good morning today we are going to see the molecular orbital theory of chemical bonding what we have seen before is the valence bond method of chemical bonding
so that is that valence bond method also a quantum mechanical method we are going to see another quantum mechanical method called molecular orbital bonding method in this method um in valence bond method ah we have a pair of electron needed for for forming a bond that pair of electron can be one two three like that but it should the electrons should be a sparse only not as one electron that balance bond theory does not talk about bonding formed by using one electrons we will see the difference while discussing about the molecular orbital theory
so those paths shared electron paths are located between atoms as far as in wells bond theory method is concerned and it is mutually shared between the atoms in molecular orbital theory we will see that um we have molecular orbitals
so as you know are are very familiar with them if you take a hydrogen atom ok there is a nucleus and one electron is there outside
so this is one to one interaction for that schrodinger equation was solved exactly and we got okay energy levels
so you got s orbital p orbital d orbital f orbital
so these orbitals are nothing but wave functions or mathematical functions wave functions because in wave mechanics electrons is treated as a wave
so ah after that this schrodinger equation
so scoring equation for this hydrogen atom that for hydrogen atom was solved exactly and we found energy levels and the orbitals sp d orbital in the same way you can you can go for molecular molecules
so when you go for a hydrogen to helium ok
so you have um your nucleus you have a nucleus and then two electrons are here one electron one electron
so this is one electron this is another electron
so this electron is attracted by this nucleus this electron is attracted by this nucleus as well as there is a repulsion between the two electrons
so it is a three body um problems which cannot be solved exactly
so there that's why we went for approximate method same way for calculating energy levels for molecules for molecules we can adopt similar way but the problem is the number of interaction is is very high
so solving the equations coordinate equation for molecules is is not is is cannot be solved um exactly solving the problem is very difficult we cannot find a exact solution then we must go for a go for approximate solutions because um you can also do
so if you follow the same way as here when you build up the electron atom higher atoms you are adding proton to the nucleus and the electron to the outer electrons outermost orbitals
so that way you can build up atoms the same way you can build up molecules by fixing the nucleus for example nucleus a and nucleus b as in the molecule some molecules a b molecule and then you have to add electron to them energy levels that is molecular orbitals ok orbitals formed by molecules ok
so that is called molecular orbital you can add electron to the molecular beta and then you can calculate alarm energy levels but doing that calculation is very tedious and cannot be solved exactly that is why we have to go for a approximate method of finding the um energy levels the ok one of the approximate method is called linear combination of atomic orbitals atomic orbitals
so it is l c a o method ok let us see what is a basic what is the basic logic behind this method for finding out the energy levels in molecules let us see in an example let us see a molecule of this type h two plus
so you have a hydrogen atom and another hydrogen atom let us say this is

hydrogen atom a this is hydrogen atom b between them there is one electrons now um in wave mechanics atomic orbitals these are the atomic orbitals which are described by wave equations okay

so if you have if you take this hydrogen atom this hydrogen atom okay it has it can be described atomic orbital of this hydrogen atom can be described by a wave function phi a and atomic orbital of this hydrogen atom can be described by a wave function phi b now um

so you have a molecule this is a prototype dihomonic diatomic molecule a very simple molecule

so two nucleus one electrons

so you can have that is a

so two there are two nucleus one electrons okay

so you have the electron here the nucleus nucleus

so it can attract here this electron can be attracted here and there can be repulsion between

so it is a three body interaction okay the equations coordinate equation for this type of interaction cannot be solved exactly

so that is the reason we have to go for m go for m we must go for a approximate method such that that will be very close to the exact values

so what is that approximate method is the um linear combination of atomic orbital the basic idea behind this linear combination of atomic orbital can be explained using this prototype molecule

so you have two hydrogen atom a and hydrogen atom b and there is one electron that electron at any time can be closer to this hydrogen atom okay then you can describe the electron or the whole molecule by using wave function of this hydrogen atom

so this can be described by wave function of hydrogen atom a if you have a another in um time you can have that electron um very close to this hydrogen atom then then the behavior of this electron can be described by using wave function of hydrogen atom b now if you have this electron in between somewhere in between these two hydrogen atom h a you have h b and somewhere in between this hydrogen atom then this situation ok about this molecule can be described by using um by combining both orbitals that is va and phi b

