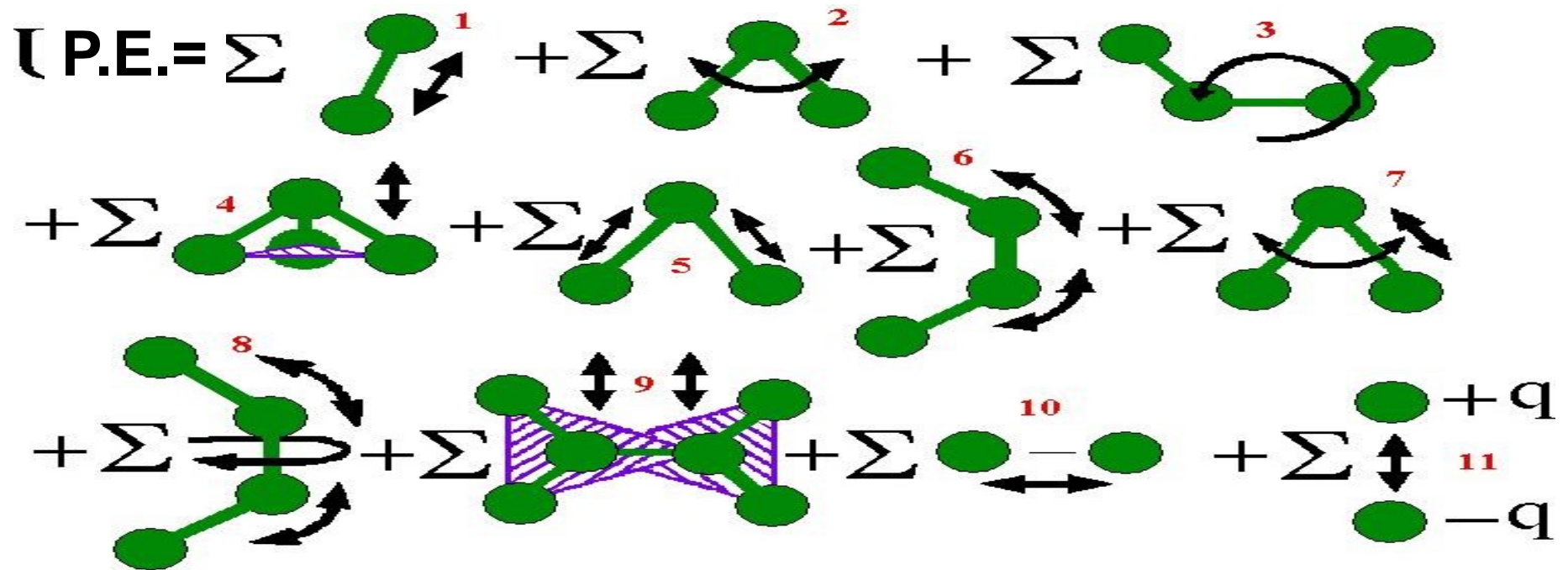
Covalent Bonding (III)

2-D schematic of the “spaghetti-like” structure of solid polyethylene



Covalent Bonding (IV)

