Thermodynamics for Biological Systems:
Classical and Statistical Aspects
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Lecture – 54
Introduction to Statistical Thermodynamics

Hello everyone, I will be teaching Statistical Thermodynamics as a part of this course Thermodynamics and Statistical Thermodynamics for biology. And I am Sanjib Senapati from IIT Madras and the part of the course the reference books what I will be following or Statistical Mechanics by Donald A. McQuarrie and Molecular Modelling: Principles and Applications by Andrew R leach.

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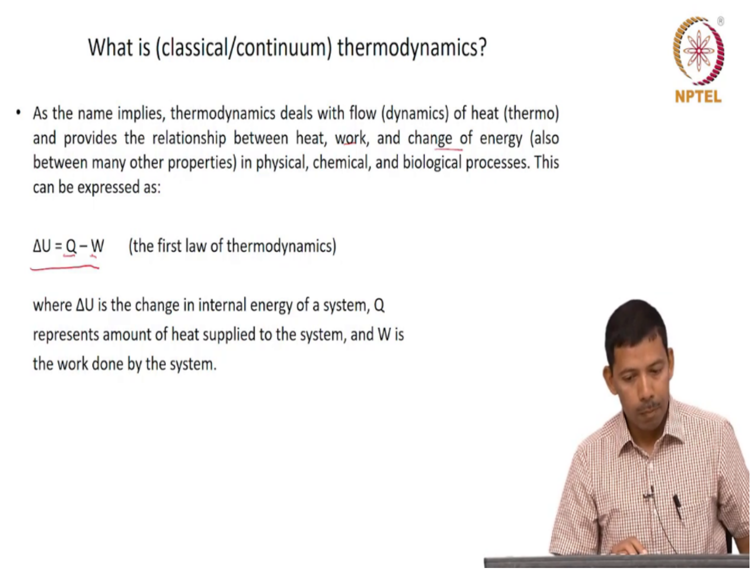

So, before we go to Statistical Thermodynamics, let us look at what we mean by Classical Thermodynamics. So, as you know, Classical Thermodynamics is also called the Continuum Thermodynamics and if you look at the name thermodynamics as the name implies it essentially talks about dynamics or the flow of heat. Dynamics is nothing but the flow and thermal is nothing but the heat.

So, thermodynamics talks about flow of heat and if you look at the first law of thermodynamics it basically gives you the relationship between heat, work and change of energy in a physical chemical or it could be a biological system. And this is the first law, the change of energy of our system is equal to the heat supplied to the system minus work done by the system on the surrounding.

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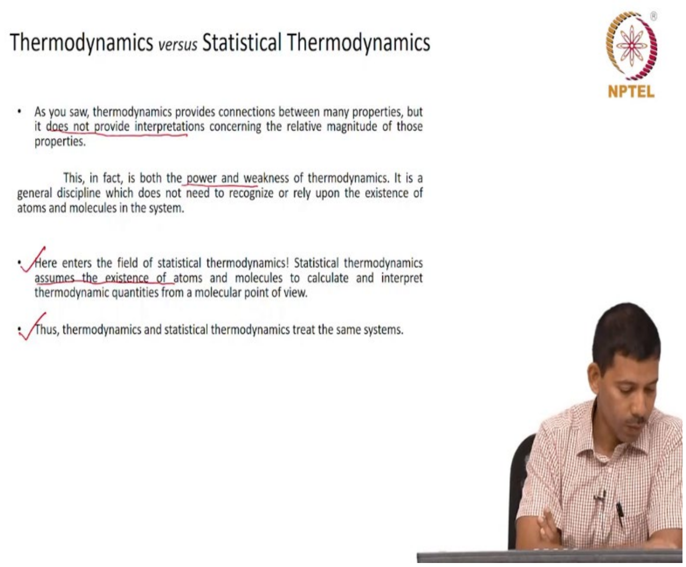

So, how Statistical thermodynamics is different than the Classical thermodynamics, as you saw the first law thermodynamics provides connection between many properties, there are many other properties you have come across in the first part of this course. One of the equations what we will be using in few minutes is

$$\Delta G = \Delta H - T\Delta S$$

So, that expression basically gives a relationship between free energy, enthalpy and entropy.

