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PHYS3009: Force and Function at the Nanoscale
Week 20 – 9:00am Wednesday – 05 February 2025

valid for 15 minutes from 8:55am
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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”?

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

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

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

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Polar interactions

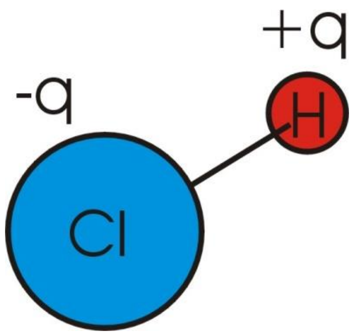
Force & function at the nanoscale

What are polar molecules?

Many molecules are electrically neutral and therefore carry no net charge

However, they can still possess an **electric dipole moment**

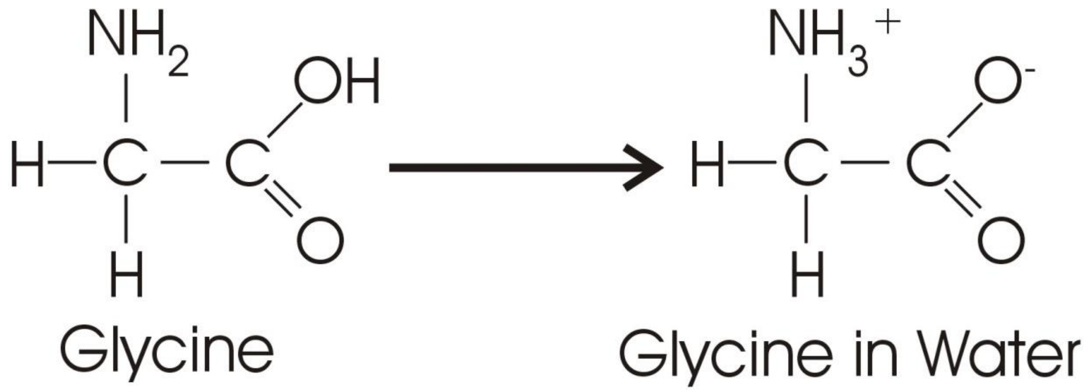
Consider the molecule **HCl** (hydrogen chloride)



More **electronegative atoms** such as chlorine have a higher affinity for electrons. In the case of HCl, the electrons are pulled towards the chlorine atom giving rise to a **permanent dipole**

Zwitterions and dipolar ions

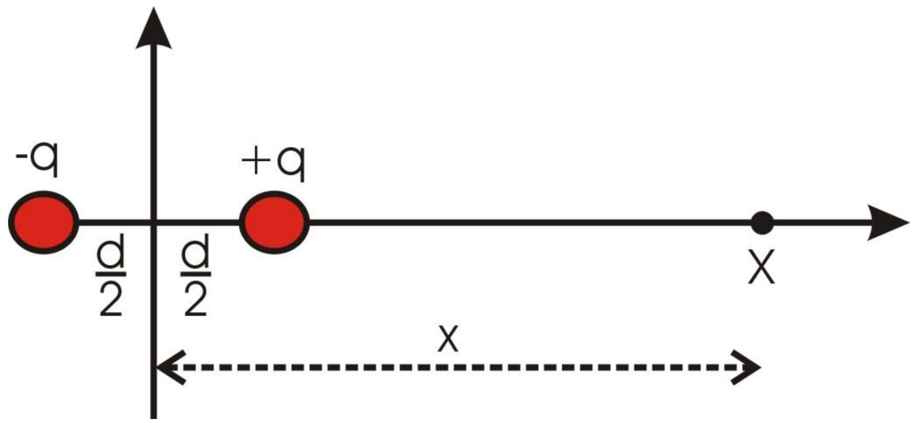
In some cases, the polar properties of the molecules depend upon the local environment (e.g. presence of solvents). Water soluble polar molecules of this type are called **Zwitterions** (Zwitter- German meaning ‘hybrid’)



Some molecules contain both a net charge and a dipole moment. These molecules are referred to as **dipolar ions**

