Introductory Quantum Chemistry

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Lecture - 44
Molecular Orbitals. The Hydrogen Molecule

Let me very briefly recollect, what we did in the last lecture. We were thinking of proton and hydrogen atom approaching each other then, we show that there is reduction in energy, that is what molecular, that is what our calculation said.

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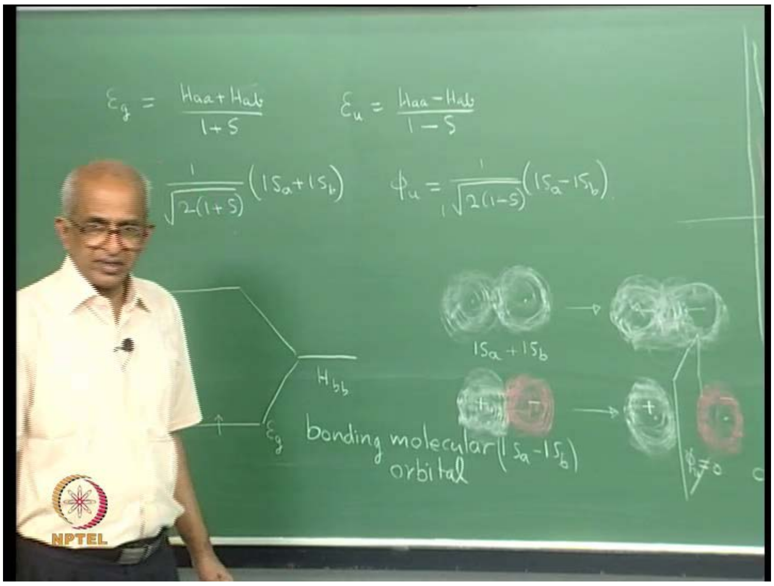

Infect, if we using variation method we found two possible states of the system, one was called E g and other was E u. The energy of E g was actually equal to H a a plus H a b divided by 1 plus S. While E u was found be equal to H a a minus H a b divided by 1 minus S. And further the wave function for these two states, which we denote by the symbol phi g and phi u where given by. And I also point out that, if you made a plot of E g or E u against R.

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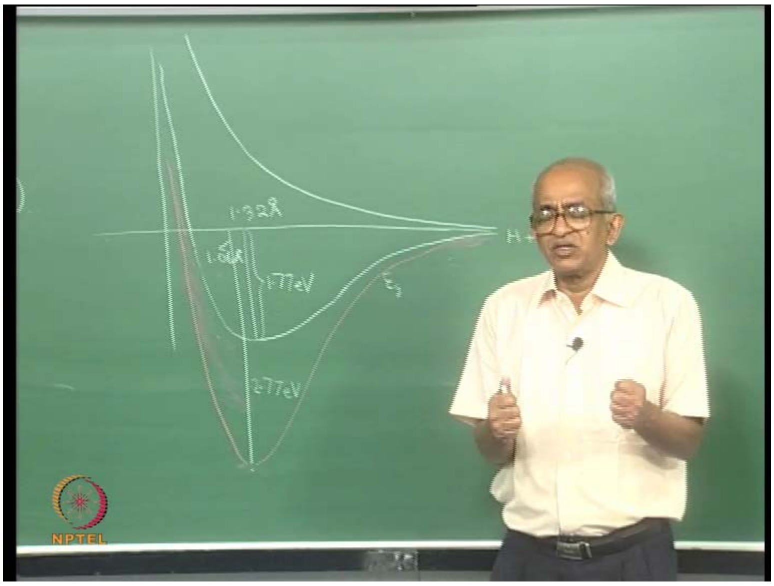

You will find the kind of curve that, I supported it drawn at far away the energy actually becomes that of a hydrogen plus a proton in atomic unit. It actually equal to minus half in atomic units, but for convenient we took that to be equal to 0. And then what will happen is that general will decrease reach a minimum and go on to increase. This is a part of epsilon g, while if you plot it epsilon u will find that energy simply goes on increasing. So, using this calculation it is possible to find the equilibrium inter nuclear distance, this distance at which energy is the minimum and if you did the calculation the answer that you get is actually 1.32 angstroms. I mean possible to determine this curvy experimentally and if you did that the curve would look something like this. Actually it is much skipper something like that and the minimum acquire at 1.06 angstrom. Theoretically is 1.32 and 1.06 is the experimental answer.

This also possible to determine this energy then energy required to dissociate the molecular, remember if the molecule is in this state, is in this possession and then the supply energy from outside. You can actually cause the molecular distance to go infinity which may the molecule will disassociate. And this height can be calculate theoretically and what you find is 1.77 where as the experimental value of the same distance is actually 2.77 electrons volts. So, this shows that our calculation is not actually great, it gives you only; I mean roughly speaking sixty percent of their dissection their roughly.

And bond length also not such a great thing, because the actual value is 1.06, but instead of that you get 1.32, but then it is actually possible to do better calculations. People have done it and in fact, I told you that it is also possible to solve the Schrodinger equation for this system exactly. And if you sold it exactly you will find essentially answers that co inside with the experimental values. So, you will get 2.77 as well as 1.06 if you can solve it exactly and I said it can be done. But then let us look at the equilibrium geometry. So, at the equilibrium geometry we are interest in the question why is that? There is just bond formation even before answering that we can actually say there are two energy levels.

That we found one is epsilon g and the other, one is not epsilon, but E g and the other is E u. So, these two allowed states, you can suppose in a figure like this. As I told you yesterday the E g is lower and E u is greater. Now, E g actually represents the energy of this particular state, while E represent of that state. Now, these are thing, we are refer to us molecular orbitals, because as we see this are orbitals that extent throughout the molecule. So, this is a molecular orbital that is a molecular orbital. So, we say that when the two spaces are brought together they to atomic orbital, they combine together to give molecular orbitals. So, suppose instead of saying that, suppose they did not combine then how much would be the energy of an atomic orbital.

