**Lecture – 44**
**SALC: BeH2**

We start with a very simple situation.

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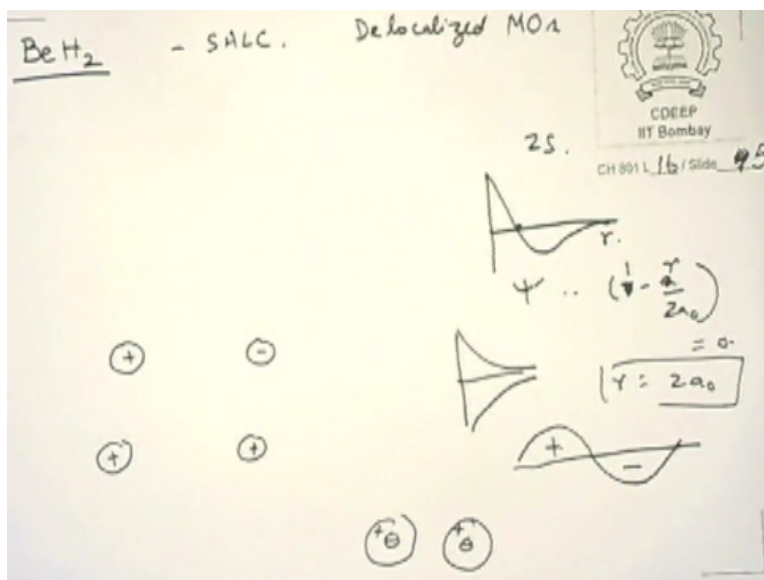


We start with a very simple molecule. What will you start with H2 is boring. So, what I will do is, I will start with a 3 atom molecule BeH2. What is the geometry of BeH2? **"Professor – student conversation starts"** (()) (00:42) No, don't say that. We are actually going to not use hybridization in our discussion. Please understand something. The shape of a molecule is not because of its hybridization. Hybridization is a way in which we try to rationalize the shape.

The shape is because of VSEPR, valence shell electron pair repulsion and did I say this in the course last semester also or not. **"Professor – student conversation ends"** What I am telling you is next you go to a birthday party of someone who cares to decorate the place with balloons, do this. Have you seen those balloons in a birthday party? Usually, four of them are tied together. **"Professor – student conversation starts"** What is the shape have you noticed? (()) (01:29) always. Provided the balloons are all of the same shape. **"Professor – student conversation ends"**

What I encourage you to do is that (()) (01:35) of celebrating the birthday take off one of those tetrahedrons. Get a toothpick, which is also available in the party, burst one of balloons. In front of your eyes, that non-planar tetrahedron will become a planar triagonal shape. There is no s-p mixing in the balloons right. It is a static effect. VSEPR is a static effect. Just burst it, it will become triagonal in front of your eyes. Burst one more, it will become linear in front of your eyes.

Hybridization is not the cause, that is what I am trying to say. Very often we think it is, it is not. Hybridization is an explanation, it is a way of explanation, that is not the cause. If hybridization at all takes place, it takes place to give you the right geometry. But, the right geometry comes from that repulsion. Lone pair-lone pair repulsion is more and that lone pair-lone pair repulsion is also not electrostatic repulsion. It is static repulsion.

Lone pair is bigger. Because it is not bound on one side, so it is kind of spread over a bigger place. That is why lone pair-lone pair repulsion is most followed by lone pair-bond pair followed by bond pair-bond pair. It is static effect and this balloon experiment is the best we often see. I think I talked about this in this course also. You have burst two balloons, it has become linear, now what you do is, you grab tetrahedron and try to tie together the tetrahedron and this linear balloon.

You will see that the balloons will shift and they will form an octahedron in front of your eyes. I have done it in many places, that is then I tried to demonstrate it with some kids who are too young and they completely hate me for bursting so many balloons (()) (03:26). **"Professor – student conversation starts"** (()) (03:32) and ended up bursting 25-30. **"Professor – student conversation ends"**

You combine the tetrahedron with the linear combination of the balloons, it becomes an octahedron in front of your eyes. Now burst one, it will become DBP, burst any does not matter whether you burst one that was from the original tetrahedron or one that we have joined. It will

become DBP. Next time, get invited to a kid's birthday party, carry a toothpick and do this experiment. It is fun. In any case, people will think that you are just celebrating.

What we do here today is that we do not even talk about hybridization until and unless we need it. Rather, we use this concept of symmetry adapted linear combination. We start with a simple system and slowly we go to a little more complicated system. $BeH_2$ is a linear molecule not because of hybridization, but because it is an AB2 kind of system. There is no electron pair on B. It is a pure AB2 kind of system that is why it is linear.