Electric field due to a dipole

Consider two charges separated by a small distance, d in a medium of dielectric constant, ε



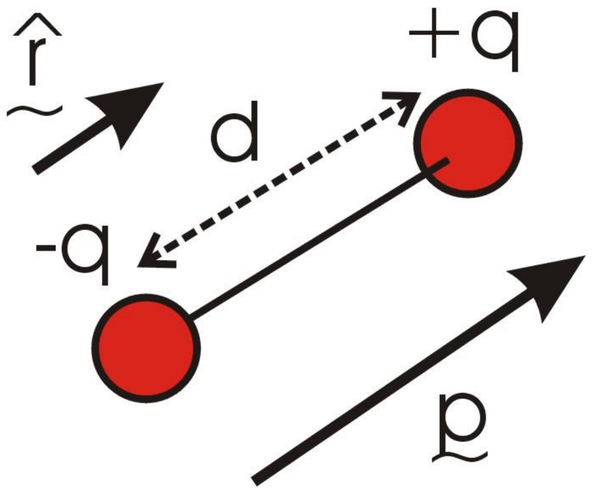
We can calculate the field at the point, x, by summing up the fields due to the two point charges

When $x >> d$, this gives the result that;

$$\boldsymbol{E} = \frac{qd}{2\pi\varepsilon\varepsilon_0}\frac{1}{x^3}\boldsymbol{i}$$

How do we define an electric dipole?

Recall from electromagnetism that a dipole consists of two charges (+q and -q) separated by a distance $\underline{d}$

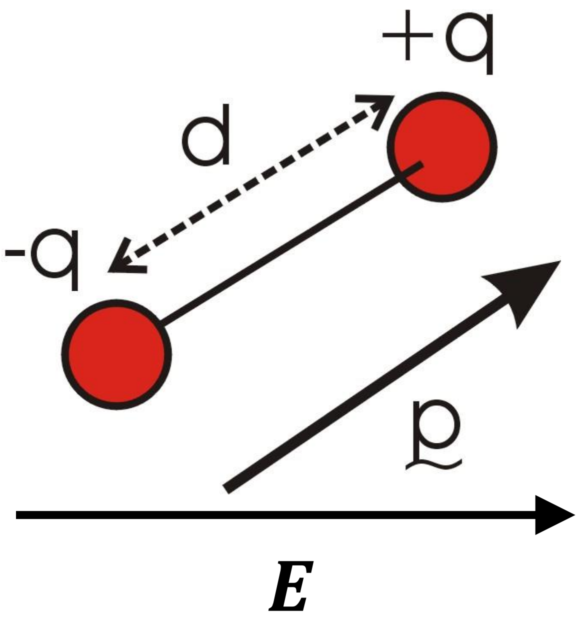


The dipole moment, **p**, is then defined as $\boldsymbol{p} = qd\,\hat{\boldsymbol{r}}$

Energy of a dipole in an external electric field

Later, we will need to determine the energy of interaction between dipoles.

We therefore need to calculate the energy of a dipole in an external electric field

