

Molecular bonds

Ionic bond

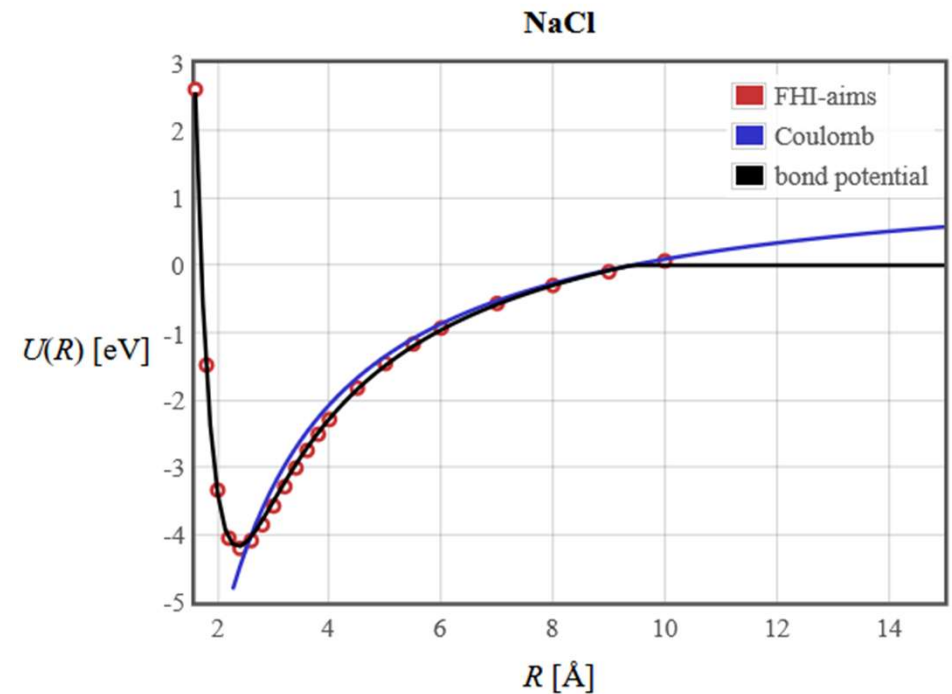
Coulomb force:

$$F = \frac{e^2}{4\pi\epsilon_0 r^2}$$

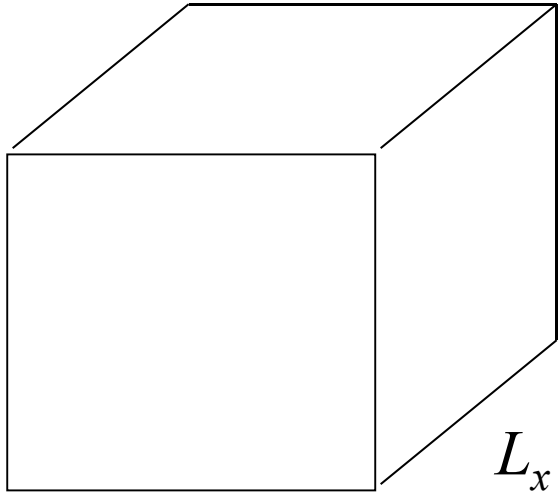
Energy needed to separate charges e and $-e$

$$E = \int \vec{F} \cdot d\vec{r} = \int_{0.2 \text{ nm}}^{\infty} \frac{-e^2}{4\pi\epsilon_0 r^2} dr = 7 \text{ eV}$$

Ionic bonds are a few eV



Covalent bond: Square well potential



L_y

L_z

L_x

$$V = \begin{cases} 0 & \text{inside the cube} \\ \infty & \text{outside the cube} \end{cases}$$