So, thermodynamics basically is providing the connection between many properties. But, it does not provide interpretation concerning the relative magnitude of those properties. It does not say why ΔH is so much why ΔS is so much why the heat why that work done by the system is so much and so on. So, this impact is both the power and the weakness on of thermodynamics.

It is a discipline where it does not need to recognize the existence of atoms or molecules in the system. And here enters the Statistical thermodynamics. Statistical thermodynamics, on the other hand, assumes that the system is composed of molecules and atoms and it calculates, it calculates and interprets the thermodynamic quantities from the molecular point of view. Thus thermodynamics and statistical thermodynamics they treat the same systems but their goal is different.

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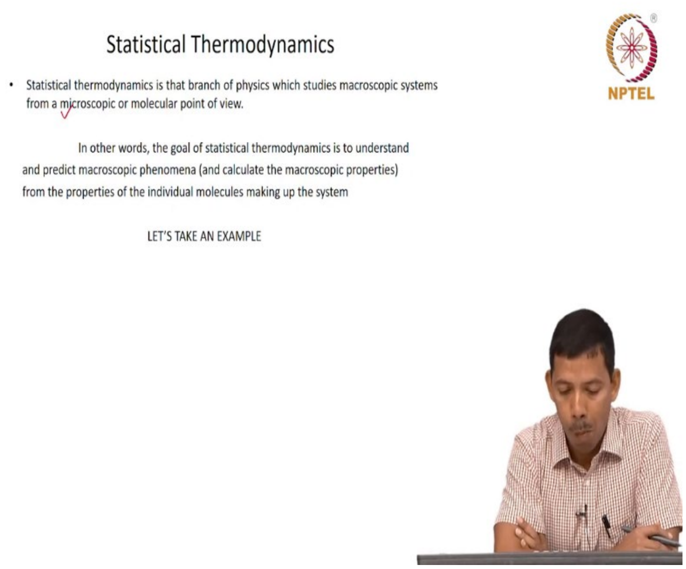

So, in nut shell, we have to define the Statistical thermodynamics we can say, is that branch of physics which studies the macroscopic system from a microscopic or molecular point of view. So, here macroscopic system by that mean the properties what you measure in laboratory. For example, pressure, volume, free energy change of energy and so on so forth.

So, how those macroscopic quantities can be obtained from microscopic information of the system. In other words, the goal of statistical thermodynamics is to understand and predict macroscopic phenomena and also calculate the macroscopic properties from the properties of the Constituent molecules or the atoms that make up the system. Let us take an example.

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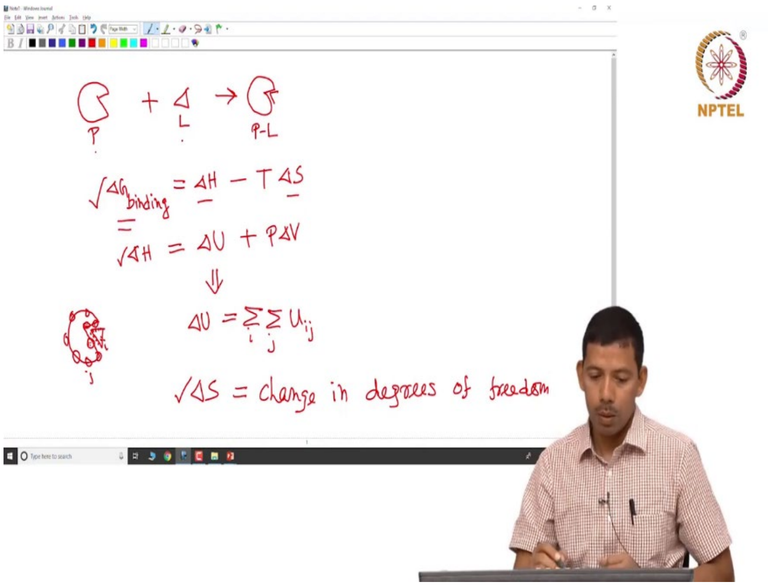

