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PHYS3009: Force and Function at the Nanoscale
Week 19 – 12:00pm Friday – 31 January 2025

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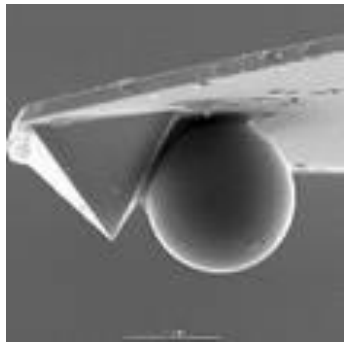
Forces and Potentials

Force & function at the nanoscale

Summary of key concepts from the last lecture

Microscopic and nanoscale forces are important in a number of areas of nanoscience, nanotechnology and biology.



These forces start to become important on the nanometre length scale.

The relevant energy scale on these small length scales is the thermal energy.

$$U_{thermal} \approx kT$$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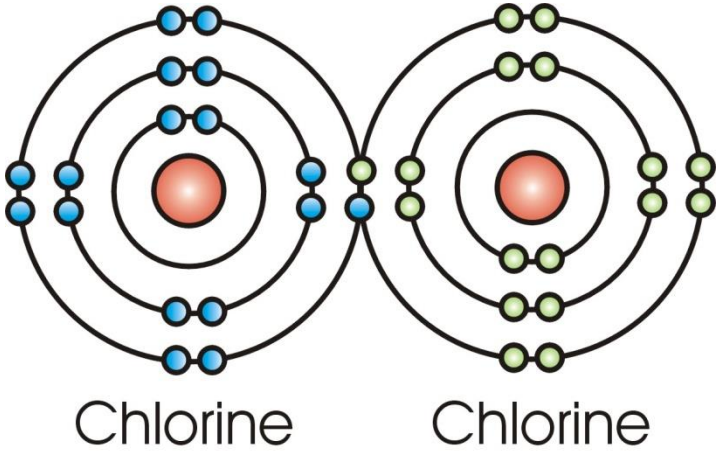
Strong interactions

Strong inter-atomic and intermolecular interactions II: Covalent interactions

Covalent bonds are highly directional and are chemical in origin (e.g. π bond created by overlap of p electron orbitals)



These interactions originate from the sharing of **valence** electrons to facilitate the filling of electronic shells within atoms → stable structures

The directionality of the bonds is caused by the mutual repulsion of the electrons in different bond orbitals

Properties of covalent bonds

Covalent forces (bonds) operate over short distances 0.1-0.2 nm

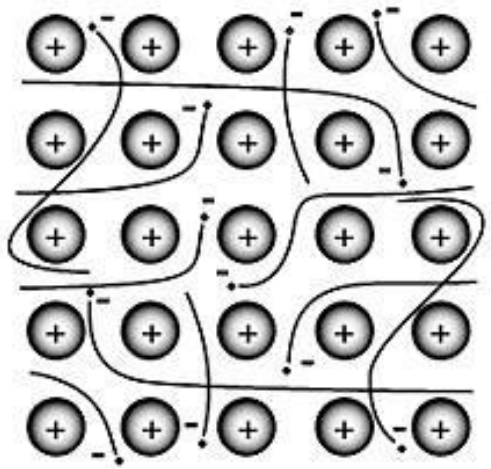
The energies associated with the formation of these bonds are typically 2 to 8 eV per bond (that's on the order of 100 times kT at room temperature)

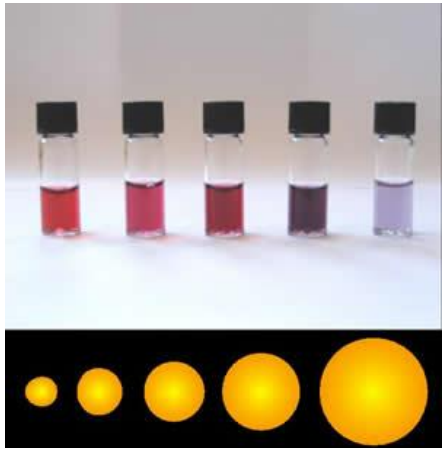
You will learn more about these in the 3rd year Solid State module

Strong inter-atomic and intermolecular interactions III: Metallic bonding interactions

Sharing of electrons between metal atoms gives rise to another form of bonding.

However, in metallic bonds, the electrons become delocalised throughout the material in such a way that they are shared between many nuclei.