so psi phi a plus or minus phi b

so by combining them or ok combining the wave function of atomic orbital of hydrogen atom a and atomic orbital hydrogen atom b ok you can describe the situation where the electron is residing somewhere between the between these two atoms

so this type of algebraic sum okay phi a plus or minus phi b is called linear combination of atomic orbitals

so you have two equation you can write

so one equation is the you just simply add phi a plus 5 b in another case you can add you can subtract wave equations phi a minus phi b

so that is called a linear combination

so linear combination of two wave function gives two equations in one case two wave functions are added in another case wave functions are subtracted

so this is called

so this combination of this one is represented by a wave function psi okay equal to v va plus phi b

so this is atomic wave function of the hydrogen atom a this is atomic hydrogen atomic wave function of hydrogen atom b combination is represented by psi p s i psi

so this is called fee this is called a fee ok now this one is represented by a another psi equal to phi a minus phi b now this situation

so because okay
so another um important parameter to be added is the normalization constant what is normalization constant that you might have studied while ah in in the while discussing or well you studied about the atomic structures
so that you will be studying more in higher classes now later let us take it as normalization constant these these are the normalization constant n added to the wave function because we are starting with the approximate wave functions
so to find the what is the um exact energy we are starting with approximate equation
so we have to add a constant that is called normalization constant
so that finding the electron is is positive probability of finding the electron is um is 1 somewhere it should be somewhere
so that is why we are adding normalization constant that right now you do not have to worry about this one we can write the wave equation without this normalization constant now we have to understand these two equations you have psi equal to phi a plus phi b and then you have another situation psi equal to phi a minus phi b what is the meaning of these two equations
so we call this when these two wave functions are added it is called bonding b when with these two wave functions are subtracted it is called anti bonding psi psi a this is psi b what is the meaning of these two equations that we have to understand clearly then only you can understand why one energy level is lower why one energy level is higher in energy now you have studied for hydrogen atom for hydrogen atom the probability function for electrons is looks like that suppose this is a hydrogen atom okay hydrogen atom a and its probability ah density function is given like that ok
so this is a probability density function now you have atom a similarly that atom a is approached by atom b and it it also has the same electron density probability density function
so this is a atom b okay when they combine when they approach each other okay there are two possible ways because the electron is treated as a wave the wave has both positive and negative regions
so when you combine two waves there is a possibility for forming constructive interference as well as for destructive interference what is that
so if you take a wave
so this is a wave is a wave this one wave you take another wave like that then the resulting wave could be like that
so yeah
so this is one wave this is another wave they added up and then the resultant wave is is having higher amplitude
so this is a resultant there is a resultant resultant wave
so this is called constructive interference suppose if you take a wave of this type and then you have a wave of this type and then resultant wave wave one is it will be like this
so this is the resultant one
so same way this is a one wave function describing atom a hydrogen atom a this is another wave function describing another atom b when they combine they can interfere ok they can interfere constructively as well as destructively
so you can write thats why ok
so va plus vb as well as va minus 5 vb
so when okay when they construct when they um interfere constructively then it looks like this
so this is the intra nuclear axis here is the atom a here is the hydrogen atom b ok this is the nucleus and this is the internuclear axis ok
so this is um ok the one way of describing the situation in another case you