I have told you this, the energy would be H a a. So, on the left hand side atom you have one orbital with an energy H a a and one the right hand side also you have an atom with an the orbital same kind of orbital beyond and this said this energy is H b b, H b b has actually equal to H a a in the case of H 2 plus. So, what is happening is that these two orbitals, these two atomic orbital, they combine and give you this molecular orbital, one is this and other is that. And energy of this orbital is lower, while the energy of that orbital higher than that of the ingudal atomics orbitals.

So, therefore, this is usual to represent by drawing figures like this, the two orbitals interact and the result is you get two new orbitals. And in the case of H 2 plus what happens is that? They one electron that is there in the system sits in this bonding molecular orbital, I say that it is bonding, because it is energy is lower, in comparison with the energies of two atomic orbits. So, it is advantages for this system to form molecular orbitals because, that will lower the energy of the system. And so, because the electron sits in this orbital, which is lower, than ether one of the atomic orbitals.

There is attractive interaction between the two spaces resulting in the formation of a bond. But then you will ask the question like I mean; how does it lower the energy? And for that we have to understand the natural of the molecular orbitals. So, let us try to understand the first molecular orbital this is the first one. So, what is it saying, it says that you take 1 s a add to it 1 s b and multiply by suitable constant, which will normalize the function that this so, that says. So, if you represent the first orbital 1 s a like this, that is the pictorial represent of 1 s a and if this is your nuclear b it also has a similar atomic orbital which you denote as 1 s b. And remember how 1 s a, 1 s b orbitals are there is a positive everywhere. And so, if you added this two up, if you added 1 s a plus 1 s b what is the result that you going to get?

Well you will realize that, in everywhere in space, the wave function would have positive value that is the first thing because, this is positive that also is positive so, were just adding them up. So, there is the resultant orbital which actually something that we refer to us, I molecular orbital it will encompass both the nuclei. So, it will be something like that. And further you would realized that, in the inter nuclear region, what is happening is that the two orbitals are added up and therefore, what is the result? The result is that there is a very large value for the wave function in the inter nuclear region. So, if you combine the two atomic orbital in this passion, what happen is that the wave function has a large value in the inter nuclear region which means the electron density.

Electron density is nothing but the square of the wave function. So, they electron density is having a large value in this region. So, if you put an electron into this molecular orbital which encamp, the molecule orbital encompass the both nuclei, but most of the time such the electron that you put in will be found in the inter nuclear region the large percentage of time, it will be inter nuclear region. And therefore, we say that there is accumulation of electron density in the inter nuclear region and that is nice, because if we have electron density in the inter nuclear region, what will happen? This nucleus is attracted towards that electron density this also is attracted towards that electron density and therefore, this system remains as one molecule. You can put in a different passion this electron density creens that nucleus from this nucleus and therefore, nucleus, nucleus repulsion is reduced right.

So, that is how the energy of the system is lower? The energy is lowed simply, because electron density gets concentrated in the inter nuclear region and that is why this orbital which I say is the bonding molecular orbital is having energy which is lower than H a a. So, we refer to this orbital as the bonding orbital. On the other hand if you think of 1 s a minus 1 s b which is what do you have in the case of the other orbital right this molecular orbit has 1 s a minus 1 s b multiplied by some normalization factor some constants. So how I will represent it? Well this is my 1 s a and 1 s b has a similar appearance, but what I have to do is, I have to multiply 1 s b with the negative sign and add, because you multiplying by negative by minus 1, I will denoted with the different colour.

So, this is positive while after multiplication this is negative and then, if you added the two up, what will be the result? The result will be you will have a molecular orbital which will be something like this. Here you see, you will have values which are positive while near the other nucleus, you will have values which are negative. And what happens in the inter nuclear region well in the inter nuclear region, if actually think of a plane like this. Suppose I think, of a plane like that, what is the special about that plane? The plane, which bisects the bond between the two nuclei. So, on such a plan what will happen is that 1 s a and 1 s b have precisely the same value, because the distance of any point in that plane from either nucleus is the same. So, therefore, in that plane 1 s a and 1 s b have the same value.

But you are actually subtracting 1 s a from 1 s b which means that, on this plan 1 s a and 1 s b will cancel each other exactly so, that the answer is going to be 0. And therefore, what happens in right in the middle, if you think such a plane, on this plane the wave function will be identically equal to 0. On this side of that plane the wave function will be positive while on the other side the wave function will be negative. So, if I do a plane something like this let me say, right on this plane the wave function phi u is actually equal to 0.

Now that is not actually surprising, because this is the lowest possible state of the system, the lowest possible state has no node. Remember this always happen lowest possible state has no nodes, but this has one node, which immediate that, this means actually represents an excited state of the system not the ground state. We has one node what is that node, it is a plane that bisects the bond right, perpendicular to the bond and this same time cuts the bond into two equals half. And if you put an electron into this orbital, there is no accumulation of electron density in the internuclear region.

In fact, electro density actually is removed from the internuclear region, because the wave function has a node. And therefore, this orbital is not a bonding orbital it is what is affect to as a anti bonding orbital, anti bonding molecular orbital. So, this one is bonding while that one is anti bonding. Now, further say if you remember 1 s orbitals are actually spherically symmetries. So, I have two 1 s atomic orbital both of it are spherical symmetric and in the first orbital phi g, what you are doing is, you just adding them up. But if you think about them, you will realize that, they have cylindrical symmetry about the internuclear axis, see imagine two nuclear here, you think of an axis passing through both the nuclei. This is what I refer to as inter nuclear axis and this are my orbitals.