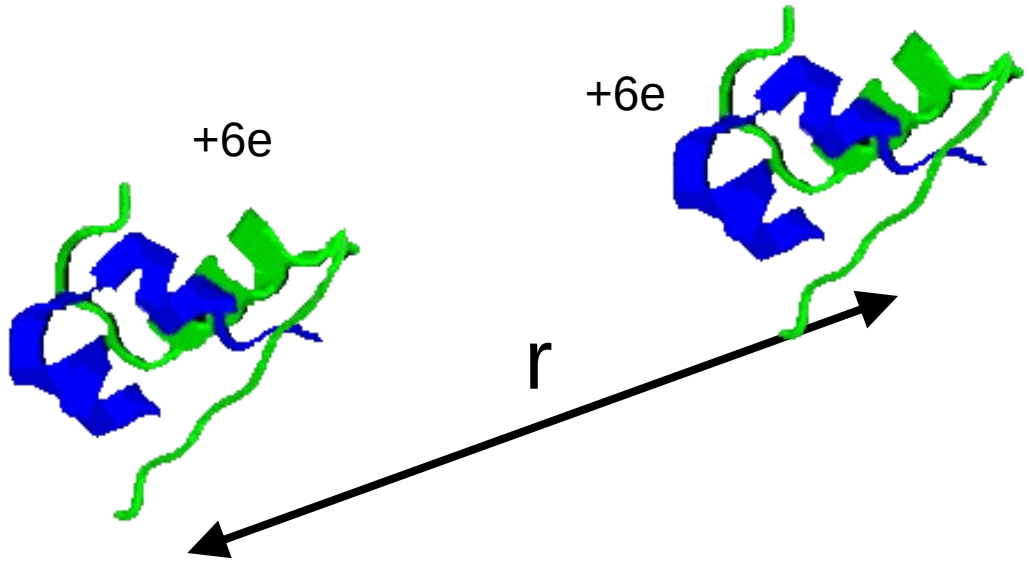




Strong inter- atomic and intermolecular interactions I: Coulomb interactions

You have already met Coulomb interactions in the first year module ‘Newton to Einstein’

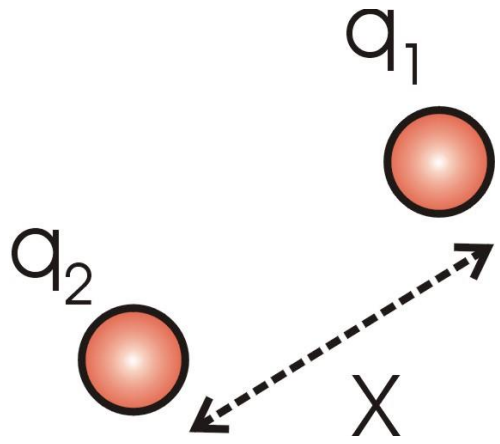
Some atoms and molecules may acquire a net charge and will interact via electrostatic forces



Electrostatic potential

The **potential energy** of two molecules having charges q_1 and q_2 that are separated by a distance, x, is given by