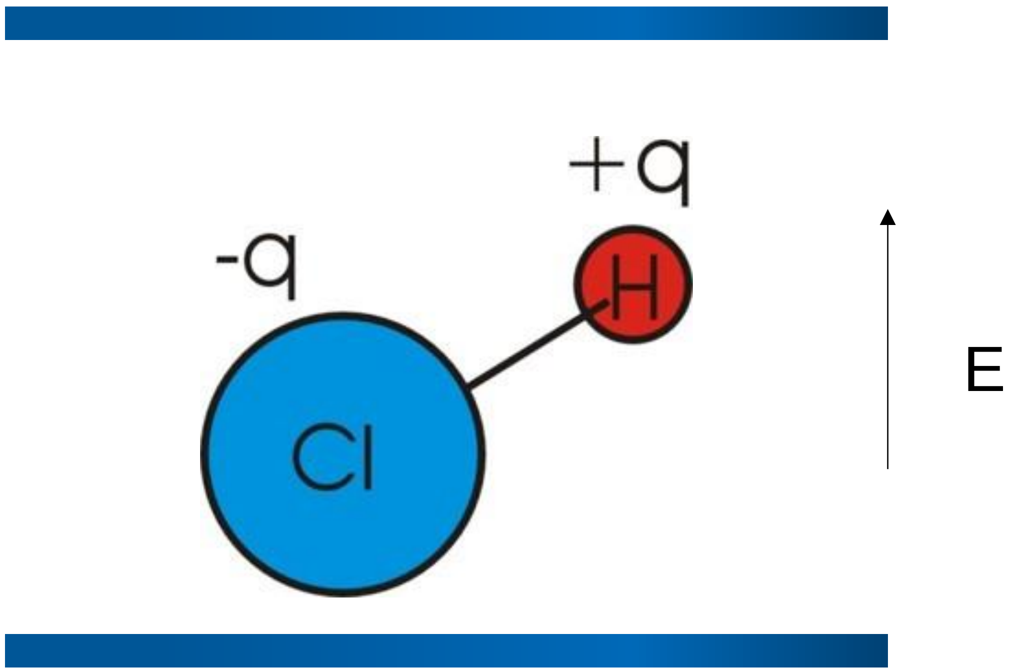


Potential energy of a dipole in an electric field

$$\boxed{U_{dipole} = -\boldsymbol{p}.\boldsymbol{E}}$$

Problem 3.3

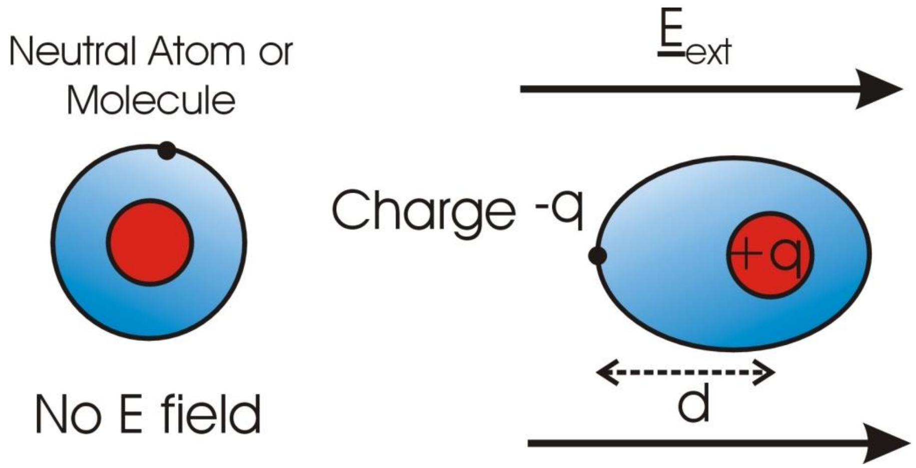
A Hydrogen Chloride molecule is placed between a parallel plate capacitor with linear electric field $1Vm^{-1}$. The HCl molecule has a bond length of 0.3nm and charges of +/- 0.1e. What is the energy change if the dipole rotates from an initial angle of 60˚ to the Electric field to aligned with it?



Polarisation using external fields

Atoms and molecules are polarised by external electrical fields.

Opposite charges move in different directions when an E field is applied



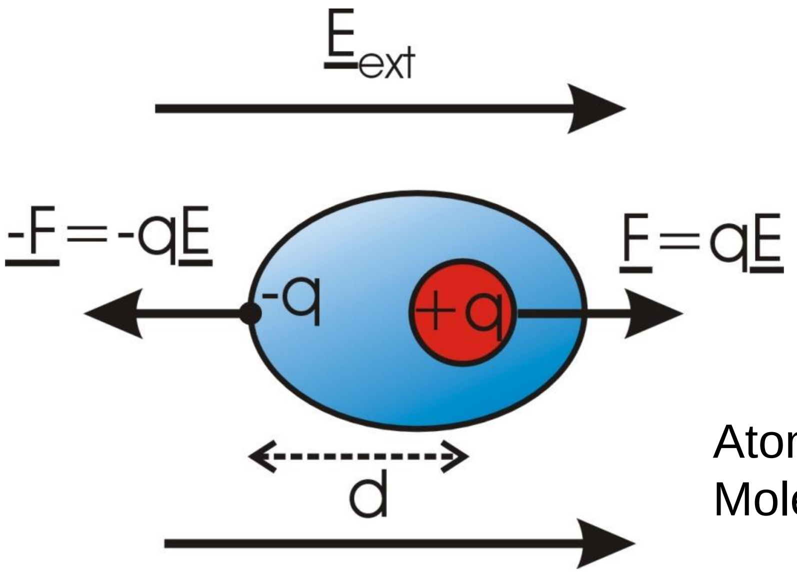
The dipole moment of an atom or molecule can be related to the external applied electric field by