So, we have a protein, unless this is the conformation of the protein, we say this is P and we have a ligand L which binds to this protein to make the protein ligand complex PL complex. Now, what will be the ΔG of ligand binding? So, this ΔG binding you will be getting from thermodynamic expression ΔH - TΔS where ΔH is changing enthalpy and ΔS is the change in entropy.

So, this is the thermodynamic relation what you got to get the change in free energy due to the binding of the ligand to the protein. But what is the magnitude of ΔH magnitude of ΔS, the classical thermodynamics does not tell you that. Now, statistical thermodynamics comes so I am writing another expression from Classical thermodynamics what you have come across is

$$\Delta H = \Delta U + P\Delta V$$

So, now, Statistical thermodynamics can explain why ΔH is this much. Statistical thermodynamics now constitutes this particular protein is composed of amino acids and each amino acid is composed of many atoms: carbon, hydrogen, oxygen, the peptide bond and so on and so forth. It also considers that my ligand is having the atoms that made of this ligand molecule.

So, now statistical mechanics will calculate this

$$\Delta U = \sum_{i} \sum_{j} U_{ij}$$

So, this U_{ij} is basically defining the inter particle interaction. So U_{ij}, is basically the interaction of i^{th} particle in the ligand with the j^{th} particle in the protein. So, ΔU is obtained from Statistical thermodynamic law which says that the inter particle interactions between the ligand and protein, if you sum them up you get the total U of the protein ligand complex.

Likewise, if you want to get the entropy so, you basically calculate from statistical mechanics the change in degrees of freedom, freedom of the ligand and protein due to the binding of the ligand to the protein active site. So, as you see, both entropy and enthalpy, you are getting from Statistical thermodynamics and those magnitude you are putting off in this expression of thermodynamics to find out what is your ΔG binding.

So, both thermodynamics and statistical thermodynamics they are applied to a same system but for different goal.

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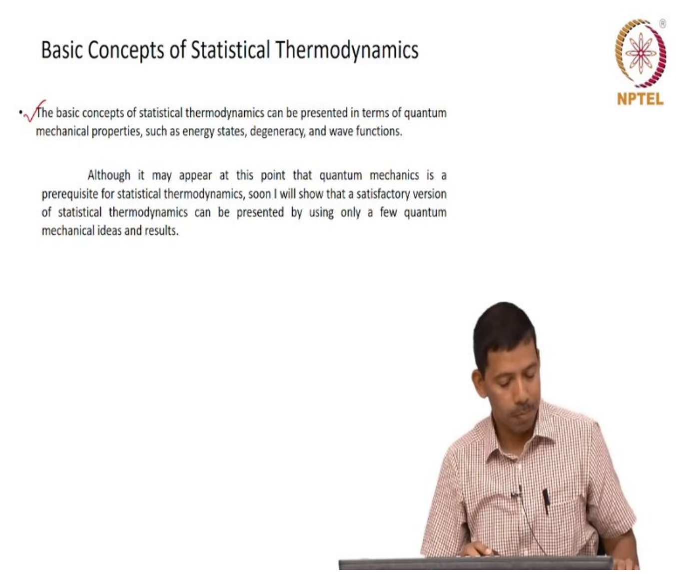

So, now we need to get a few basic concepts of Statistical thermodynamics. And the basic concepts of Statistical thermodynamics can be presented in terms of few quantum mechanical properties such as the energy states, the degeneracy, the wave function and so on. But so from my this statement it might appear that there you need up quantum mechanical you know quantum mechanical knowledge, but that is not the case.

As soon; so, that a satisfactory version of statistical thermodynamics can be presented by using only a few quantum mechanical ideas and results;