$$U(x) = \frac{q_1 q_2}{4\pi\varepsilon\varepsilon_o x}$$



ε_o=8.85 x 10^{-12} $C^2N^{-1}m^{-1}$

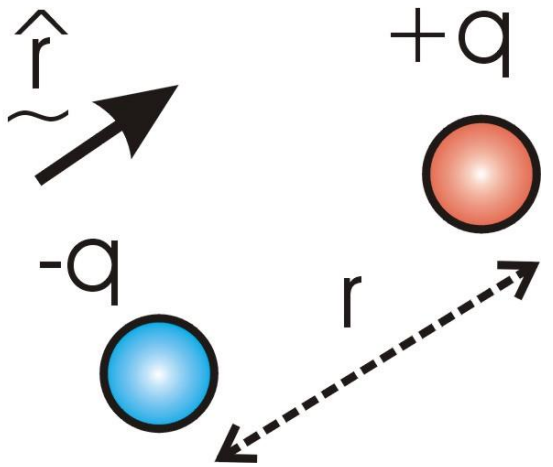
ε=relative permittivity

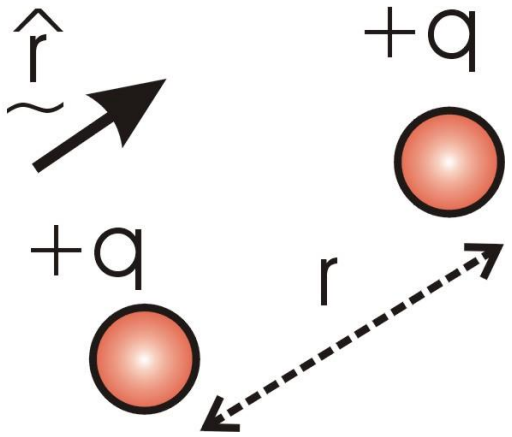
Inverse power law dependence (x^{-n}) is typical of many different types of potential

The ‘sign’ of the potential

When the potential energy is negative the interaction is favourable

Potential energy $U < 0$





When the potential energy is positive, interactions are unfavourable

Potential energy $U > 0$

Problem 2.1 Range of electrostatic interactions

We can obtain an estimate of the range X_{range} below which the interaction between two atoms/molecules matters

$$|U(x)| = kBT$$

Problem: A positively charged sodium ion Na^+ and a negatively charged Chloride ion Cl^- are 20nm apart in a vacuum. Is the Coulomb force between them significant?

$$U(x) = \frac{q_1 q_2}{4\pi\varepsilon_o X_{range}}$$

e = 1.602×10^{-19}C
$\varepsilon_0 = 8.854 \times 10^{-12}$ Fm^{-1}
$k_B = 1.38 \times 10^{-23}$ m^2 kg s^{-2} K^{-1}
T = 20°C

Range of electrostatic interactions

Rearranging gives

$$X_{range} = \left| \frac{q_1 q_2}{4\pi\varepsilon\varepsilon_o kT} \right|$$

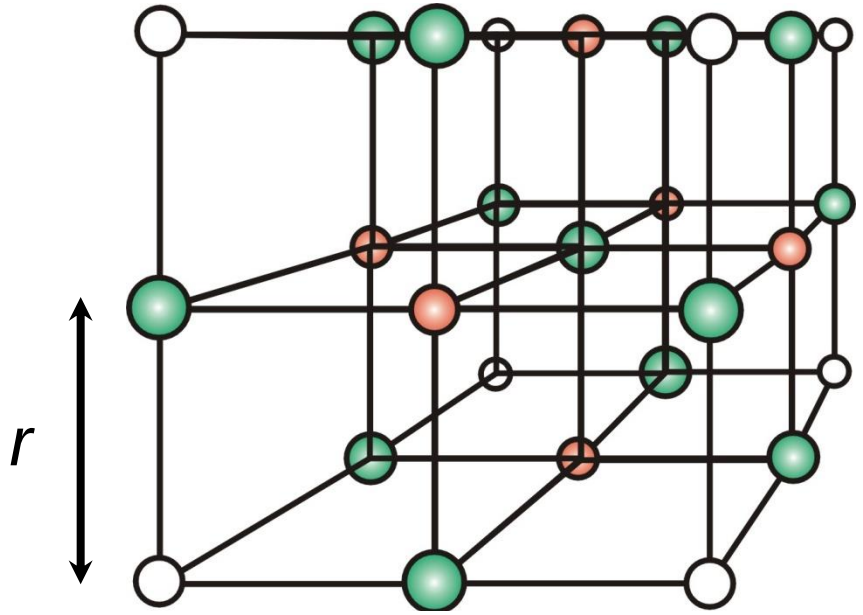
$x \geq X_{range}$ *electrostatic interactions become unimportant*

$x < X_{range}$ *electrostatic interactions start to influence atoms/molecules*

Ionic Crystals

Electrostatic interactions are responsible for the formation of ionic crystals

For example, consider NaCl (salt)



Cohesive energy of ionic crystals

We can calculate the (cohesive) energy per ion pair holding the crystal together by summing up the contributions to the potential energy from all neighbours

$$U_{coh} = -\frac{e^2}{4\pi\varepsilon\varepsilon_0 r}\left(\frac{6}{1} - \frac{12}{\sqrt{2}} + \frac{8}{\sqrt{3}} - \cdots\right) = -\frac{\alpha e^2}{4\pi\varepsilon\varepsilon_0 r}$$

where α is called the Madelung constant (α =1.748 for NaCl and anything else that has the same crystal structure)

e is the electronic charge (1.6 x 10^{-19}C)

"Strong" or "weak"? – Boltzmann Equation

However, if |U(x)| > kT this **does not** mean the interaction is stable indefinitely

The probability of 2 objects which are held together by an attractive interaction escaping due to thermal fluctuations is given by the Boltzmann probability.

$$P(x) \propto exp^{-U/k_B T}$$

Proportional

Potential of interaction

The ratio U/kT determines how likely 2 objects are to stay "stuck" to one another.