Potential energy of system of covalent bonds

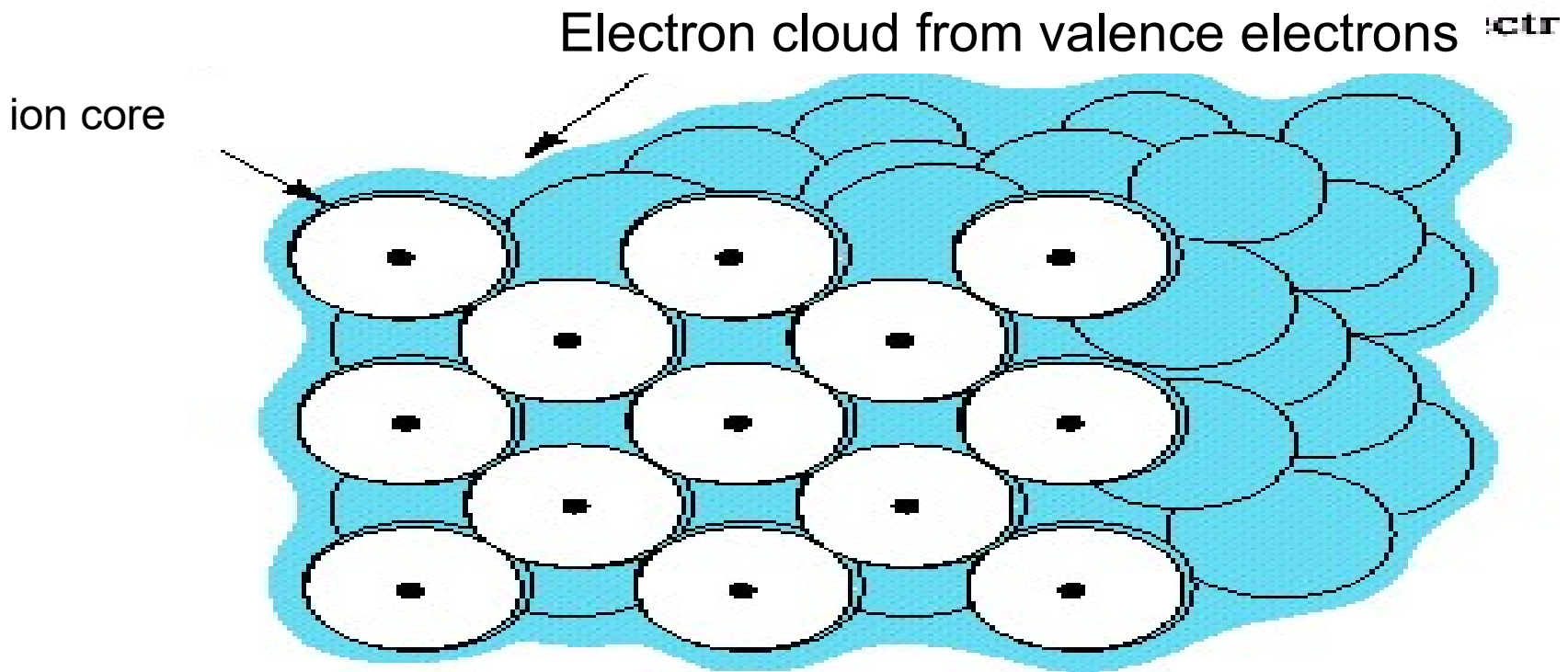


Depend on **distances** between atoms
AND angles between bonds

Metallic Bonding III

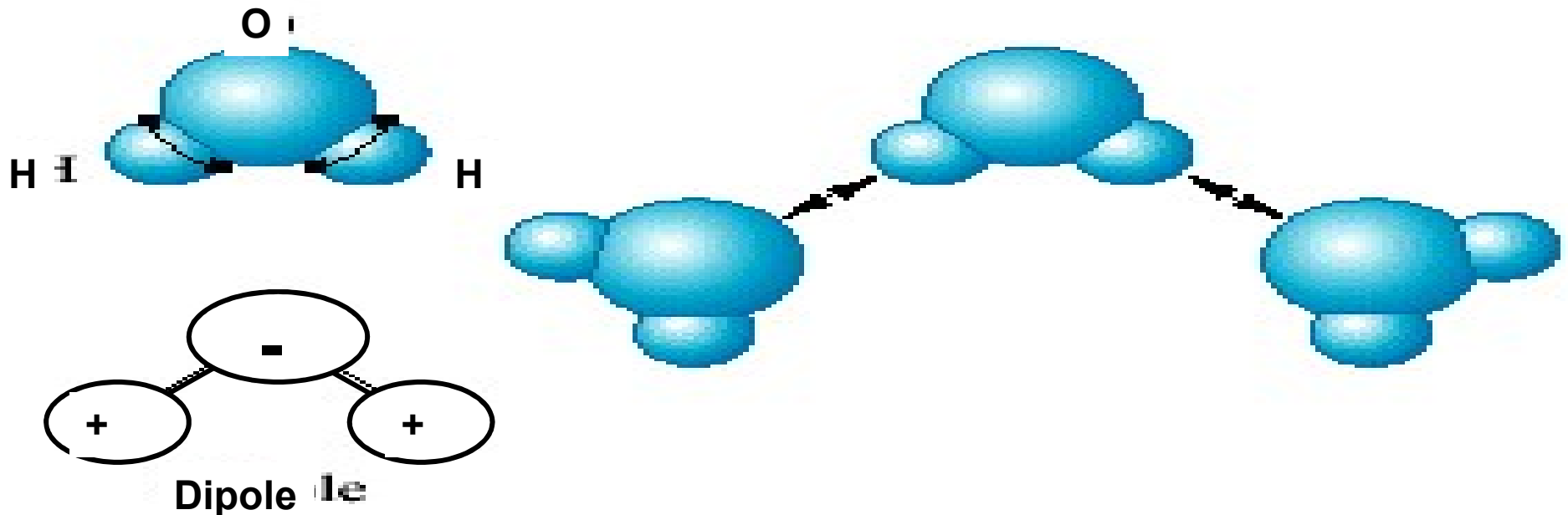
**Valence electrons are detached from atoms
Spread in an 'electron sea'
that "glues" the "ions" together**