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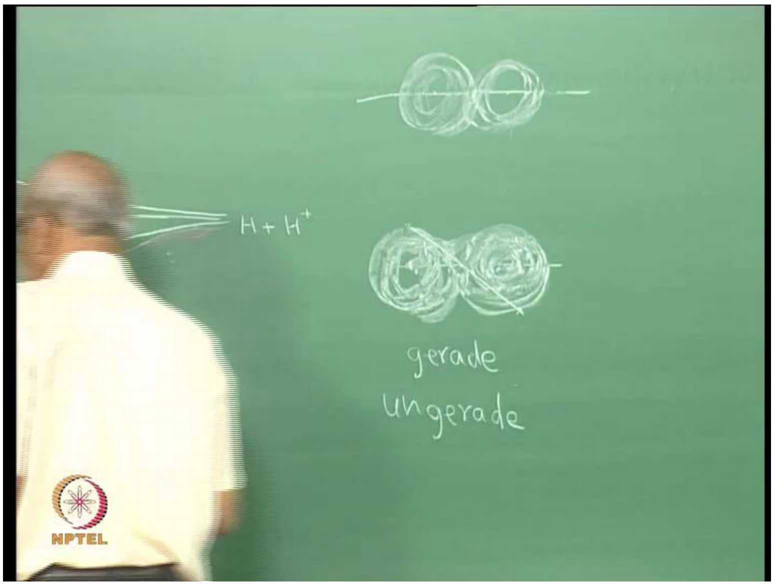

Now, you would realize that, if I rotated both the orbitals about this axis, the appearance is actually going to be unchanged, because there actually having a cylindrical symmetry about this axis. As a result of that, even this combination 1 s a plus 1 s b if I rotated about this axis the appearance is actually unchanged and therefore, people say that this is a sigma type molecular orbital. Similarly with the anti bonding orbital this same kind of thing happens, if you rotate this orbital about the internuclear axis, you will find that the appearance of the orbital is unchanged and so, this also is a sigma type molecular orbital fine. And H 2 plus is a molecular ion which has the center of symmetry. So, suppose you perform the operation of inversion about the center of symmetry, what is the result? Well how do you perform the operation of inversion, the answer is extremely simple, imagine this is yours molecular ion with the two nuclei and this is yours bonding molecular orbital something like that.

And remember that the molecular orbital is actually completely positive everywhere, it is positive everywhere. So, to perform the operation of inversion, what you do is, you think of any point in space may be a point somewhere here and what you do is? You draw a line from that point passing through this center of the molecule; the center of molecule is right in between these two nuclei. So, that is the center of molecule. So, you draw such a line and then you extent that line on the other side, in such a fashion this distance and that distance are the same. And then what you do is you look at the value of your function at that points and construct the new function in a such fashion that a value of the new function at that point is equal to the value of the previous function at the original point right. So, if you did this operation with this molecular orbital you would realize that the molecular orbital actually remains unchanged; that means, after the performing you do it for all the points.

After performing that operation, you will see that as for as this molecule orbital is concerned, if you perform the operation of inversion nothing happens, the orbital remains unchanged. And therefore, people use a German word gerade to describe this orbital which essentially means that, the orbit remains unchanged as a result of this operation of inversion. So, this is actually a gerade and that is a reason why I was actually using this simple g, because it is a gerade or I can more specifically says that this is the sigma g orbital. I said it is the sigma type orbital, but now, I am more specific it is a sigma g orbital and it has been obtain by combining together 1 s a and 1 s b. So, that also I will indicate and say that it is sigma g 1 s orbital. Now, suppose we performed the operation of inversion with this orbital, then what you will find is that, when a perform the operation of inversion, this positive region it will go to the other side and this negative region will come to this side.

And therefore, that is actually equivalent to taking the original orbital and multiplying it by minus 1. So, therefore, I say that, this an orbital that is anti symmetric under inversion and they use the German word ungerade, you had an u n and say that this orbital is ungerade. And that is actually indicated by saying that, this is the sigma u type molecular orbital, this is sigma type when it is ungerade this orbital and it has arise from 1 s atomic orbital. So, therefore, you will say sigma u 1 s and further in addition to this orbital is actually anti bonding and the anti bonding orbital usually are indicates by putting star.

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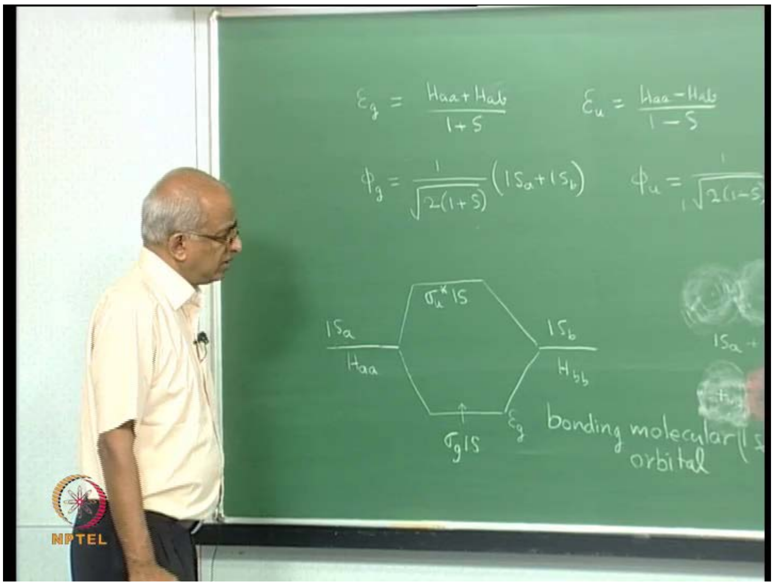

So, therefore, we now say 1 s a, this is my 1 s a, this is my 1 s b what have they done? They have combine together they gets, they give rise to a sigma g 1 s orbital which is bonding and a sigma u star 1 s orbital which is anti bonding. And there is one electron sitting in sigma g 1 s. Now, suppose by some means, I have the molecular ion sitting in the lowest possible state which made the electron is sitting here and suppose, I allow into interact with electromagnetic radiations and it absorps a proton, as a result of that proton absorption, this electron let me say is promote to that orbital. Now you see, if the electron was sitting there, then the system is stable, but the moment that, promoted the electron then what will happen, there is no stability for the system right, this system is unstable and therefore, what will be happen? Once I promote the electron, the molecular ions will actually dissociation. I can show that in this picture you see, you starting from here and if you exciting it to their right.