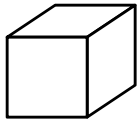
$$-\frac{\hbar^2}{2m} \nabla^2 \Psi = E \Psi$$

$$\Psi = \frac{2\sqrt{2}}{\sqrt{L_x L_y L_z}} \sin \frac{n_x \pi x}{L_x} \sin \frac{n_y \pi y}{L_y} \sin \frac{n_z \pi z}{L_z} \quad n_x, n_y, n_z = 1, 2, 3 \dots$$

$$E_{n_x n_y n_z} = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right)$$

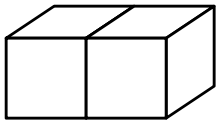
Covalent bond

$$E_{n_x n_y n_z} = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right)$$



Energy of a particle confined to a cube $L \times L \times L$

$$E = \frac{3h^2}{8mL^2} = \frac{12h^2}{32mL^2}$$



Energy of a particle confined to a cube $L \times L \times 2L$

$$E = \frac{9h^2}{32mL^2}$$

Decrease in energy:

$$E = 2 \times \frac{3h^2}{32mL^2} = \frac{3h^2}{16mL^2}$$

Two electrons

For $L = 0.2 \text{ nm}$ $\Delta E = 14 \text{ eV}$

Polar bonds

Partly covalent and partly ionic. The more electronegative element will have more negative charge.

0 ————— ————— 4
electronegativity (Pauling's)

Electronegativity

1 H 2.1																	2 He				
3 Li 1	4 Be 1.5															5 B 2	6 C 2.5	7 N 3	8 O 3.5	9 F 4	10 Ne
11 Na 0.9	12 Mg 1.2															13 Al 1.5	14 Si 1.8	15 P 2.1	16 S 2.5	17 Cl 3	18 Ar
19 K 0.8	20 Ca 1	21 Sc 1.3	22 Ti 1.5	23 V 1.6	24 Cr 1.6	25 Mn 1.5	26 Fe 1.8	27 Co 1.8	28 Ni 1.8	29 Cu 1.9	30 Zn 1.6	31 Ga 1.6	32 Ge 1.8	33 As 2	34 Se 2.4	35 Br 2.8	36 Kr 3				
37 Rb 0.8	38 Sr 1	39 Y 1.2	40 Zr 1.4	41 Nb 1.6	42 Mo 1.8	43 Tc 1.9	44 Ru 2.2	45 Rh 2.2	46 Pd 2.2	47 Ag 1.9	48 Cd 1.7	49 In 1.7	50 Sn 1.8	51 Sb 1.9	52 Te 2.1	53 I 2.5	54 Xe 2.6				
55 Cs 0.7	56 Ba 0.9	57 La 1.1	72 Hf 1.3	73 Ta 1.5	74 W 1.7	75 Re 1.9	76 Os 2.2	77 Ir 2.2	78 Pt 2.2	79 Au 2.4	80 Hg 1.9	81 Tl 1.8	82 Pb 1.8	83 Bi 1.9	84 Po 2	85 At 2.2	86 Rn				
87 Fr 0.7	88 Ra 0.9	89 Ac 1.1	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt													
58 Ce 1.1	59 Pr 1.1	60 Nd 1.1	61 Pm 1.1	62 Sm 1.1	63 Eu 1.1	64 Gd 1.1	65 Tb 1.1	66 Dy 1.1	67 Ho 1.1	68 Er 1.1	69 Tm 1.1	70 Yb 1.1	71 Lu 1.2								
90 Th 1.2	91 Pa 1.4	92 U 1.5	93 Np 1.3	94 Pu 1.3	95 Am 1.3	96 Cm 1.3	97 Bk 1.3	98 Cf 1.3	99 Es 1.3	100 Fm 1.3	101 Md 1.3	102 No 1.3	103 Lr								

Bond potentials

Morse (covalent)

$$U(r) = U_0 \left(e^{-2a(r-r_0)} - 2e^{-a(r-r_0)} \right)$$

Lennard - Jones (van der Waals)

$$U(r) = 4\epsilon \left(\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right)$$