will have like this you will have like this
so this is a atom a this is atom b
so this one represent a buildup of electron density between two nuclei
so this is a electron density as you have seen before if you take here atom a you have a buildup of electrons and density this is a buildup of electron density buildup electron is maxima here but there are
so much electron density here here
so that is around atom a similarly you have electron density around atom b which is represented in this way
so when these two are combined you can have like this ok
so that is
so this ok in atom a atom b and between them
so much electron density
so this is ok from here here
so much electron density between on the other hand if they in ok um for this type of situation in this situation ok they can combine destructively as well
so that the resultant one is like this one here nucleus a nucleus b and in between them okay
so there is a reduction in electron density
so this one represent a reduction in electron density electron density
so here there is a ah increase in electrons density that in other words the wave function of atom a ah and wave function of atom b reinforce each other that is they strengthen each other between them as a result there is a buildup of electron density between them
so what will happen if there is a buildup of electron density
so that means the electrons are attracted by this nucleus similarly electrons here are attracted by this nucleus here in between you have a mixture of electron the electrons from this nucleus from this atom electron from this nucleus in other words as well that electron of this atom is attracted by nucleus of this atom and vice versa that is electron of this atom is attracted by the nucleus of this atom
so that ok that can happen if there is a buildup of electron density between two hydrogen atoms
so that is represented by this type of graph
so when there is a reduction in electron density there is m
so you can have there is one electron density brow okay and then you have a ah electron density zero here electron density zero and then there is a increase electron density here
so you can see here between nucleus a and b and there is a reduction in electron density that means if there is a electron density between two nuclei then the nucleus or nuclei are shielded and they are protected by the electrons when there is no electron b density between them they repel each other actually electron densities on other side
so b here behind this there is some electron density similarly after this nucleus there is electron density
so these electron densities are not mutually attracted
so as a result there is a repulsion between the two nuclei here but here the atoms are attracted to each other that is what this is this situation is represented by this equation
so this situation is discovered ok is described by this equation ok is it clear
so so when there is a attraction mutual attraction energy of this system is lowered energy
so that is called bonding situation when there is a repulsion between the nuclei energy is higher

so that situation is represented by antibonding
so this is bonding situation this is anti-bonding situation and the bonding situation okay wave functions reinforce each other okay wave function psi a and psi phi b reinforce each other here va and vb cancel each other as a result there is a reduction in electron density between the two nuclei
so this situation is bonding this anti-bonding and here the electrons are attracted mutually here electrons are not attacked mutually that's a higher energy
so this is lower in energy lower in energy this is higher in energy
so you could under its becomes clear now that what is the meaning of these two equations these two equals still one can represent these two equation in a diagram like this
so you have a atom a okay hydrogen atom a interacting with another hydrogen atom b and then there is one energy level lower in energy another energy level higher in energy this energy level okay or or the result of interaction between the two hydrogen atom hydrogen atoms
so this one is phi a plus phi b this one is phi a minus phi b
so this is a bonding this is bonding ok
so hydrogen atom you have oneness orbital you have oneness orbital which are singly occupied here there is one electron there is one electron which are given here
so this is atomic orbitals ok are combined to give molecular orbitals
so this is called molecular orbitals bonding molecular orbital you can say that bonding molecular orbital
so this one is called on the antibonding molecular orbital ok simply m orbital you can write like that is higher energy compared to this one now you can see here two atomic orbitals are combined to give two molecular orbitals one is lower energy another one is higher in energy okay
so this situation ok
so with this lower energy is described by this wave function combination of wave function higher energy orbital is described by this type of combination of atomic orbitals now if you take m ok
so if you take a hydrogen molecule itself
so your hydrogen a hydrogen hydrogen then here it is a hydrogen molecule then these two electron will occupy the lowest energy level
so it will both will go to this lower energy state
so lower energy molecular orbital energy level molecular orbital this higher energy electron will go to this one
so here electrons um filling up follow the same principle that was followed for filling up atoms in atoms for building up of atoms electrons are added by following the half of principle you have one has to follow poly exclusion principle and whose rule of maximum multiplicity multiplicity
so using those principles same principles were usually here also to fill up molecular orbital energy levels
so here there is one electron here is another electron and both electron will go to a level its energy is lower energy lower
so both of them will come to this level that is bonding molecule orbital they will not go here okay
so the difference between this level and this level ok is delta e that is a bond energy delta e is a bond energy bond energy of two hydrogen the bond energy of the bond between two hydrogen atom
so when two hydrogen atoms are combined this is the amount of energy released that we have seen in terms of electrostatic potential model energy model we have seen that in case of valence bond theory

