Molecular bonds

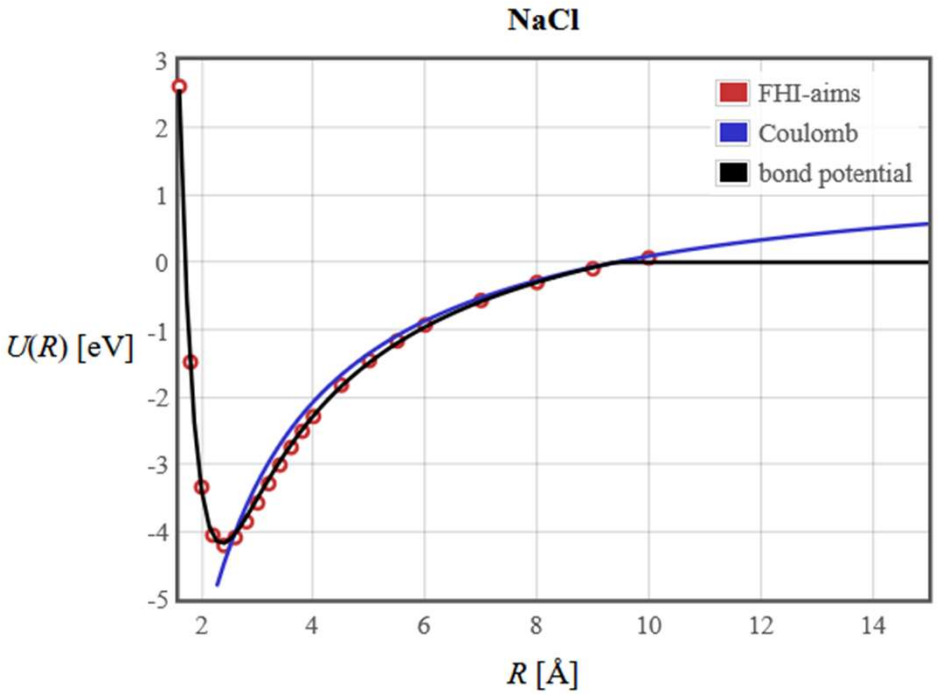
Ionic bond

Coulomb force: $$F = \frac{e^2}{4\pi\varepsilon_0 r^2}$$

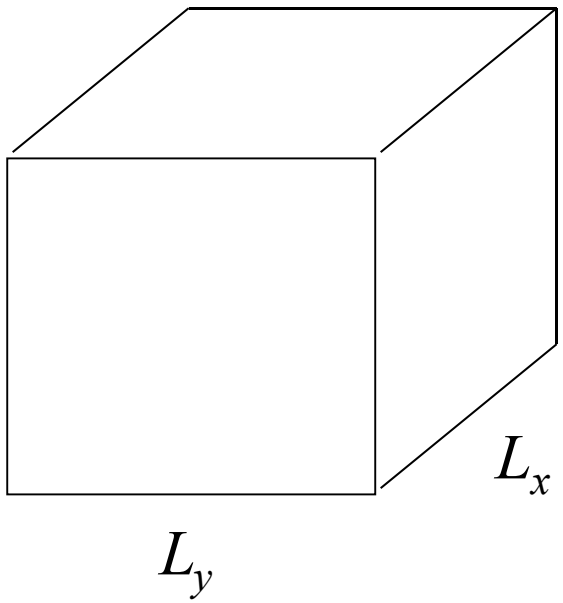
Energy needed to separate charges e and $-e$

$$E = \int \vec{F} \cdot d\vec{r} = \int_{0.2\text{ nm}}^{\infty} \frac{-e^2}{4\pi\varepsilon_0 r^2} dr = 7\text{ eV}$$

Ionic bonds are a few eV



Covalent bond: Square well potential



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

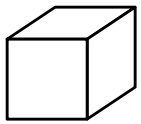
$$-\frac{\hbar^2}{2m}\nabla^2\Psi = E\Psi$$

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

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

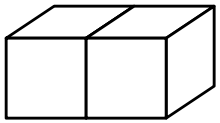
Covalent bond

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



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:

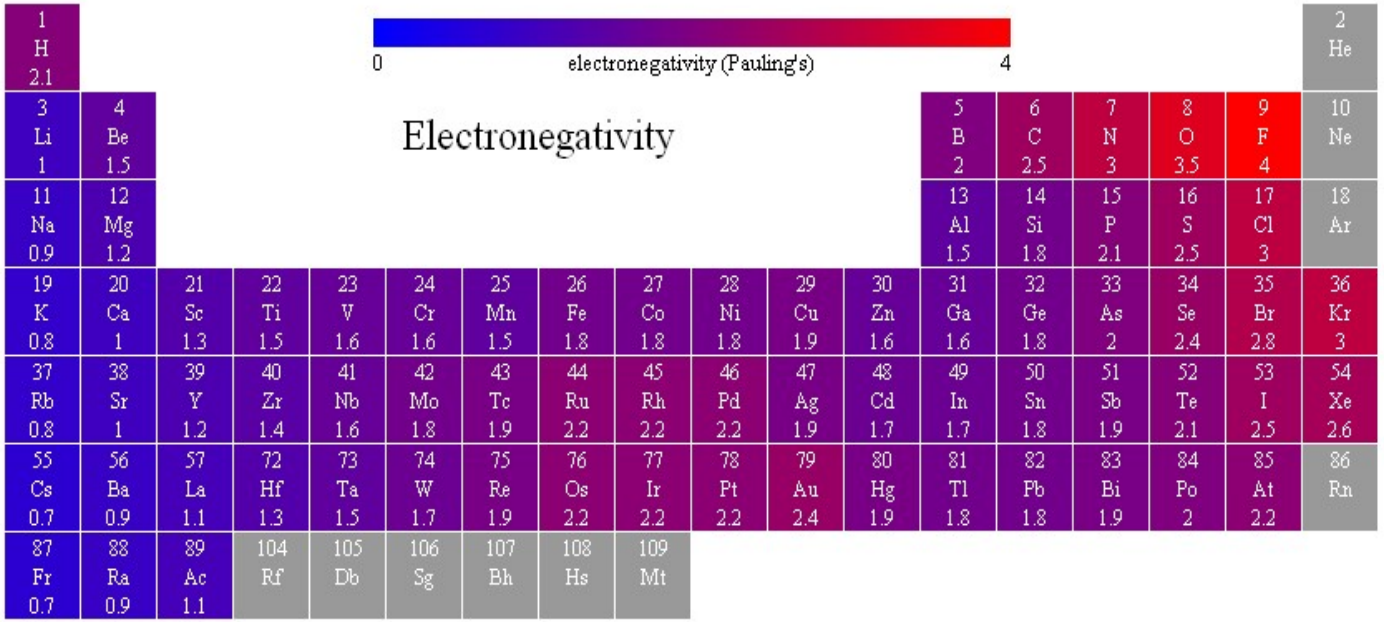
$$E = 2 \times \frac{3h^2}{32mL^2} = \frac{3h^2}{16mL^2}$$

Two electrons

For $L = 0.2$ nm $\quad \Delta E = 14$ eV

Polar bonds

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



http://www.webelements.com/ http://www.chemicalelements.com/ http://www.chemicool.com/

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)

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