Biophotonics
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Lecture - 7
Fact of Matter - Part 2

(Refer Slide Time: 00:13)

Welcome back. So we shall continue our discussion on the quantized state of matter or as I like to put it, the fact of matter, pun intended of course. So in the previous class, we discussed about the quantization state of electrons or quantization state of atom itself.

When we have a nucleus that puts some amount of conditions on to the electron that is moving around. It cannot be too close, it cannot be too far. So there is an overall boundary, the so called Goldilocks Zone, where it can exist.

And whenever you have put these kinds of conditions onto an electron, the electron further restrict itself into discrete levels. These discrete levels are discrete in nature, i.e. they have a whole number associated with it, there is nothing continuous about them.

So there will be areas where it can stay. And then there will be areas where it cannot be stay, much like the steps of a ladder, you can only put your feet in a specific step of a ladder, you cannot put your feet in between.

So having said that, with electrons distributed in peculiar or somewhat cumbersome areas, cumbersome locations around the nucleus as orbitals describe, let us ask ourselves a fundamental question.

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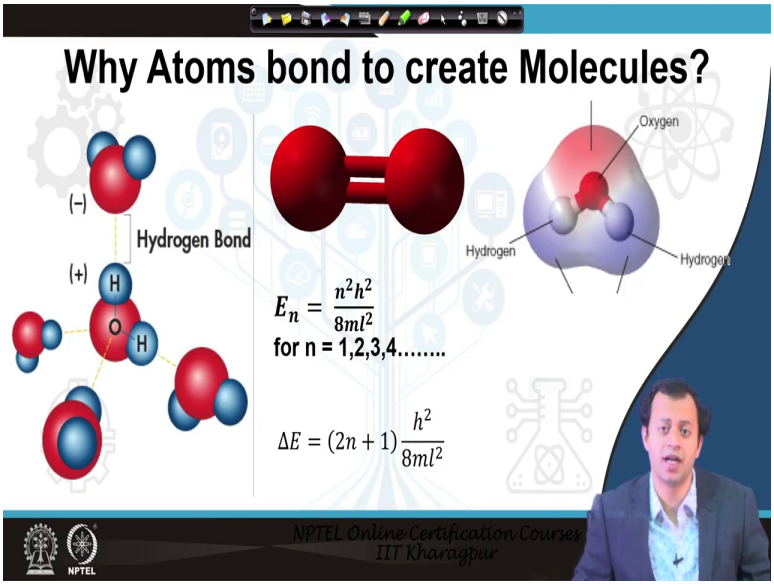

Why atoms bond to create molecules? What is the requirement for atoms to create molecules? Now, remember when I am asking this question, it is not as easy that you might think it is. You will obviously say, oh well, it has to fulfill the final valence electrons, it needs to fulfill all those valence states, and it forms electron, it forms bond so that it stabilizes.

But is there a degree of stability? How many times does it need to form bonds with how many different, different types of molecules? One particular atom say, for example, carbon. Carbon forms bond with thousands of different atoms in different manner.

Has it not received or has it not achieved the stability that it has been looking for? All it needs is 4 more electrons. So it can get 4 more electrons. So why is there a propensity for all these elements or all these atoms to form a molecular bond? Stability granted. I am not discarding that fact that atoms need to form molecules to stability, but might be there is something more to it. Might be there is something more to it.

Now, this is an example of what bond look like but then again, by this time, you must understand that atoms do not have the straight lines between them by which they hold, these are not hands

basically. Atoms do not possess hands by which they hold another atom. And therefore these 2 combined form molecules. This is just a schematic representation.

The idea what we want to know is that what is the requirement. Stability is fine. We have had stability. Stability has achieved in h2 itself. Hydrogen atom has combined with another hydrogen atom and formed h2, diatomic hydrogen. So it is not satisfied with its stability? Why does it has to go around and have bonding with so many different elements, so many different atoms?

Maybe, just maybe the Schrodinger wave equation that we discussed last time is going to give us a clue. Remember, Schrodinger wave equation from last class? The energy state as n square h square 8 ml square and the gap between energy is l.

Now, check this out. Your energy is indirectly proportional to the length. Previously, we have discussed this x as 0 to l. So x is equal to l is the full length. What does that mean? What does that actually mean? Meaning if somehow the length increases, if somehow the length increases, energy reduces. Energy is inversely proportional to the l. l is the length representing the x.