so here again the same amount of energy release can be calculated by this way by molecular orbital method
so um ok now we can what we have done is um combination of atomic orbitals what are those atomic orbitals those atomic orbitals are from different atoms not from the same atom in valence bond theory method atomic orbitals are combined using which are present in the same atom but in molecular orbital theory atomic orbitals are combined from different atoms that is a difference and then you have molecular orbital energy levels that is this orbital is called sigma sigma orbital this orbital is called sigma star orbital to represent anti bonding
so you have a sigma orbital sigma star orbital then you have pi orbital pi star orbital and then you have delta orbitals okay you can have that you are not going to see
so you have like 1 s 2 s 2 p like that you have sigma sigma star pi pi star molecular orbitals in in molecules
so there ok their energy levels are filled by following paulie's exclusion principle and hoons rule of maximum multiplicity now for hydrogen atom formation
so you have combined for this diagram you have oneness orbital of atom okay of one hydrogen atom combined with oneness orbital of another hydrogen atom to give a sigma orbital this is nucleus another nucleus and it is everywhere positive it is positive the wave sign of the wave function is positive
so this is called a sigma orbital which is cylindrically symmetrical about the internuclear axis
so this is one combination another combination is the phi minus phi b
so you have your atomic orbital one hydrogen atom minus atomic orbital of another hydrogen atom one s orbital and then they give this type of situation and you have to put the nucleus very close to this border very close to this border ok
so so that they repel each other there is no buildup of electron density between two nuclei between these two nuclei
so there is a node node means a plane where finding the electron is zero
so this is called node there is one node
so compared to bonding anti bonding orbitals have one additional node
so that is what is happening
so there is no node here there is one node here
so node means finding electron in that region is zero
so nucleus a nucleus b they repel each other then you have to give the sign this is plus this is minus that is the sign of the wave function
so this is called a sigma star orbital
so molecular orbital ah of this one looks like this molecular orbital of this of this type looks like this one okay
so because this nuclei ripple each other energy of this orbital is higher
so that is why higher compare the contributing parent atoms
so how much it is decreased that much is increase
so total energy remains the same
so this much in decrease in energy same level increase that is possible if the two hydrogen atom two atoms are same if they are different it will not be like that that we are we will see later or you will be studying higher classes
so what we have seen formation of sigma orbital that is bonding molecule orbital sigma star orbital that is anti-bonding orbital by combining oneness orbital they can be combined in this way
so this is s plus s this is yes minus s
so two combination linear combination s plus s s minus a because two orbitals of this one wave function this another wave function they can be combined in a ok by linear combination method to give this wave function and then this wave

function which are and the energy levels are like this now you can also combine p orbital to form sigma bonds
so you have um like um oneness orbital you have a two p orbital let us say two z p z orbital 2 p z orbital which can interact with another piece of p z orbital because its energy level is almost same as this orbital okay
so combination of atomic orbitals um is possible only if they have um following conditions for example for combination of atomic orbital they should have same or almost um they should have equal energy almost equal energy or same energy then only they can combine another important condition is that they should have same symmetry ok
so oneness orbital can combine with oneness orbital oneness orbital cannot combine okay cannot combine with two s orbital because two s orbital is higher in energy compared to one s orbital they cannot combine
so these two orbital can combine to give a molecular orbital provided they have same energy or almost um equal to each other but you cannot combine oneness orbital with 2s orbital because 2s orbital is higher energy
so when when they differ
so much they cannot combine to give molecular orbital ok
so energy should be same
so energy must be must be almost equal almost equal another one is a symmetry should be the same must be the same for example p x can combine with p another p x p x cannot combine okay p x cannot combine with p z orbital this cannot combine okay because symmetry is different they cannot overlap because p x is along the x axis p z are is along the z axis
so they cannot come symmetry is different
so they cannot combine
so symmetry must be the same for combination of atomic orbital energy must be almost equal for combinational atomic orbital and then third one is the they should overlap very effectively such that um the bonding ok the bonding is stronger
so overlap must be must be okay must be greater they must overlap better otherwise there will be no bond formation because overlap is related to the bond strength higher the overlap higher the bond strength
so they must overlap
so these are the three condition must be made for combination of the atomic orbital to form molecular orbitals
so you can combine
so what we have seen is the combination of bonus orbital with another oneness orbital now we are seeing combination of p orbital with another p orbital
so you if you take p z orbital as the um axis where the internuclear axis internuclear as the internuclear axis then you can draw the interaction diagram of this type
so p c orbital interact with the two p c orbital then you will have one energy level lower energy another one higher energy
so which are connected by this type of ok diagram
so this dotted lines or solid line you can draw represents interaction between okay these two orbitals after interaction two energy levels are formed
so they can combine each other because symmetry is same the energies are same and they can also overlap by head-on overlap that we have seen yesterday um
so you can describe um the overlap of the pc orbital in this way if you take atom a having p z orbital this is a nucleus positive this is negative that is sine of the wave function combine with another p orbital this nucleus this is positive negative
so this is p plus p will give sigma orbital of this type this is positive