Because once you change the orbital, the electron change the place have change the orbital which the electron is sitting the orbital. The electron is order from this state to that state as a result of which the molecule or ion will dissociate. So, it is actually possible to us for photo dissociation of H 2 plus, because the you are changing the electron from the bonding to the anti bonding orbital. Now, many of this thing that, I have told you are that available in my power point presentation.

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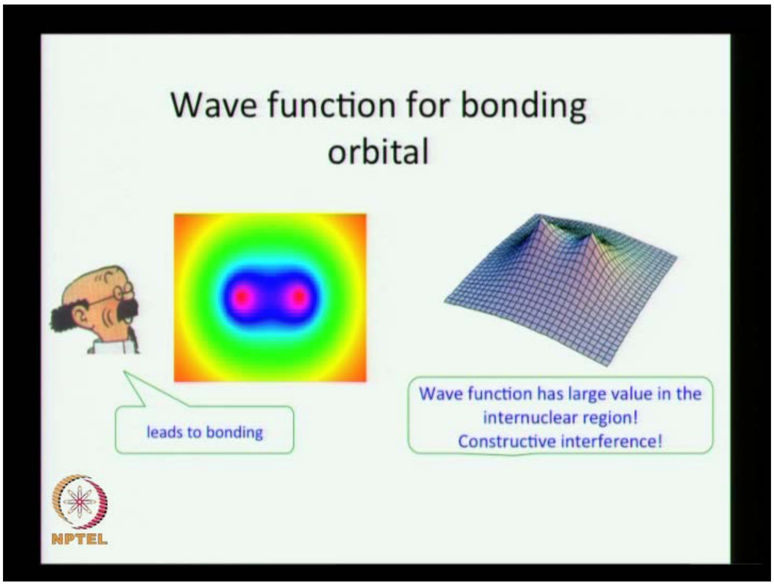

Wave function for bonding orbital

leads to bonding

Wave function has large value in the internuclear region!
Constructive interference!

So, you will have a brief look at the power point presentation. This actually is the density plot, if we look at this, you see these are points, these two are points where the nuclei sitting and this surrounding thing that you see, are actually values of the wave function difference values being represent by different colours and as you go away; obviously, the wave function will decrease. And the next picture I have a similar I have a slightly different kind of representation, what is being done is, I have the two nuclei in a plane, let me say in the x y plane. So, in that plane what I will do is, I will evaluate the wave function that each point right, at this point I evaluate the wave function and show the value that obtain along the vertical axis.

And you know that, this orbital have a large value at the nucleus as a result of, which you have these two tent or these two tips sitting there. They actually are position were the nuclei are and as you go away from there, the value of the wave function actually decreases, which is shown by the that. Notice further that in the inter nuclear region there is a build of electron density and so, essentially what you would says that, you see there is the constructive interference in that region, because the two atomic orbitals as you are getting added up. So, once says that there is constructive interference in the internuclear region and that constructive interference actually causes the electron density into internuclear region to grow up and that result in the formation of the bond. In comparison with this, for may be, before going to that.

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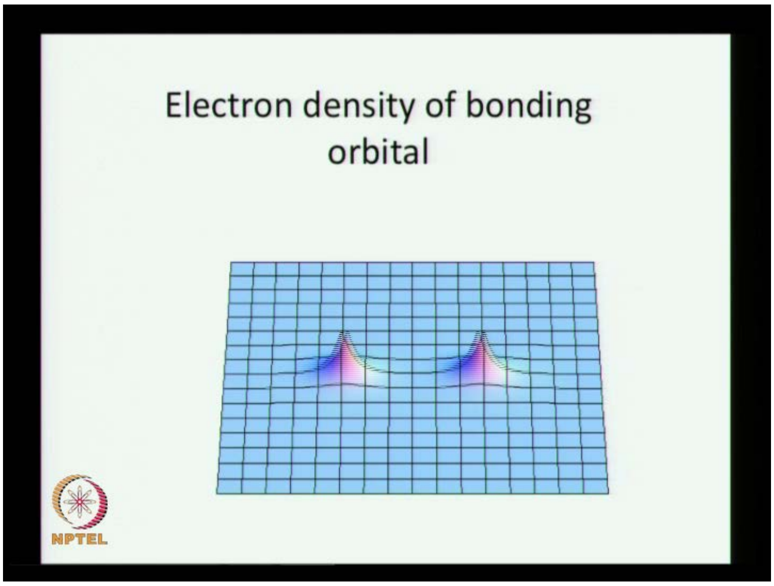

Electron density of bonding orbital

Let us look at what happens to the electron density as the two nuclei are coming together. This is an animation that have created you can see that, the nuclei are sitting at this point where the tips of this two tenser and this can see you would realize that they are electron density in the internuclear region is increasing as the two nuclei come together. In the animation that you have seen just now, the two nuclei start at large distance and then they come close and close and then eventually after coming close, we allow them to separate that is actually animation, but because the animation is elude, what you see is appearance in which the two nuclei are oscillating that is not actually the animation should be, I said it is just because animation is being to look that you get the appearance. That the nuclei are oscillating or that you should look at is just one approach like that and then one separations going away.