So, when molecules, when atoms, when atoms bond with another atom, the electron is shared between 2 nucleuses. That is the idea, sharing of electrons. Covalent bond is basically sharing of electrons. So, the electron previously was moving around 1 particular nucleus. Now, because of the bonding the electron has the chance to move around 2 nucleus or more, how many atoms have it had bonded with.

So overall, the length increases. The overall length in which the electron can find itself increases. It is now l2. Previously, it was l and now it was, it is l2 and so on and so forth. So, if the length increases, energy decrease. Now, you must know that this is the property of nature, everything wants to occupy to the lowest energy level, lowest energy state, everything comes down from high energy to low energy. Very little, you have to actually supply energy from outside to make something go from lower energy level to higher energy level.

But from higher energy level to lower energy level, it is in nature, you do not have to do most of the time anything, it will simply dissipate and come back. That is how it works, water, high pressure to low pressure water falls from top to bottom, gravity, wherever you see. At the end of the day, every matter wants to come back to a lower energy state.

Now, previously the lowest energy state E1 was for a particular l_1, but now since l_1 has increased to l_2, E has now reduced. So, there is a compelling argument, there is a compelling argument, there is a compelling reason for atoms to form bonds. Atoms are constantly looking to lower their energy or any matter for that matter, pun intended. Anything wants to lower its energy. Atoms are constantly looking to lower their overall energy state. Whenever they form bond, the length increases where the electron can move around and the overall energy reduces. That is one of the fundamental reason for atoms to create molecules, granted there is something additional to it as well.

So by this time, you must know that there would not be any straight line forming between 2 atoms to form bond, but instead by this time, since there are this electron cloud, the probability distribution of electrons around each atom, whenever atoms form bond, they overlap their electron cloud as seen here. They overlap their electron cloud and the overall distribution of the electron cloud in an equilibrium state, in a stable state determines tremendously on how the molecules will be, how the overall molecule will react, how the, what will be the nature of overall molecule.

So, this image is more true version than this particular image or this particular image, where you have simply lumped couple of atoms, basically nucleus on top of one another. So, let us continue with this. Also, one more thing that I need to tell you, and that is this energy gap. Whenever we form bond this energy gap also reduces. So, previously the discrete level where electrons can exist was like this. After forming bond, the gap reduces.

So see now, this particular image here, the electron which was previously surrounding only the hydrogen nucleus or only the oxygen nucleus now have all this path to move around. Thereby, l increases, E reduces. That is the fundamental aspect, why atoms create molecules. Several of you, again, knew it already, but maybe the interpretation that I gave is slightly different.

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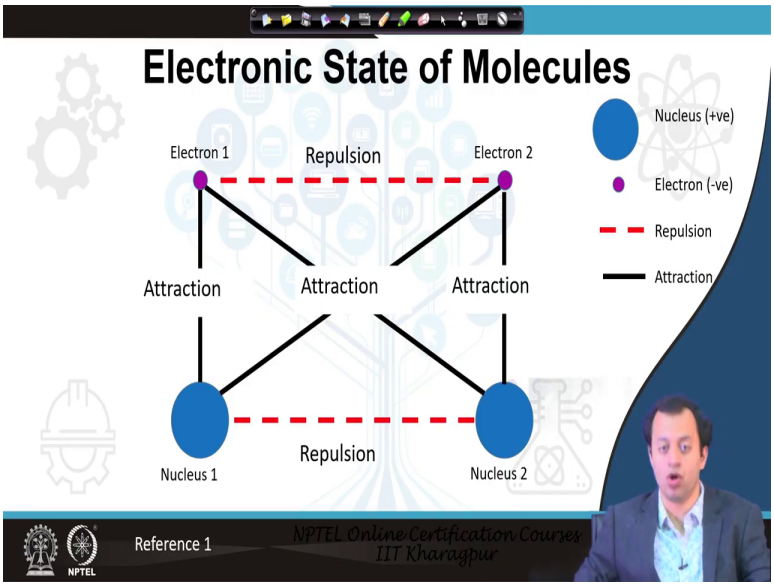

So, how exactly do atoms come together to form a molecule or what is the nature of bonding or how do they bond? Remember, 2 sets of forces are simultaneously working on atoms, nucleus and electrons when they come together, the nucleus 1 and nucleus 2. For example, let us consider the simplest example. This is the nucleus of hydrogen with 1 electron, this is the nucleus of hydrogen with another electron.