Metallic bond is non-directional → atoms pack closely



Secondary Bonding (I)

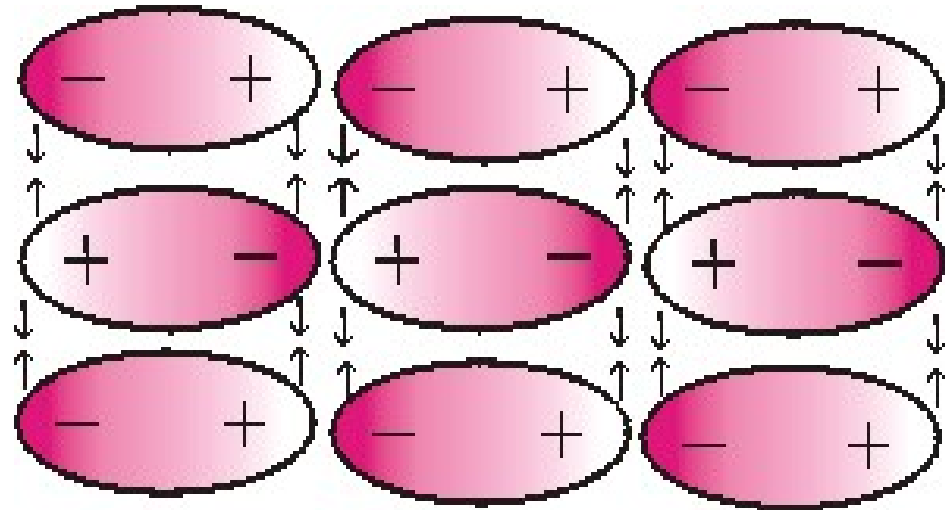
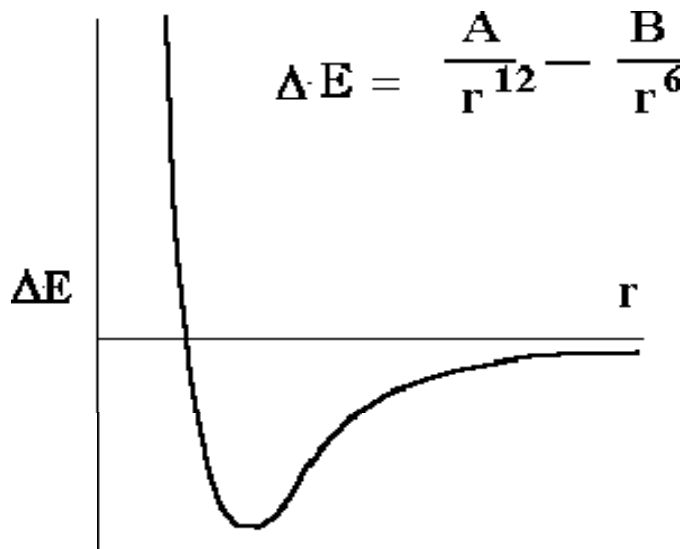
Example I: **hydrogen bond** in water. The H end of the molecule is positively charged and can bond to the negative side of another H_2O molecule (the O side of the H_2O dipole)