negative this is negative
so there is a node two nodes are here two nodes are there
so this is a sigma orbital sigma orbital formed by p orbital
so sigma orbital the corresponding antenna ok some antibonding orbital is represented in this way this is p minus p will have like this like this
so this is minus plus minus plus and there are these are the nodes
so you can see that compared to sigma orbital this is sigma star beta that is anti-bonding orbital formed by p r beta
so compared to bonding orbital in antibonding orbital there is one additional node that is three here here two is
so there is one additional node
so this is a sigma orbital formed by p orbital antibonding orbital sigma star bit are formed by p orbitals same way
so we have seen combination of s s plus s s minus s p z minus p z as well as p z minus plus okay both common linear combination of p r beta p p c orbitals now what about p x and or p y they are almost equal for forming five banana pi bonds
so p x we have seen p x can combine with another p y p x or p y or p y plus p y can give ok pi bonds or p y plus p y can give pi bonds let us see how do they look like
so if you take this is a p x orbital or p y orbital p x or p y ok this is p x r p y and then two energy levels are formed two molecular orbitals are formed this is atomic orbital or one atom this atomic carbon orbital of the another atom combined to give two molecular orbitals
so this is a pi bonds which are connected to the um parent atoms this is pi star like sigma star you have pi pi star here
so this is a pi orbital formed by p x or p y orbital how do they look like if you take this is the inter nuclear axis atom a ok and this has a p x orbital this plus this minus p x r p y okay then combining with another atom b okay its orbital p x orbital is this one plus minus ok this is a nucleus this is a this b can give this inter nucleus this is a nucleus on top of the nucleus there is a cloud of electron on top of below this plane there is another cloud of electron density
so this is positive this negative
so that is the sign of the wave function there
so there is a node along the inter nuclear axis if you combine the orbital in the reverse
so this is a px plus px now you take another combination p this is a this plus minus px r p y minus nucleus b having a p a x orbital plus this minus this p x orbital can give like this this inter nucleus axis this is atom nucleus and then you have like that like that there is a like that you have like that now how many nodes are there there is a node along the internal axis as well as there is a node along the perpendicular to that perpendicular to the inter nuclear axis
so additional node is present there
so this is called
so this is a plus minus plus minus
so this is called pi star orbital this is called pi orbital okay contains electron density above the above this plane above the plane formed by these two atoms and there is electron density below that plane okay here you have um nucleus between the nucleus electron densities decrease
so they repel each other
so that's why higher end energy like sigma star orbital pi star beta is higher in energy
so these are the molecular orbital pi pi star sigma sigma star orbitals now from the molecular orbital theory um we can talk about the stability of the

molecules that stability can be um zero based on the number of electrons present in the ion bonding orbitals as well as from the number of electron present the antibonding orbitals if you take hydrogen molecule

so you have a hydrogen atom had an atom a combining with hydrogen atom b and this is a molecular orbital it has one electron it has one electron both electrons go to

so lower energy sigma orbital this is sigma star orbital okay now we can talk about the stability of the hydrogen molecule we know that it is very stable how because ok because there is a pair of electrons between the two hydrogen atoms that pair up electron is located in the sigma star sigma in the sigma orbitals

so if you consider this as a bonding bond electrons

so the number of ok okay as nb

so the number of electrons in bonding orbital as okay n b similarly the number of electrons in antibonding is taken as n a then the then we can then we can talk about the stability of the molecule by using the concept called bond order bond order is the multiplicity of the bonds between atoms

so bond order is equal to just difference divided by two

so in number of electron present in the bonding orbital bonding molecule orbital minus number of electron present in the antibonding molecular orbital divided by two

so from this bond order we can talk about the stability of the molecules the bond order should be positive for stable molecules

so the b ok

so this is a bond adder the bond order ok should be positive ok then only the molecule can be stable should be positive for stable molecule if the bond order is zero or negative this unstable if the bond order equal to zero molecule is unstable molecule is unstable