So, 2 hydrogen atoms have come together. There will be a force of repulsion between the positive nucleus 1 and positive nucleus 2. These 2 nucleuses are exactly identical. There will be a force of repulsion between the electron of nucleus 1 with electron 2 of nucleus 2, But at the same time, there will be an attraction of electron 1 to nucleus 2, there will be attraction of electron 2 to nucleus 1. And of course, there is this original attraction that presents between nucleus 2 electron 2, electron 1 and nucleus 1.

So simultaneously, 2 different type of forces will be working on it. Here, we have, I am saying 2 different forces, 2 types of forces, attraction and repulsion between 2 different atoms. Simplest case, I have taken and that is the hydrogen atom, that is the hydrogen atom. Remember or try to understand how complex this chart will become when you have a very complicated organic compound, say

for example, benzene or butadiene, and you can see how the attraction and repulsion forces are coming together. Here also, since nucleus 1 and nucleus 2 is identical, electron 1 and electron 2

are identical, the force of attraction and the force of repulsions are all same, but in complicated molecules, they start becoming quite different. And thereby, it determine whether 2 or 3 or 4 different types of atoms will bond or not.

If, they come together, if the attraction forces prevail, if the distribution of the electron cloud around the 2 nucleus happens in such a way that all of them are attracted towards one another, we form a bond.

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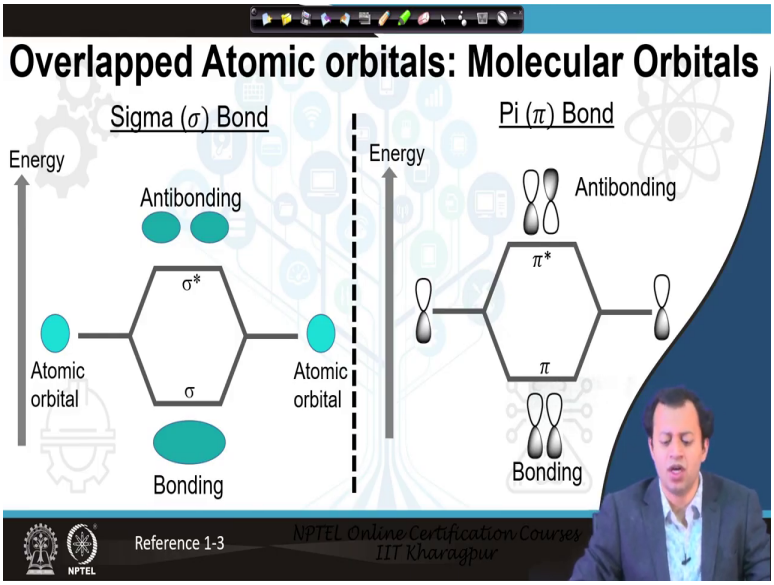

This is very-very easily shown by this example of s-orbitals. s- orbitals 1s, 2s, these are the closest orbitals, one of the closest orbital, we are talking about 1s or 2s, this can be applied to anywhere. These are the closest orbital to the nucleus. So say, you have an atomic orbital s here, atomic orbital s there, they can come together, remember the previous chart that I showed you. And overall, the attractive forces prevail and there is a bonding, there is a distribution, there is a delocalization, there is a redistribution of the electrons around each nucleus.

Like you saw in the H_2O schematic diagram. It is stable enough and there is a bonding. The length has increased for the electron to move around and energy has reduced overall and you have bonding. There is however another case, where the repulsive forces have been together, the repulsive forces have prevailed, the repulsive forces have won, and therefore they have repulsed each other.

So, 2 of these atoms are coming together, they have redistributed. The nucleus of this atom is attracting the electron of this atom, the nucleus of Atom number 2 is attracting electron number 1. And overall, they have distributed, they have married together, they formed a bond. It may also happen the opposite case, where the electron of this and the electron of this have repelled each other, the nucleus of this and the nucleus of this have repelled each other, and they are apart from one another. That is your anti-bonding, that is anti-bonding, where the overall energy has increased. Why?