Now, in the next figure you will see same kind of plot for the wave function for anti bonding orbital. So, this is actually density plot for anti bonding orbital, this region one can say is positive that region is negative and right in the middle as I have already told you there is a nodel plane. I have one more picture showing this, this will correspond to the possession of first nuclei while somewhere here will be the function for sorry, will be the possession of the second nucleus and somewhere in the middle is your node right. And therefore, you can see that, the wave function has negligible value that point.

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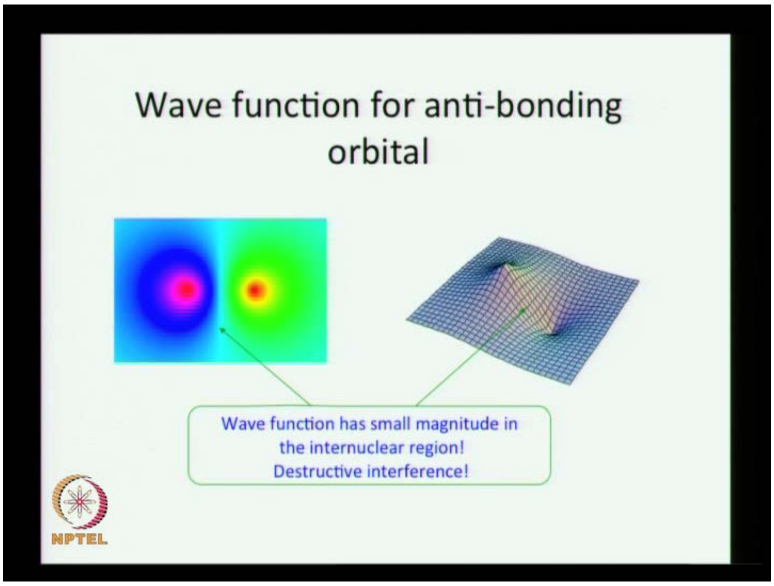

Wave function for anti-bonding orbital

Wave function has small magnitude in the internuclear region! Destructive interference!

Which will become clearer, when I look at the electron density? Now, in this case what is happening is that your subtracting one 1 s atomic orbital from the other. And therefore, in the internuclear region you can say there is distractive interference. And so, it is distractive interference which causes the electron density to be taken a wave or the wave function to be taken away from the internuclear region and that is the reason, why there is no bond. In fact, this is anti bonding orbital. So, this is the wave function, an animation showing the wave function as the two nuclei approach.

And in the next animation, I have the electron density. And if you look at this animation you would realize that, even that two nuclei approaching at the right in the middle, right in the center, there is no buildup of electron density and that is why this orbital is anti bonding. Now, that actually completes my discussion of H 2 plus, I shall now, think of more complex system so; obviously, the next more complex system is hydrogen molecule, having understood H 2 plus we should look at H 2 molecule. So, as usual, we will start with the Hamiltonian for H 2 molecule, well in the case of H 2 molecule, you have two nuclei, which we will call a and b and we have two electron so, electron 1 electron 2.

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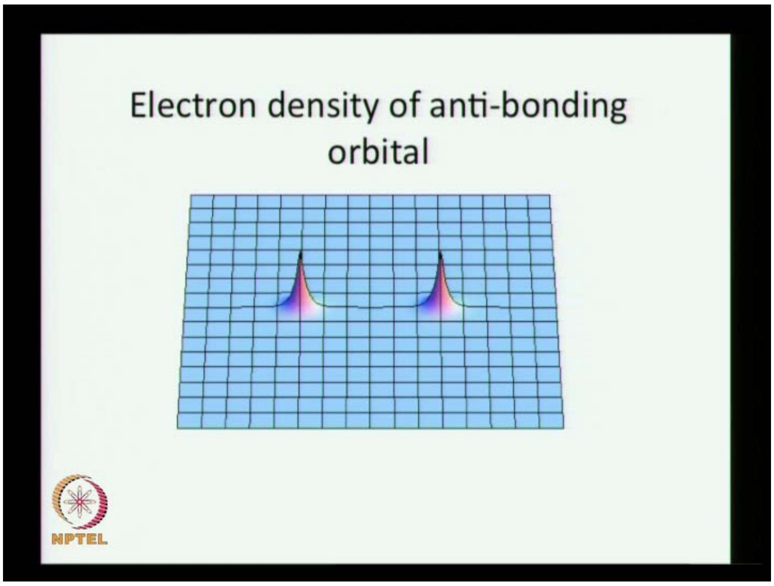

Electron density of anti-bonding orbital

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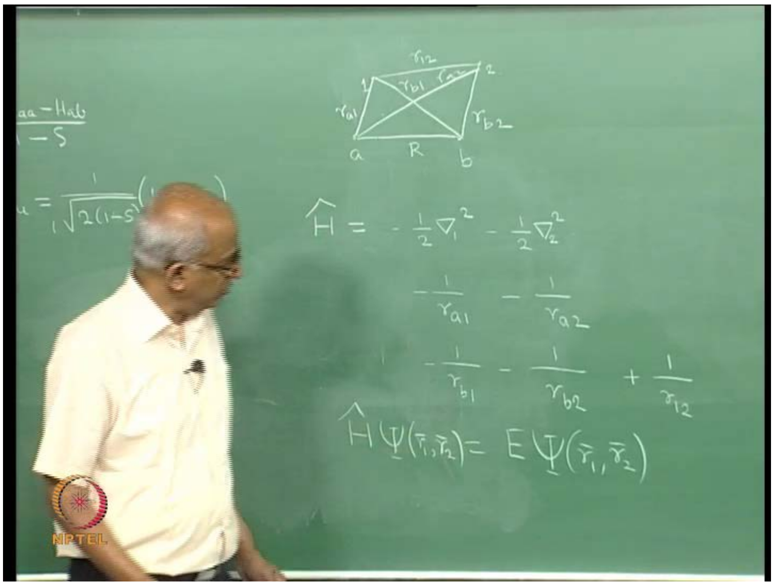

Now strictly speaking, when I write the Hamiltonian, I will have to include kinetic energy is from the motions of both the nuclei as well as the motions of the electrons. But just as in the case of H 2 plus we will assume that nuclei may be taken to be stationary and that different internuclear distances, I can go ahead and make a calculation of just the electronic energy. So, therefore, were the Hamiltonian that, I am going to write down, will assume that the two nuclei are kept fixed at the particular distance which I denote by symbol capital R.