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

Example 2: van del waal (second bonds)

Molecules can attract each other at moderate distances and repel each other at close range. The attractive forces are collectively called "van der Waals forces". Van der Waals forces are much weaker than chemical bonds, and random thermal motion around room temperature can usually overcome or disrupt them.

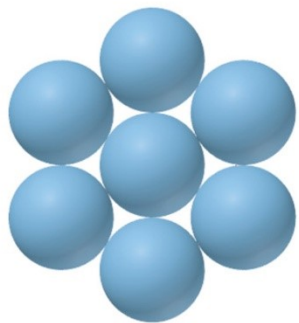


Now, we already know:

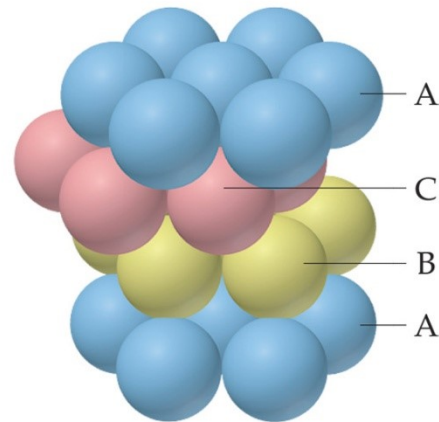
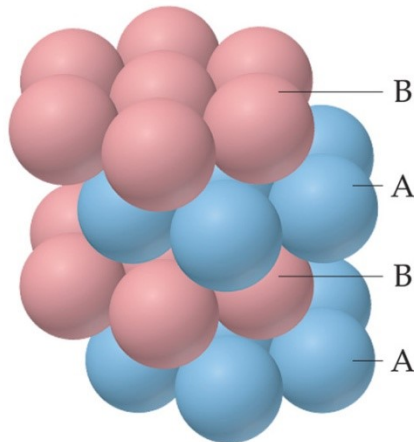
- Can be chemically bonded
 - Ionic
 - Covalent
 - Metallic
 - Hydrogen
 - Van der waals

Attractions in Ionic Crystals

In ionic crystals, ions pack themselves so as to maximize the attractions and minimize repulsions between the ions.