$$\boxed{\boldsymbol{p} = \alpha \boldsymbol{E}_{ext}}$$

Where α is the **polarisability** of the atom/molecule

Polarisability of atoms and molecules

We can determine the polarisability of an atom/molecule in an applied external field



Atom or Molecule

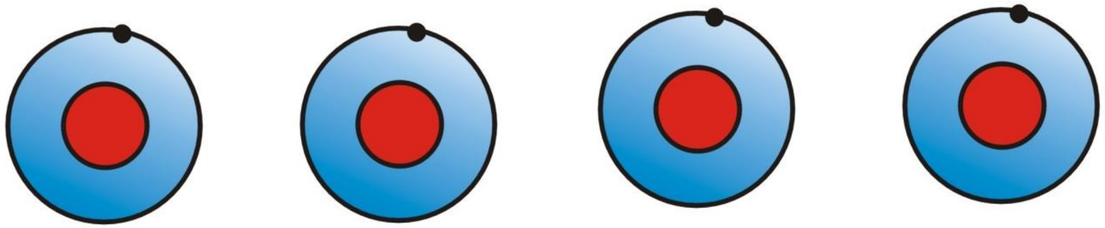
$$\alpha = 4\pi\varepsilon_0 d^3$$

d is typically smaller than, but comparable to radius of atom/molecule *R.*

α scales with volume of atom/molecule *(V~R^3)*

Dispersion Interactions

Consider what happens in a piece of material containing all neutral atoms

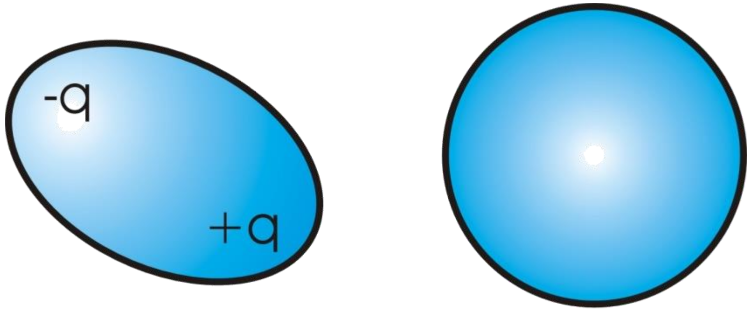


Dispersion forces

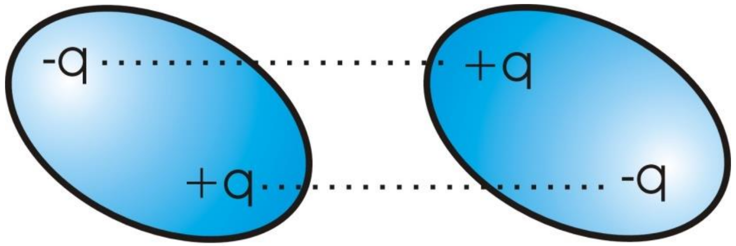
Dispersion interactions act between all atoms and molecules (in contrast to other types of interaction e.g. ionic, covalent etc. which depend upon the type of molecule).

These interactions arise as the result of **temporary local fluctuations in charge density on atoms/molecules**

They always result in an attractive force between them and their neighbours.



Atom 1 Atom 2



Atom 1 Atom 2