So, then what is going to be the Hamiltonian, I shall write in atomic units, the first time will be minus half del 1 square, this represents the kinetic energy of electron 1, I had put a H cross m everything equal to one. So, therefore, the term looks very simple then I would have minus 1 by 2 del 2 square representing the kinetic energy of electron 2. And then I have to worry about the interaction of electron 1 with the nucleus a, it is interaction with nucleus b. So, the distance of electron 1 from nucleus a, I will called it r a 1, this distance will call r b 1, that will be r a 2 and this will be r b 2. And of course, there is a repulsion between the electrons 1 and 2.

So, naturally this distance also is important, that I will call r 1 2, so, the notation is actually obvious. And if you wanted to write the potential energy of the system, what will happen? I will have minus 1 by r a 1. Remember this is atomic unit that is why it is look nice and simple. This is the attractive interaction between electron 1 and the nucleus, similarly you have that attractive interaction between electron 2 and nucleus a. Maybe, I will write in slightly different fashion the same term, set of term, I am going to write like this minus 1 by r a 1, minus 1 by r a 2 then I would have the interaction with nucleus b, which will be minus 1 by r b 1 minus 1 by r b 2 correct. And of course, you have interactions between the two electrons which is actually 1 by r 1 2 and what I would like to do? I would like to solve this equation H psi equals to E psi. And what about psi, psi will depending upon the possession coordinates of the first electron; it will also depend upon the possession coordinates of the second electron. So, it is the function of six possession coordinates, coordinates of the first as well as the second electron, remember I am not included spin right, we can worry about spin later. And; obviously, this equation is simply cannot be solved, because you have right, you have six coordinates right, that means you have six partial differentiation.

So, this is a partial differential equation involving six variables and almost impossible to solve, I mean not say almost, it is impossible to solve. And if you look at the problem, what is the term that makes like difficult, what is that makes solution of this equation impossible, the answer is that, there is 1 by r 1 2. Which tells you that two electrons repeal each other, this is the problem, this is the reason why thing are difficult, because of this term what does the electron do, that they always try to avoiding each other. That may there motion is co related were that they have used earlier and as a result of that it is not possible to solve this equation and if it is not possible to solve this equation.

I would like to know at least what will happen in the ground state of the system. Imagine I have two hydrogen atoms and they bring them together would there be an attractive interaction between the two leading to the formation of a bond, if the system is ground stage. So, if I slowly imagine, I slowly bring together two hydrogen atom would there be a lowering of energy; that means, would bond form or not that is the kind of question that I am interested in. So, therefore, I am very much interested in the ground stage of the system H 2.

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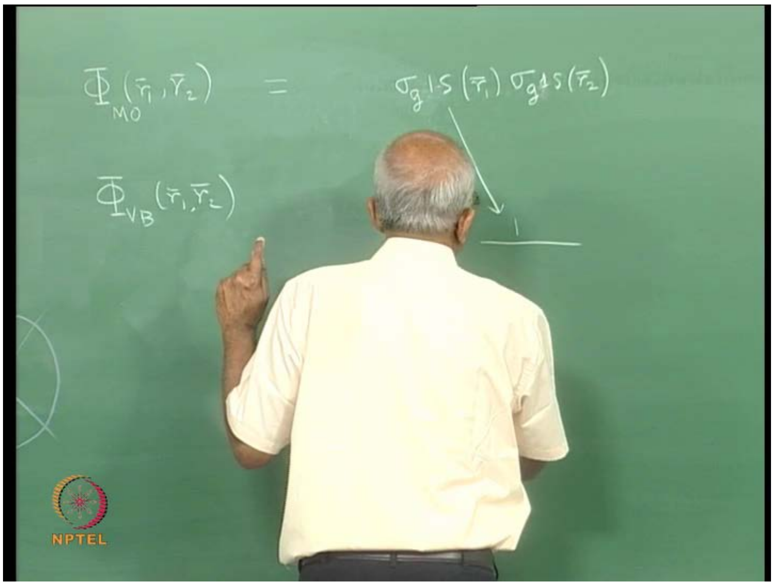

And if you wanted to answer this the question like this, what is if that, you will have to do you will have to write down in suitable trail function phi r 1 r 2 for the molecule for the system right. And the question is what is the most the or best suitable trail function using which I can perform calculations and there have been two sets of trail functions, one set actually is refer to us the molecular orbital approach. So, you can say phi M O which is what I will discuss now, and the other is a actually refer to us phi V B. First I shall discuss this approach which is refer to us the molecular orbital approach to the case of H 2 molecules. And this means I am going to approximate the wave function for the actual system by some the procedure which is based upon molecular orbitals.

So, what is the approach for, what is the bases for the approach, let us now, imagine that I take this Hamiltonian and for this Hamiltonian, I actually cannot solve this Schrodinger equation why is that, I cannot solve it the answer is that there is, this electron, electron repulsion 1 by r 1 2 that is the reason. So, imagine for a minute that this term was a absent, suppose this term is not there, maybe temporarily I will strike it off to emphasize that. Suppose I imagine that, this term was not there, then what is the problem? The problem is now extremely simple, why because you have two nuclei they are stationary at some fixed distance and we have two electron, the electrons are moving around both the nuclei.