What we do is we try to see which orbitals can participate in the molecular vital formation and go ahead from there. You could take approaches, first is you could use hybridization and generate what is the called the localized molecule orbitals, but in any case I do not want to do that, so we will focus on the delocalized molecule orbital all the way. Because that is the strength of MOT. It allows you to handle more than 2 center 2 electron bonds. We better use the strength to the maximum extent possible.

What we do is, first of all we think what are pendant atom and what is the central atom. In this case, $BeH_2$, Be is the central atom and the hydrogen atoms are pendant atoms. You know what is the meaning of pendant? Sometimes girls wear chains and there is a locket, the locket is also called pendant. Pendant means something that hangs at the end. The hydrogen atoms are the pendant atoms.

Which orbitals of this pendant atoms that are likely to participate in the bonding. **"Professor – student conversation starts"** S, which S, 1S. **"Professor – student conversation ends"** What I will try to do is, I will try to see in how many ways I can arrange these 1S orbitals. One that I can think of is, + and + and other that I can think of is + and -. Can you think of any other combination – and – is just minus of + and +, and – and + is just minus of + and –. So, these are the two basic combinations.

These are the SALCs, symmetry adapted linear combinations. The mathematical constructs of the atomic orbitals of the pendant atoms, what we do is, we construct them, look at the symmetry

and then we try to find orbitals on the central atom that would match these symmetries and then we will only consider combination of the SALCs and the central atom orbitals that have matching symmetries.

**"Professor – student conversation starts"** Yeah, (()) (07:19) what do we (()) (07:21) to the minus sign. **"Professor – student conversation ends"** Do you remember this radial distribution function of 2S orbital. You just take a section through 2S orbital, it looks like this. Why does it look like this because in the expression for the wave function, there is something like 1-r/2a0. When you equate this to zero, when will the wave function be equal to zero, when r = 2a0. This is where it becomes zero and that is where it changes sign. This is called a node.

A node is a point where wave function changes sign. So, + or − is just the sign of the wave function, nothing else. You think of a simple sine wave, the value is + here and the value is − here. It is also called the phase, + phase and − phase. "Professor – student conversation starts" No node in 1S. No node in 1S. What I can do is I can draw 1S like this or I can draw it like this who is going to stop. I am taking linear combinations.

When I take linear combination, I can just add a − sign. **"Professor – student conversation starts"** (()) (09:12) what was that, yes. One structure a + and − are different. See what I have done. I have taken a combination of + and −, here I have taken combination + and −. If it is 2S then what will happen. This is one combination. Now I think you get the answer. **"Professor – student conversation ends"**

In fact, this node in 2S has very important implications in your hybrid orbitals. Once again, I diagnose a little bit, does anybody remember the shape exactly of SP orbital. If I ask you to draw the contour for SP orbital what will you draw? I will draw it for you.
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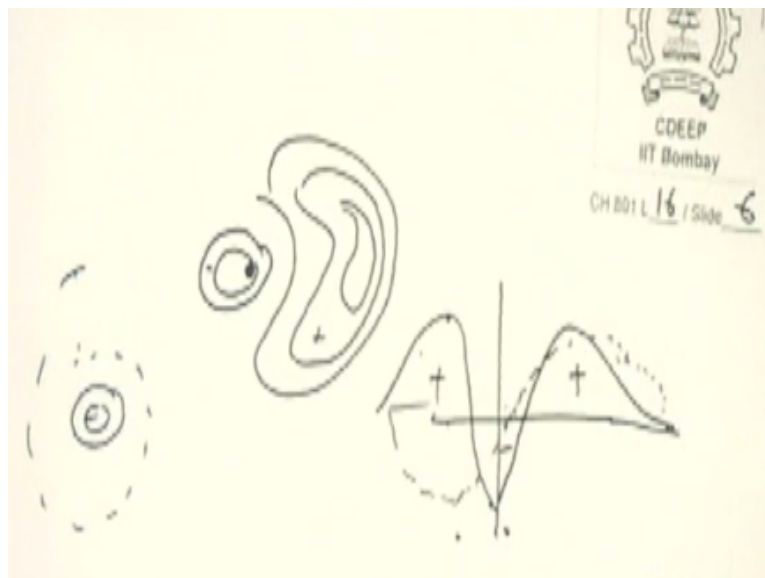
We will use that also, may be today we will run out of time, but tomorrow we will need it. If I ask you to draw the contours of SP orbital, this is what you always draw. You remember this? This is +, this is −. My question is where is the nucleus? Here, then, somewhere here. Why? Because what are you mixing, you are mixing 2S and 2P. What is 2S? 2S has a node. This is minus, outside only you have +.

