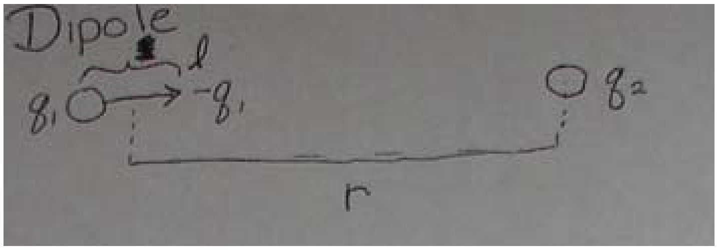
20.310 Section 9/19/06

(HW: radius of interaction… mcs & cells)

Dipole



$$E = \frac{q_1 q_2}{4\pi e_0 r} = \frac{1}{4\pi\varepsilon_0}\Sigma\frac{q_1 q_2}{r_{12}}$$

$$= \frac{1}{4\pi\varepsilon_0}\left(\frac{-q_1q_2}{r-\frac{l}{2}} + \frac{q_1q_2}{r+\frac{l}{2}}\right)$$

$$= \frac{1}{4\pi\varepsilon_0}\left(\frac{-q_1q_2}{r}\right)\left(\frac{1}{1-\frac{l}{2r}} - \frac{1}{1+\frac{l}{2r}}\right)$$

Let $x = \frac{l}{2r}$

$\therefore$ $E = \frac{1}{4\pi\varepsilon_0}\left(\frac{-q_1q_2}{r}\right)\left(\frac{1}{1-x} - \frac{1}{1+x}\right)$ where $\frac{1}{1-x} - \frac{1}{1+x} = \frac{(1+x)-(1-x)}{(1-x)(1+x)} = \frac{2x}{1-x^2}$

or $(1\pm x)^{-1} = (1 \mp x + x^2 \mp x^3 + x^4 \ldots)$

$$= \frac{1}{4\pi\varepsilon_0}\left(\frac{-q_1q_2}{r}\right)\left[(1+x+x^2+x^3+\ldots) - (1-x+x^2-x^3+\ldots)\right]$$

$$= \frac{1}{4\pi\varepsilon_0}\left(\frac{-q_1q_2}{r}\right)\underset{\uparrow}{(2x)} = \frac{1}{4\pi\varepsilon_0}\left(\frac{-q_1q_2}{r}\right)(2)\left(\frac{l}{2r}\right) = \frac{1}{4\pi\varepsilon_0}\left(\frac{-q_1q_2 l}{1}\right)\left(\frac{1}{r^2}\right) \sim \frac{1}{r^2} \qquad \surd$$

dominant term in series

Molecular Mechanics in General

$$\underset{\substack{\uparrow\\ \text{energy}\\ \text{function}}}{E(R)}=\frac{1}{2}\sum_{\text{bonding}}\underset{\substack{\uparrow\\ \text{bond}\\ \text{stiffness}}}{K_B}(b-b_0)^2+\frac{1}{2}\sum_{\substack{\text{bond}\\ \text{angles}}}K_\theta(\theta-\theta_0)^2+\frac{1}{2}\sum_{\text{torsion}}K_\phi(1+\cos(n\phi-\delta)+\sum_{\substack{\text{nonbonding}\\ \text{interactions}}}(\underset{\substack{\nwarrow\\ \text{repulsive}}}{\frac{A}{r^{12}}}-\underset{\substack{\uparrow\\ \text{attractive}\\ \text{(van der Waals)}}}{\frac{B}{r^6}}+\underset{\substack{\uparrow\\ \text{Columbic}\\ \text{interaction}}}{\frac{q_1q_2}{Dr}})$$