But the two electrons are not repulsing each other; because I say imagine this is not there. So, therefore, the two electrons are actually not feeling the presence of one another, but each one will feel the presence of the two nuclei right. So, each electron will move as see, if it is an H 2 plus molecule, because you see the electron does not feel the presence of the other electron, but it feels only the two nuclei. So, each electron feels only the 2 nuclei right. And I know what will electrons which feels the presence of two nuclei will do they will form right. The system will form molecule orbitals and the first electron will sit in a bonding molecular orbital of H 2 plus and similar the second electron also I aspect will sit in a bonding molecular orbital of H 2 plus. So, therefore, what will be the wave function for the system? The wave function would even by this I will say that, the first electron is sitting in a sigma g 1 s orbital, because that is the bonding orbital sigma g 1 s this is electron 1 and the second electron also sitting in the same orbital sigma g 1 s r 2.

Now to be very clear, I want to tell you what this function is even though, I have written use this as chhotta notation this actually means, I would have this, what I have written here, I would have 1 by square root of 2 into 1 plus S right.

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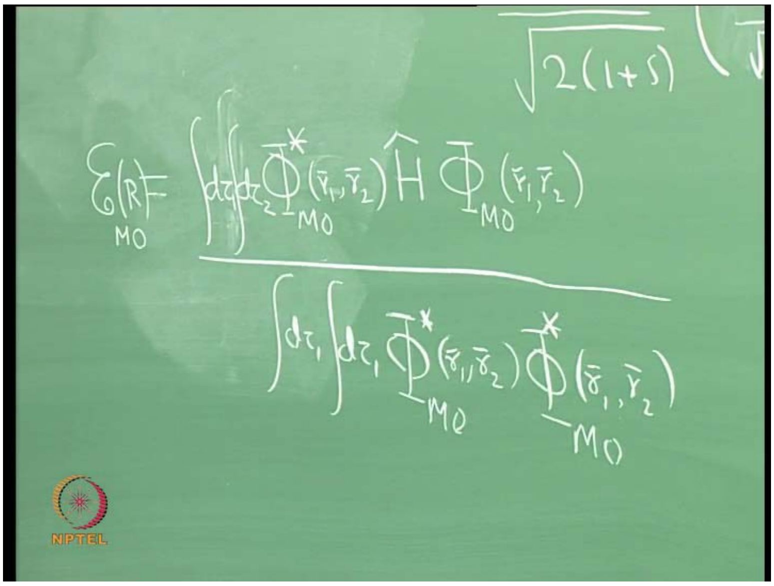

$$\sqrt{2(1+S)}$$

$$\mathcal{E}_{MO}(R) = \frac{\int d\tau_1 \int d\tau_2 \, \Phi^*_{MO}(\bar{r}_1, \bar{r}_2) \, \hat{H} \, \Phi_{MO}(\bar{r}_1, \bar{r}_2)}{\int d\tau_1 \int d\tau_1 \, \Phi^*_{MO}(\bar{r}_1, \bar{r}_2) \, \Phi^*_{MO}(\bar{r}_1, \bar{r}_2)}$$

1 s a plus 1 s b right, that is what it means, but 1 s a itself, I would like to write in a slightly more detail form that is actually equal to 1 buy square root of phi e to the power of minus, that is precious form of 1 s a, e to the power of minus r a right. Constants are not there, because I am using atomics units, plus 1 by square root of phi e to the power of minus r b, but here you say r a and r b are actually for the electron 1, because electron 1 is sitting in sigma g 1 s. So, therefore, I should strictly speaking, I should say r a 1 and r b 1 and similarly if you throughout of this it expression is going to be similar.

you are going to get 1 by square root of 2 into 1 plus S, 1 by square root phi e to the power of minus r b sorry, r a 2, because I am concern with the second electron, plus 1 by square root of phi e to the power of minus r b 2. So, the actual function which I mean when I write such a thing is this function. So, this is my approximate wave function. And so, what I am going to do is, you see this is actually valid provided electron, electron repulsion is not there, but I can use it as a trail function in my calculation. So, I take this trial function and what will I do? I will calculate script E. How will calculate script E? The answer is very simple, you will take this approximate function which I denote as phi M O it depends r 1 and r 2.

Allow the Hamiltonian to operate upon it multiply the result by phi M O star r 1 r 2, and then you will have to integrate over d Tau 1 for the first electron, d Tau 2 for the second electron and divided by integral d Tau 1, d Tau 2 phi star r 1 r 2 M O, phi star r 1 r 2 M

O so, this is the way in which I will calculate script E. Now this is not a simple calculation, it is quite and involved calculation. So, we will not going into the details, but it is enough for our purpose to say that, I know what this function is and it is also possible for me to calculate this script E. And I can calculate the script E at a different value of the internuclear distance so; that means, I can get this as a function of capital r. For each capital r, I will do this calculation and what is the result? The result is something that I will refer to us E with a subscript M O, because this is the result of my molecular orbital approach to the wave function. So, after that you can make a plot E M O of r against R.

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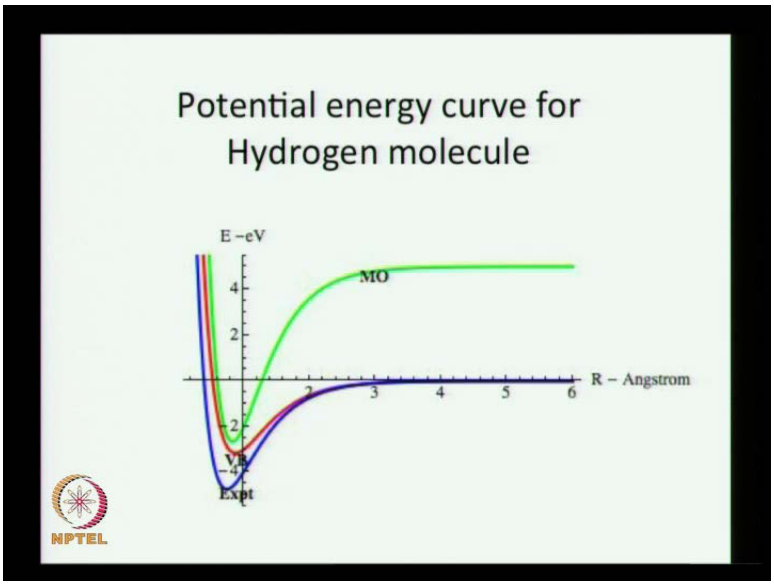

Potential energy curve for
Hydrogen molecule

And if you did that, the result is actually shown here. In this picture may be best thing is for me to draw in the board. Far away you have two hydrogen atoms the energy of two hydrogen atoms an imagining that, I bring that to together.