Once again, dig a section, this is what 2S is going to be, something like this, - close to the nucleus and + away from the nucleus. What about 2P? 2P is something like this. It is zero at nucleus, right or wrong, cross-section of 2P. You know what 2P looks like anyway. I have just taken a cross-section. Now see in the immediate vicinity of the nucleus, it is the value of 2S that is going to be dominated, not 2P. Because 2P is just 0. Add 0 to a negative quantity, you get a negative quantity.

In the immediate vicinity of the nucleus, it has to be minus. No matter whether you are on this side or whether you are on this side. All that happens is that of this side, what happens on this side let us see. What did I just draw, the other side of 2S. When you go far away from the nucleus, here on this side, this + and − start cancelling each other with destructive interference. That is why this low is so small. Thus, far away from the nucleus, these are the last positive value 2S, 2P has a large negative value, they cancel each other.

But in the immediate vicinity of the nucleus, on both sides 2P has negative value, 2S has a value of 0, so it will be 0 all the way and if you go this side, you have constructive interference all the way. That is why you have a bigger low here. Thus here values are being added up. May be next day I will bring you a nice cartoon where it shows how 2S and 2P mix and SP is formed. I will show it to you next day.

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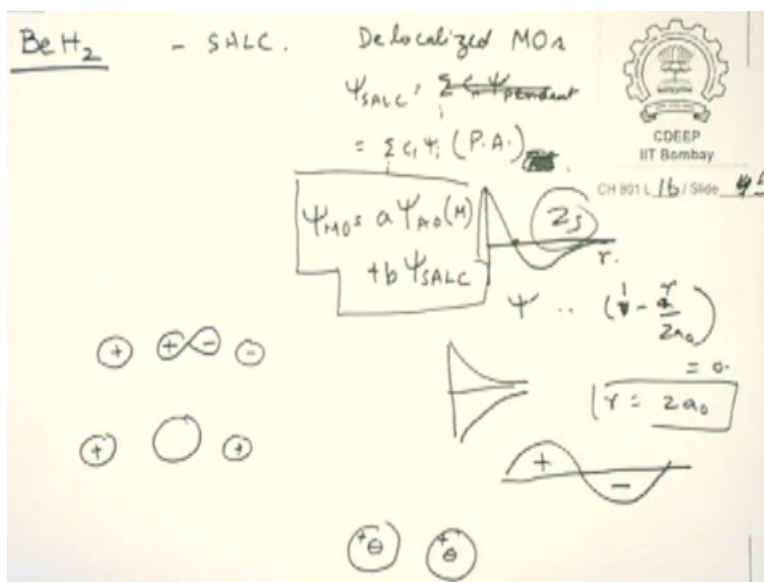


We just (()) (13:14) this, let us come back here. We were talking about BeH2 and we said that we can have two kinds of combinations of the 1S orbitals of the pendant hydrogen atoms. What are the (()) (13:36) that have the right symmetry to combine with this SALCs. One of the atomic orbitals of beryllium. **"Professor – student conversation starts"** What is the electron configuration of beryllium. (()) (13:50) 1:2: that is it. Right. But, then 1S is much lesser in energy, we can consider 1S to be (()) (14:05) completely. Not participating in the bonding.

So, 2S 2P, only valence shell. 1S energy is much less, so only the valence shell reacts isn't it. We only concern ourselves with valence shell usually. (()) (14:25) It is 2S2, so what is the valence shell? It is 2. So, 2S and 2P can actually contribute. Does 2S match the symmetry of any of these? And 2P matches the symmetry of this. **"Professor – student conversation ends"**

Now, what we are saying is first of all we will construct the SALCs. What are the SALCs, I will write like this psi SALC = sum of i Ci psi I pendant atoms. That is what I did first. I took the 1S

orbitals of the hydrogen atoms and made linear combinations and then psi MO should be equal to a psi ao (M) + b psi SALC. This is how I am going to construct my molecular orbitals. The approach we are taking is basically linear combination of atomic orbitals.

