**Density functional theory**

Density-functional theory (DFT) is a successful theory to calculate the electronic structure of atoms, molecules, and solids. Its goal is the quantitative understanding of material properties from the fundamental laws of quantum mechanics.

**Permeability**

Permeability is therefore a measure of the ability of water to move through a porous material.

Permeability = number of water molecules/ (area x time x applied pressure)

**Hydration radius of ion**

It is defined as the radius of ion and closely bound water molecules. It is inversely related to the atomic radius of an element. The ions with larger size and low charge hold water molecules less tightly and therefore have a smaller atomic radius.

**Potential of mean force**

The potential of mean force provides a free energy profile along a preferred coordinate, be it a geometric or energetic coordinate, such as the distance between two atoms or the torsional angle of a molecule. This free energy profile describes the average force of all possible configurations of a given system (the ensemble average of the force) on particles of interest.

**Optimized potential for liquid simulations OPLS**

OPLS is basically a force field containing different parameters for the liquids. These potential functions have a simple form and they have been parametrized directly to reproduce experimental thermodynamic and structural data on fluids.