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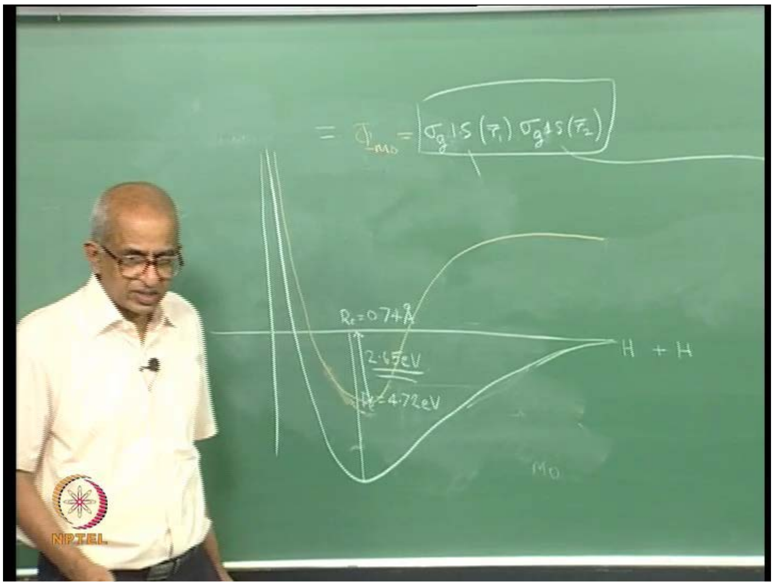

So, acutely what I would expect is, that as you bring to together the energy will decrease, this what you would expect, Energy would decrease reach a minimum and then you will expect to increase, why does it increase? Because the two nuclei are close together they are going to be repel each other. And experimentally, you can determine the dissociation energy this height can also determine R e, R e is found to be 0.74 and the dissociation energy D e experimentally it is found to be 4.72 electron volts.

Now, this particular wave function phi M O, this particular function phi M O, if you used it and calculated the value of script E, then what you find is that, the curve looks something like this. Well first of all, the think that you notice is that the behavior of the curve is actually quit wrong, because far away when I increase the distance between the two nuclei the energy actually should go to the energy of two hydrogen atom which we take to 0, but we does not do that. So, therefore, there is some problem, but the other thing is, inspite of that, if I why calculate it dissociation energy by taking this energy difference. So, what is the energy difference? The energy difference is the difference between the energy of the system at the equilibrium in the internuclear distance and the energy of the two hydrogen atoms that you can find out. You will find that, it is actually 2. 65 electron volts.

So, you can say this is my estimate of dissociation energy which is 2.65 and in compression the experimental value is actually 4.72 electron volts. And you can also determine the equilibrium internuclear distance, the equilibrium internuclear distance according to the calculation is 0.83, maybe I should write the table which gives you these values.

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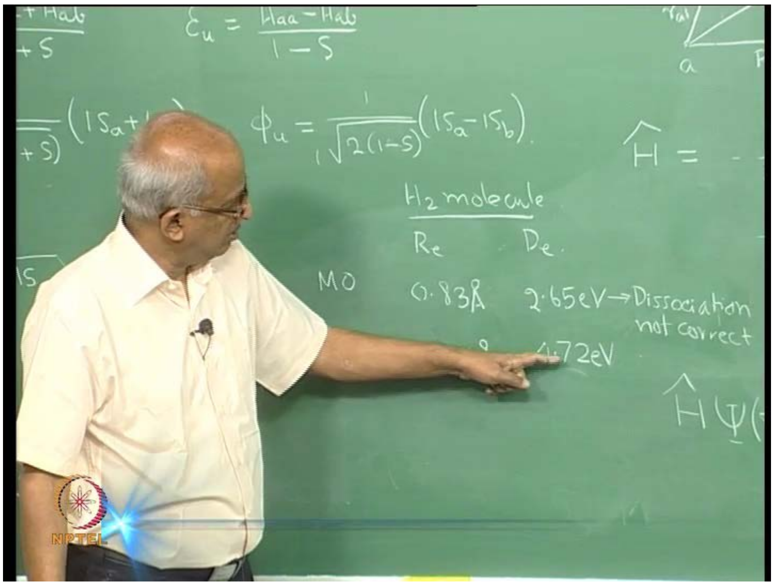

This is for H 2 molecule, I am using molecular orbital calculation, here is my value of R e it is my dissociation energy, this is found to be 0. write the value probably not 0.83 angstroms, the theoretical calculation, angstroms. And disassociation energy this found to be 2.65 electron volts, in comparison experimental values are 0.74 angstroms and 4.72 electron volts.

In addition of course, I pointed out that, this does not described the dissociation of the system currently, there is some problem. Because, if I calculate the energy of the dissociated system it should co inside the energy of two hydrogen atoms, but I does not do that. Now again if you compare the bond length, it is not actually very great it is 0.74 and 0.83, but the disassociation energy itself you find that it is roughly speaking something like 55, 60 percent of the actual value. I think I will stop here, and continue in the next lecture.

Thank you.