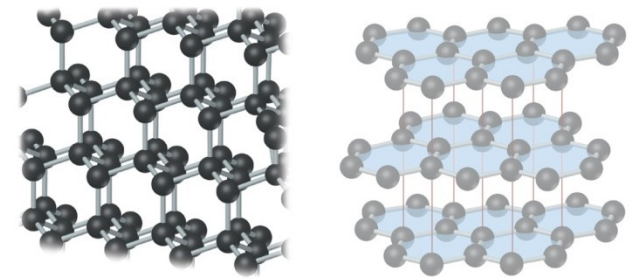


Close-packed
layer of spheres

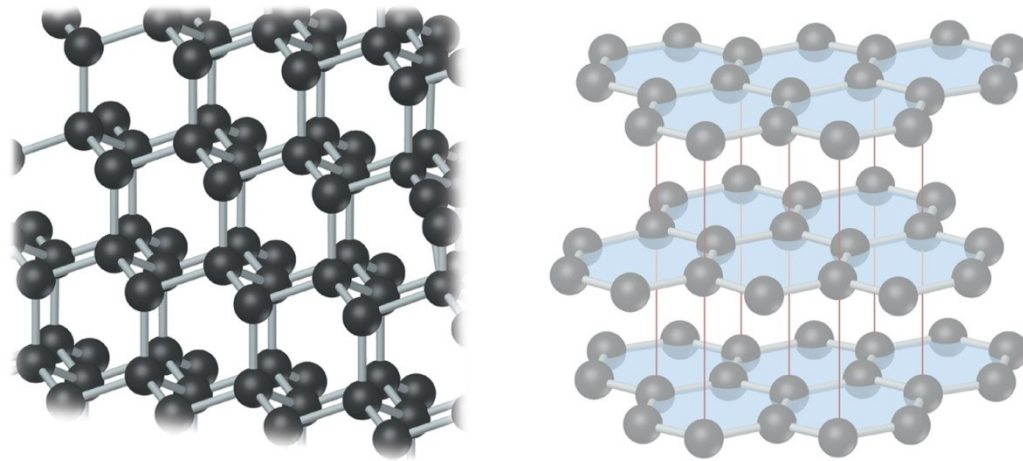


Covalent Network Solids

- Special group of covalently bonded molecules or atoms
- Consists of atoms that are covalently bonded together into 2-D (sheets) or 3-D networks
- Formed from nonmetals
 - Elemental (same element throughout C)
 - Or 2 nonmetals (examples: SiO_2 (quartz) or SiC)

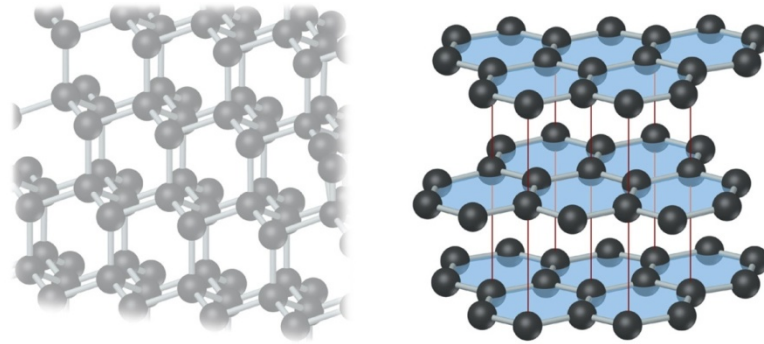


3-D Covalent-Network Solids



- 3-D network is rigid and hard because covalent bond angles are fixed
 - They tend to be hard and have high melting points.
 - Example: Diamonds (C atoms)

2-D Covalent-Network Solids



- Atoms are bonded covalently into 2-D sheets that are held together with van der Waals forces.
 - They tend to be softer and have lower melting points than 3-D network solids because the 2-D layers can slide past each other relatively easily
- Graphite is an allotrope of carbon (same element bonded in a different arrangement)

Covalent network solids

- Typically formed from elements in Carbon group because of their ability to make 4 covalent bonds