so from that we can tell what we can tell from the molecular orbital whether the molecule is we can draw a interaction diagram or molecular orbital diagram of this type and then we can talk about the stability of the molecule by looking at the number of electron present in the bonding orbital and then number of electron present the antibonding orbital by using a concept called bond order the bond order refers to bond or bond order can be one okay bond order can be equal to one that means it is a single bond if it is two it is a double bond if it is three its a triple bond and

so on and

so on

so we can

so higher the bond order higher the stability of that molecule ok

so then the bond is sensor there is a relationship between the bond order and bond length higher the bond order shorter the bond length when you compare the bond distance between single bond and triple bond single bond distance is always higher for the same molecule for the same atoms higher compared to or the single bond distance is longer than the double bond distance or triple bond distance bond order is higher means multiple bonds multiple bond descents are lower compared to single bond distance now uh for hydrogen molecule let us calculate the bond order

so for hydrogen molecule the bond order equal to number of electron present in the bonding orbital is two minus number of electron presence the handy bonding orbital zero divided by two okay it is just one half of them difference between the number of electron present in the bonding and the antibonding electrons

so equal to

so two ok zero equal to one

so the bond order for okay is one

so that is why there is a single bond present between the two hydrogen atoms
so bond order is one the molecule is stable ok
so stable molecule is stable now let us see another molecule after hydrogen you have a helium whether it is stable or not let us see from the electronic configuration you have oneness orbital for for helium atom is a oneness orbital which is completely there are two electrons in there
so another helium atom you have oneness orbital it has it has two electrons
so they interact and form two molecular orbitals which are represented in this way okay now this hydra this helium atom has two electron similarly this helium atom has two electrons
so we have to fill up the molecule orbitals
so you have to start with ah start from the lower energy level
so this is a lower energy level both electrons
so because like atomic orbital molecular orbital can also accommodate only two electron and the spin should be opposite each other that is poly exclusion principle same principles are usually here super max maximum multiplicity poly exclusion principle then another two more electron will go to the anti bonding orbital
so this bonding sigma orbital this anti bonding sigma ok this is sigma this is sigma star orbital
so molecular electronic configuration return sigma oneness orbital containing two electrons sigma star orbital formed by oneness orbital contain two electron that is a molecular electronic configuration for he2 now bond order if you calculate one order equal to number of electron present the bonding electron two minus number of electron present in the antibonding two divided by two equal to zero okay
so that tells that there is no bond between two helium atom
so helium is unstable is unstable okay that means it does not exist that is true excellently found that it is it does not exist
so there is no he2 molecule in the world
so because there is no bond between two helium atoms thats how we can do that
so this is a molecular electronic configuration let us see another molecule after helium you have lithium li 2 let us see whether it is stable or not
so in lithium electronic configuration is 1 s 2 2 s 1.

so we have to combine two atomic orbital oneness orbital two s orbital
so let us start here okay
so here you have oneness orbital of one one helium atom another one is orbital of another helium atom and then you have a molecular orbital formed between them
so always remember as you go up energies increases
so energy increases then you have um 2s orbital here is a 2s orbital and there is a sigma bond there is a handy bonding orbital and the interaction is shown as a dotted line and then we have to
so this is one lithium atom this another lithium atom you have here li2 molecule formed between them ah now it has two electron here two electron here both will here go here another two will go here now if you look at that there is one electron here one electron here there is one electron here then both will go to the ion bonding molecule capital
so this is sigma sigma star this is sigma sigma star now the molecular electronic configuration is sigma orbital formed by oneness orbital containing two electron then sigma star orbital formed by oneness orbital containing two electron and then you have a sigma orbital formed by two s orbital containing two electron only
so in total six electron because two lithium atom is combined one lithium atom

three electron in taut after li two contains six electrons
so two plus two plus two six electron the number of electron is the same after forming molecules okay number of molecular orbitals would be the same after forming molecular orbitals now you can see that how to calculate now we have to find out whether it is stable or not okay this bonding cancelled by the anti bonding of this
so two electron canceled by another two electron present in the antibonding now here bond order ok
so you have to here you have work here here the number of electron in the bonding is two minus number of electron and the bonding is zero divided by two equal to one
so alloy there is a bond between two lithium atoms a single bond is formed
so it is stable
so that's how we can talk about bonding between atoms as far as molecular orbital theory is concerned thank you you