**"Professor – student conversation starts"** (()) (16:29) here, no, no, no this is different. 2S is the label for this. **"Professor – student conversation ends"**

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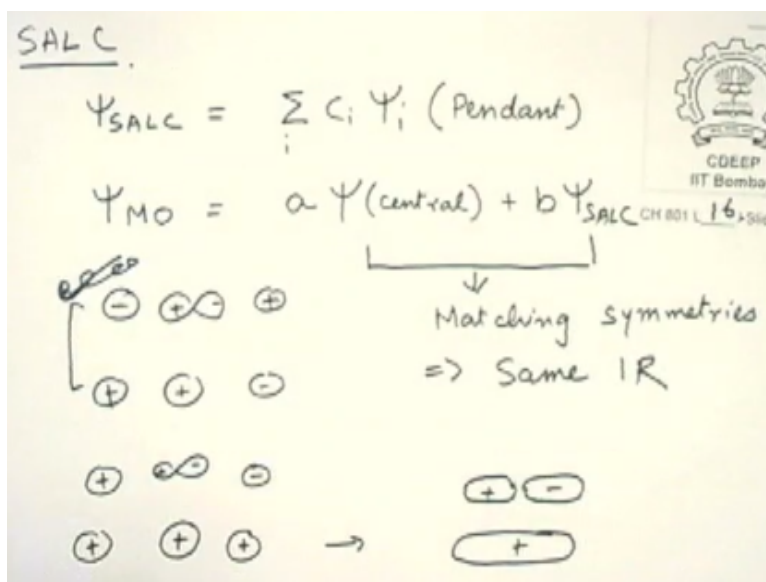


You want me to write in a little neater way, I can do that. SALC approach, what you do is you construct the symmetry adapted linear combinations from the atomic orbitals of the pendant atoms that are likely to participate in bonding and then you say that you construct the molecule orbitals by taking an appropriate linear combination of the psi of the central atom + the SALC. What is the restriction, this psi central and psi SALC must have matching symmetries.

In the language of root theory, they must belong to the same irreducible representation. Then, what we said was, first of all I am going to take these linear combinations, plus-plus is 1 and plus-minus is another 1, 2S of beryllium has the right symmetry for this plus-plus combination. 2P of beryllium has the right symmetry for the plus-minus combination. But, whatever I have drawn here is basically bonding interaction.

You can have anti-bonding interaction also. How will I get the anti-bonding interaction? I can keep the central atoms the same, central atoms ions, but I can change the sign of the SALCs. Instead of plus-plus, I can write minus-minus and what all that it means is that b has become –b and this can become minus-plus. So far, all this we can do without even bothering about (()) (19:29). That is why we are doing it first.

What kind of MO will you get if you combine these, what will it look like? Something that is delocalized over all the atoms. What will this MO look like? It will look like the big sister of P orbital. You know what the energy level should be in these cases. I will just show you what you expect then. **"Professor – student conversation starts"** Out of these two, which one will be of lower energy? This one will be of lower energy isn't it. That one will be. No, no, right. This one will be of lower energy. **"Professor – student conversation ends"**

Whatever I have done, I think I made some mistake somewhere. Suppose I take this, suppose I try to combine this with something else, suppose I try to combine this with plus-minus, then what will happen? **"Professor – student conversation starts"** (()) (21:13) and then suppose the same thing will happen there. **"Professor – student conversation ends"**
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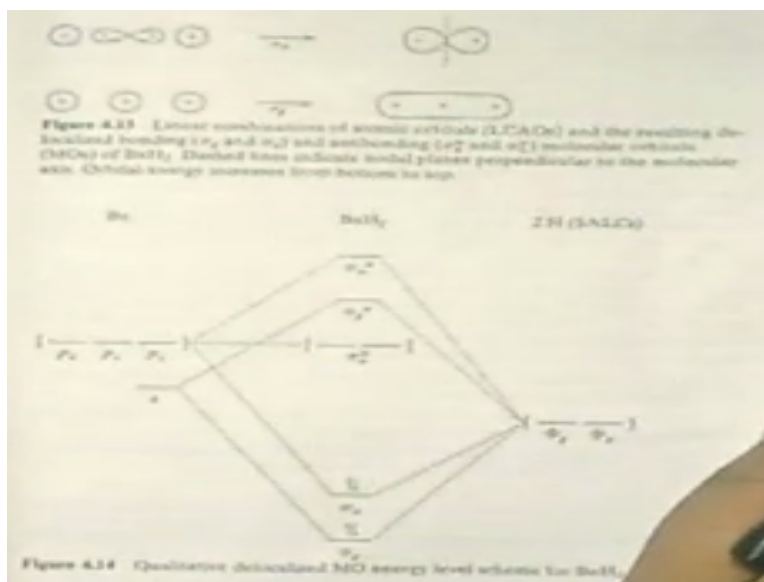


So, this is the order of energy that you are going to get. That you can figure out. These are the atomic orbitals, these are the atomic orbitals of pendant of the central atom, you combine them, I

think you know how to construct the energy diagram. Thing is we do not want to leave it as qualitative as this. Eventually, we want to know how we can use the character table to do this.