Because, the length has reduced. Previously, the electron was more or less around this area.

Now, it has got a repulsion force from outside, now it has got a repulsion force from outside, the electron has moved slightly inner, slightly inward because, from outside it is getting a repulsive force. So length has reduced, if length has reduced energy has increased. That you absolutely need to understand, the difference between bonding and anti-bonding.

From wave point of view, you can consider bonding as constructive interference where crest and crest meets, false equivalency I understand, but still it is easier to put, imagine bonding is this constructive interference, crest and crest meets you get 2 times the intensity bright field and crest and trough meets, that is anti-bonding where it is destructive interference and you do not see anything coming out dark, dark pattern.

The same thing can happen with pi bonds as well. pi bonds are basically the overlapping of p-orbitals where you can have bonding as well as anti-bonding.

Remember, anti-bonding is always at a higher energy level. Anti-bonding makes sure that the bond dissociates. Bonding on the other hand, lowers the energy and thereby it stabilizes the overall structure. Sigma bonding happens when 2 s-orbitals merge, 2 or more. pi bonding happens when p-orbitals merge. I think, I would stop it here about the bonding part because these things have already been discussed. One more thing, the energy part.

So, whenever you are bonding, a bonding has happened, well pi bond is weaker compared to sigma bond, you know this already. Sigma bond happens mostly in similar atomic orbitals. So, H_2 diatomic molecules usually form sigma bonds. pi bonds are formed, well different types of carbons, organic molecules can form pi bond.

So, you know this already. I am simply repeating myself. Also remember, bonding means lower of energy. This is the energy scale. Bonding means lower of energy. Anti-bonding means higher of energy. So if you have a molecule, which is at this stage, where bonding has happened and you want to break it, you want to break the bond, you have to supply enough energy, so that the bonding goes to anti-bonding level. Anti-bonding is where no bonding takes place. Anti-bonding is where the bond dissociates. In order for you to break the bond, this much amount of energy needs to be supplied.

So, moral of the story, when atoms forms molecules, their orbitals, the orbitals that they have with their electrons try to overlap with the orbitals of the foreign atom, with the other atom. If this overlap is constructive, bonding happens. If the overlap is destructive, no bond happens. Win, lose or draw.

Draw is non-bonding, which, basically no bonding is happening. Anti-bonding is where there is a huge amount of energy and it is falling apart because high energy is usually unstable. If you remember this, you remember more or less, the rest of the things coming up. Obviously, not everything will be s to s bonding or p to p bonding, we also have sp3 hybridization, so where s orbitals and p orbitals combine together.

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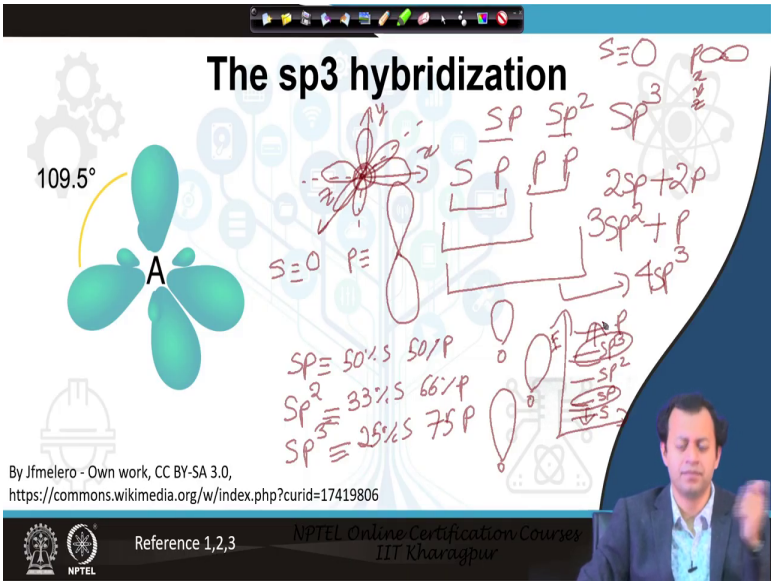

. So, let us try to see if I will be able to draw something here. So suppose, you have x y and z coordinate system. So, in the middle there is supposedly the s-orbital. The p-orbital is usually

dumbbell shape. So, the s-orbital is equivalent to like spherical and the p-orbital is usually a dumbbell shaped.