For a covalent bond U/kT ~ 100. → $e^{-100} = 3.7 \times 10^{-44}$ → "Stable" or "Strong"

Suppose U/kT ~ 2 → $e^{-2} = 0.13$ → Probability is "Significant" but "Weak"

Problem 2.2 – Dissolving salt

1) Calculate the cohesive energy of a NaCl crystal in

a) water ($\varepsilon = 80$)

b) toluene ($\varepsilon = 2.38$)

$$U_{coh} = -\frac{e^2}{4\pi\varepsilon\varepsilon_0 r}\left(\frac{6}{1} - \frac{12}{\sqrt{2}} + \frac{8}{\sqrt{3}} - \cdots\right) = -\frac{\alpha e^2}{4\pi\varepsilon\varepsilon_0 r}$$

$\alpha = 1.748$, $\varepsilon_0 = 8.854 \times 10^{-12} \mathrm{Fm}^{-1}$, $k_B = 1.38 \times 10^{-23}\ \mathrm{m^2 kg s^{-2} K^{-1}}$, $T = 293\mathrm{K}$

the nearest neighbour spacing between Na^+ and Cl^- ions is r = 0.282 nm.

2) Use your answers to parts a) and b) to explain why ionic crystals dissolve in water, but not in organic solvents.

3) Why does heating the water help the salt dissolve faster?

Relationship between force and potential

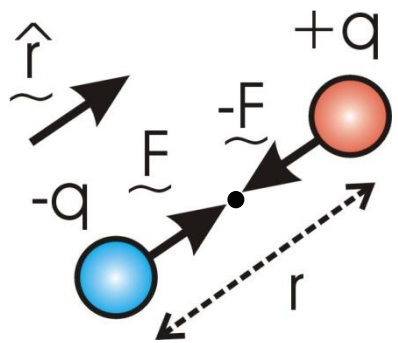
The force, *F,* on an object can be related to the gradient in its potential energy, *U,* with respect to distance, x, by the formula

$$F(x) = -\frac{dU}{dx}$$

This is an extremely important formula in physics and we will use it a lot.

The ‘sign’ of the force

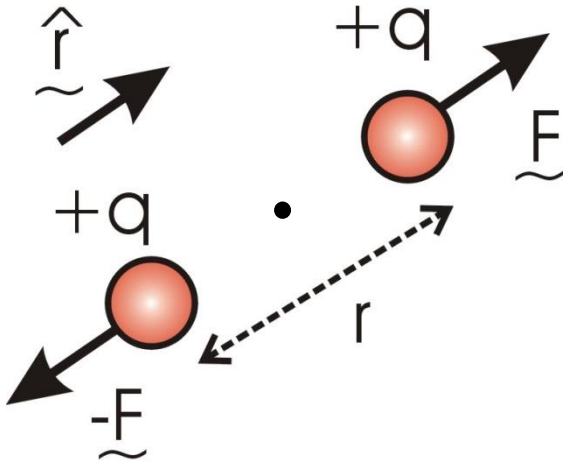
Negative forces are attractive



$|\underline{F}| < 0$

Positive forces are repulsive

$|\underline{F}| > 0$



Electrostatic forces

The **force acting between** two point charges q_1 and q_2 separated by a distance, x, is given by

$$F(x) = -\frac{dU}{dx} = \frac{q_1 q_2}{4\pi\varepsilon\varepsilon_o x^2}$$

The sign of the force depends upon the signs of the charges

If $q_1 q_2 < 0$ **force is attractive** (negative sign)

If $q_1 q_2 > 0$ **force is repulsive** (positive sign)

Summary Key Concepts

The range of an interaction determines whether it is important at different distances

How likely an interaction is to be disrupted by thermal fluctuations defines them as “strong” or “weak”?

$$P(x) \propto exp^{-U/k_B T}$$

The force can be calculated from the derivative of the potential:

$$F(x) = -\frac{dU}{dx}$$