Click on an element for more information

1												18																							
1 1	H											1 2	He																						
2 3	Li	2 4	Be											2 5	B	2 6	C	2 7	N	2 8	O	2 9	F	2 10	Ne										
3 11	Na	3 12	Mg											3 13	Al	3 14	Si	3 15	P	3 16	S	3 17	Cl	3 18	Ar										
4 19	K	4 20	Ca	4 21	Sc	4 22	Ti	4 23	V	4 24	Cr	4 25	Mn	4 26	Fe	4 27	Co	4 28	Ni	4 29	Cu	4 30	Zn	4 31	Ga	4 32	Ge	4 33	As	4 34	Se	4 35	Br	4 36	Kr
5 37	Rb	5 38	Sr	5 39	Y	5 40	Zr	5 41	Nb	5 42	Mo	5 43	Tc	5 44	Ru	5 45	Rh	5 46	Pd	5 47	Ag	5 48	Cd	5 49	In	5 50	Sn	5 51	Sb	5 52	Te	5 53	I	5 54	Xe
6 55	Cs	6 56	Ba	*	6 72	Hf	6 73	Ta	6 74	W	6 75	Re	6 76	Os	6 77	Ir	6 78	Pt	6 79	Au	6 80	Hg	6 81	Tl	6 82	Pb	6 83	Bi	6 84	Po	6 85	At	6 86	Rn	
7 87	Fr	7 88	Ra	**	7 104	Rf	7 105	Db	7 106	Sg	7 107	Bh	7 108	Hs	7 109	Mt	7 110	Ds	7 111	Rg	7 112	Cn	7 113	Uut	7 114	Fl	7 115	Uup	7 116	Lv	7 117	Uus	7 118	Uuo	
LANTHANIDE SERIES				+	6 57	La	6 58	Ce	6 59	Pr	6 60	Nd	6 61	Pm	6 62	Sm	6 63	Eu	6 64	Gd	6 65	Tb	6 66	Dy	6 67	Ho	6 68	Er	6 69	Tm	6 70	Yb	6 71	Lu	
ACTINIDE SERIES				**	7 89	Ac	7 90	Th	7 91	Pa	7 92	U	7 93	Np	7 94	Pu	7 95	Am	7 96	Cm	7 97	Bk	7 98	Cf	7 99	Es	7 100	Fm	7 101	Md	7 102	No	7 103	Lr	

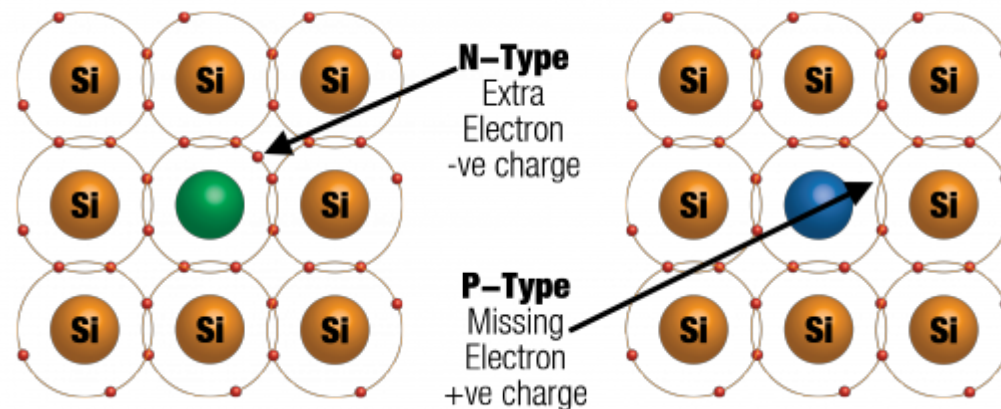
Another example for Covalent network solids

- Silicon
 - Covalent network solid and semiconductor
 - Forms a 3-D network similar to carbon
 - Doping (adding slight impurities by using a different element in the network solid) silicon's covalent network structure can increase its conductivity