So, depending on px, py and pz, you have their orientation. So px is oriented in this particular direction, py is in this particular direction and pz in this particular direction. Funny question, why are the orbital shaped like this? if you have known from high school people usually memorize, but I have a question for you. Why are p-orbitals dumbbell shaped? It can be spherical, but it is not, it is dumbbell. Think about the answer, and maybe I will try to tell you at the end.

So carbon, which basically forms all of those organic compounds, which basically forms life, and since we mostly deal with biological material, therefore we need to know very-very little of organic chemistry, very little, I promise, not much can form s and p orbitals sp2 orbitals hybridization and s and p 3 orbitals all. All 3 are possible with carbon and we see all of them happening.

So, you have spx, spy and spz. When we have s and p merging together, we have 2sp plus 2p. So, this 2p are separate, they have not been merged. s and p have merged. When 3 of them have merged, we have 3 sp2 orbital plus p, one of the p has remained empty. And when you have all of these 3 merging together, you have 4 sp3.

When s and p merged, remember s is like this 0, and so I will draw it again. s is like a sphere, and p is, when s and p merge for s and p orbital, which is 50 percent s and 50 percent p, we see this type of overlapped structure forming.

When we have sp2, which is 33 percent s and 66 percent p, we see. And when we have sp3, which is equivalent to 25 percent of s characteristic and 75 percent of p characteristic where s has merged with all of the p, we see this kind of structure.

So if we draw an energy curve where s is as the lowest level and p as the highest level, remember s is the strongest bond, hence lowest energy, p is weaker than that. You have here, starting sp, here starting sp2 and here starting sp3. sp is very close to s and sp3 is also very close to p. From this diagram, can you tell me which one is the weakest bond and which one is the strongest bond? You need to know it, because carbon can form all 3.

Carbon can for sp sp2 and sp3. In organic chemistry, remember, if from your high school classes probably you have been given this test where couple of organic compounds have been given to you, randomly selected, and you have to look at the carbon atom, and then you have to determine whether it is sp bonded sp2 bonded or sp3 bonded.

If you have forgotten, do not worry about that at all. We are as I promised little bit of organic chemistry, the concepts of organic chemistry will be required, but overall now you understand what the bonding is.

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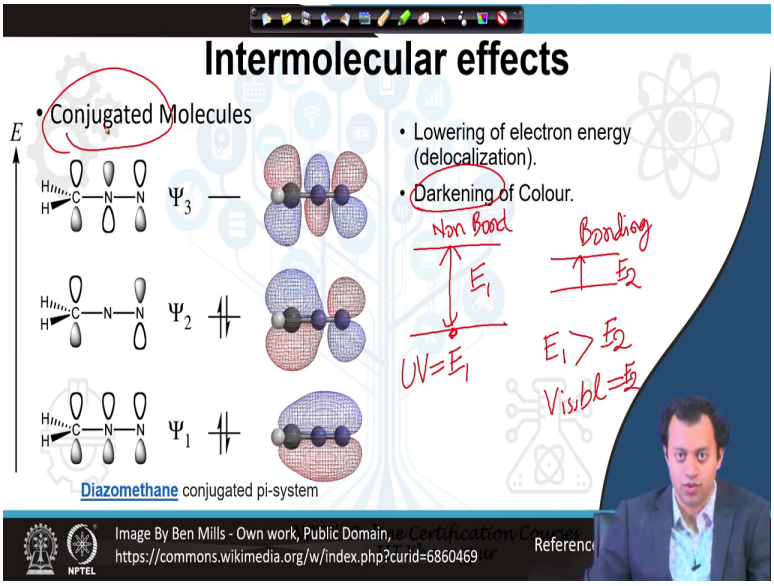

Now, obviously that was the easiest example of sp3 bonding. When you have something complicated like diazomethane, you see the intermolecular effect, a conjugated molecule where hydrogen carbon and nitrogen combines together and it forms these kinds of complicated, overlapped structure.

From this image, I would ask you to tell me, which one is the most stable one, where delocalization of electron has taken place, where the length has increased, and where the length has actually reduced, which one is better, which one can survive which one has lower energy and hence stable. I will leave that discussion to you.

But remember one more thing, conjugated molecules, I polymeric chains where carbon can form this chain bonding increases there is a darkening of color. Can you tell me, why there is a

darkening of color? I will show you something. Previously, the energy level was like this. So, you have to send Energy 1 for the electron to go from one level to another level.

Now, after bonding the length has increased, the energy has decreased. Now, you have to send E_2 energy and E_1 is greater than E_2. This is non-bonding, this is bonding. Or this can be considered as anti-bonding as well.

Moral of the story, in bonding, the energy has reduced. So, less amount of energy needs to be supplied to the electron to go from lower level to higher level. What are the applications or what are the manifestations of it? Previously, it was very colorful, these kinds of structures were very colorful.

You send visible light, the visible light get reflected or transmitter usually reflected. And only when you are sending high energy ultraviolet light, the electron will move from lower level to higher level.

But now, the energy has reduced. The energy has now reduced because of the bonding, and you can, now have to put visible, light lower energy light, that the electron will absorb and go to the upper level. What happens when visible energy or visible light is absorbed? You have darkening of color.

So, one handy trick, when you are observing a biological molecule, if you see the color darkening up, there can be several other reasons, but whenever you are observing a biological molecule and you clearly see that the color is darkening up maybe just maybe, not always, there is conjugation happening where the molecule is forming several different new bonds with it's surrounding molecules. So, that is more or less the topic that I wanted to discuss for today.

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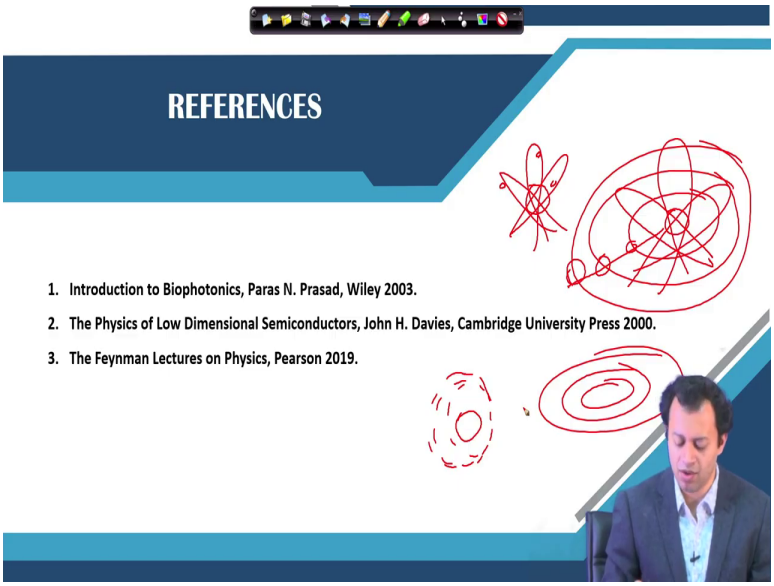

The conclusions are quite straight forward, but remember henceforth if people ask you what is the requirement for atoms to form bond, if there is one information that you take away from all this lecture, atoms form bond, atoms from molecule to lower their overall energy.

Every matter, every object, everything in this universe is trying to come back to lower energy. Lower energy, more stable; high energy, unstable. Everything is looking for stability. With this, I finish my lecture for today.

There are the references. Please go through the reference once you get time. From exam point of view, it will be pretty good, also better for your knowledge as per say. I have 1 question before I leave. Tell me this thing, the original example of atoms.

You saw, this is the nucleus and there are the strain tracts of electrons moving around. Even if we discard it, there is this distribution of electron around it. The distribution is three dimensional, all p_x, p_y, p_z is three dimensional or s-orbital is three dimensional. It is a sphere.

Wherever, however, when we look at our solar system, the solar system is not three dimensional, it is always a disc. From the Sun, the planets are like a disc. Not like this. You do not have Sun, the Mercury surrounding sun in this orbit, the Earth is this orbit, Jupiter is in this orbit, it is always, always a disc. What could be the reason for that? I know this has nothing to do with biophotonics per se.

But maybe you can think about it that it is not exactly a carbon copy, this and this are not same. With these thoughts, I finish today's lecture. I shall see you in the next class where we are going to discuss more about interaction of light in matter.

You have now learnt little bit about light, you have now also learnt little bit about matter. It is time to combine these 2 together, and try to understand what happens when light interacts with matter. Thank you and goodbye.