Click on an element for more information

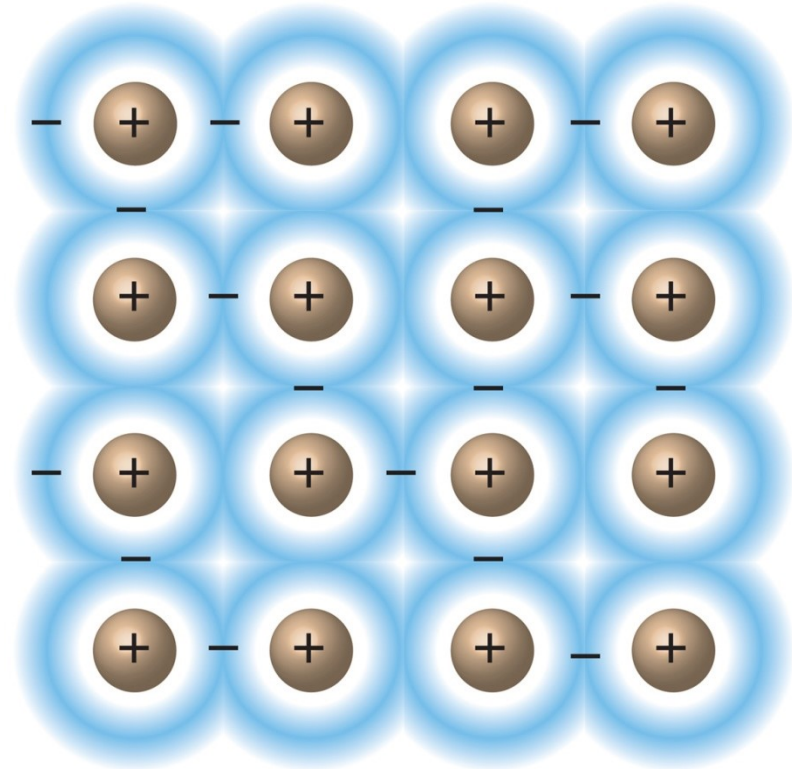
1																	18																		
1	H																	He																	
2	3	2	4											13	14	15	16	17	10																
2	Li	Be											B	C	N	O	F	Ne																	
3	11	3	12											3	13	3	14	3	15	3	16	3	17	3	18										
3	Na	Mg											Al	Si	P	S	Cl	Ar																	
4	19	4	20	4	21	4	22	4	23	4	24	4	25	4	26	4	27	4	28	4	29	4	30	4	31	4	32	4	33	4	34	4	35	4	36
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr																	
5	37	5	38	5	39	5	40	5	41	5	42	5	43	5	44	5	45	5	46	5	47	5	48	5	49	5	50	5	51	5	52	5	53	5	54
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe																	
6	55	6	56	*	6	72	6	73	6	74	6	75	6	76	6	77	6	78	6	79	6	80	6	81	6	82	6	83	6	84	6	85	6	86	
6	Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn																	
7	87	7	88	**	7	104	7	105	7	106	7	107	7	108	7	109	7	110	7	111	7	112	7	113	7	114	7	115	7	116	7	117	7	118	
7	Fr	Ra		Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo																	
LANTHANIDE SERIES				*	6	57	6	58	6	59	6	60	6	61	6	62	6	63	6	64	6	65	6	66	6	67	6	68	6	69	6	70	6	71	
				**	7	89	7	90	7	91	7	92	7	93	7	94	7	95	7	96	7	97	7	98	7	99	7	100	7	101	7	102	7	103	
ACTINIDE SERIES					7	Ac	7	Th	7	Pa	7	U	7	Np	7	Pu	7	Am	7	Cm	7	Bk	7	Cf	7	Es	7	Fm	7	Md	7	No	7	Lr	

- N-type (negative charge carrying)
semiconducting: doping with an element with one extra valence electron
- P-type (positive charge carrying)
semiconducting: doping with an element with one less valence electron
 - By adding and removing electrons from structure makes electrons that are available to flow and conduct electricity
 - Junctions between n-doped and p-doped materials can be used to control electron flow in electronics



Metallic Solids

- Metals are not covalently bonded, but the attractions between the electrons.
- In metals, valence electrons are delocalized throughout the solid.



Boiling Points of Solids

- Determined both by intramolecular (type of bonding) and intermolecular forces present
 - Generally:
 - ionic compounds have the highest boiling points
 - Metallic
 - Covalent network solids
 - Covalent compounds that have H bonds
 - Covalent compounds that have dipole-dipole forces
 - Covalent compounds that have london dispersion forces
 - If covalent compounds have similar forces, compounds with larger masses/sizes will have higher boiling points