Physics of Nanoscale Devices
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Lecture - 59
Quantum Dot Devices

Hello everyone. In today's class, we will discuss Quantum Dot Devices or in other words The Nanostructure Devices, the devices based on nanostructures, molecules or the devices that are extremely small in dimensions and let us quickly review what we have seen in this regard so far.

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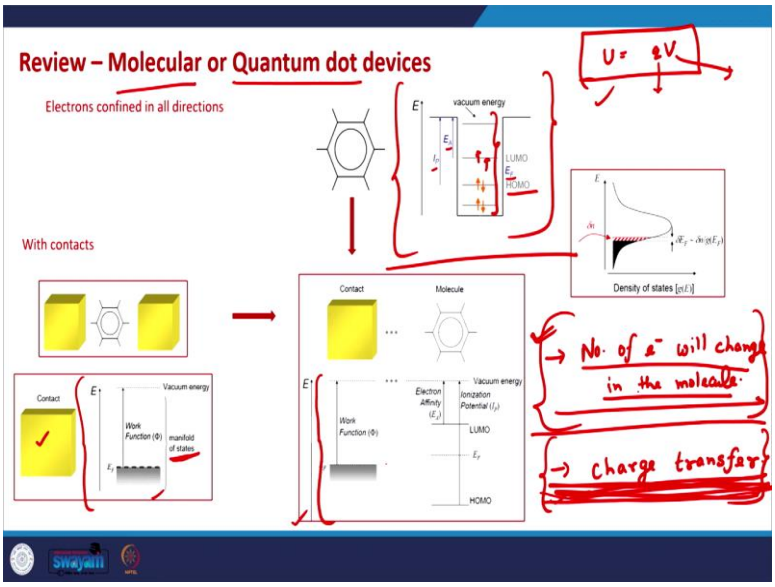

So, what we have seen is, that a quantum dot system, also in other words a molecular system can be, I would say the energy structure of this system can be understood in this way, that we have a highest occupied molecular orbital which is the orbital up to which electrons are filled in this system.

And there is this LUMO which is the Lowest Unoccupied Molecular Orbital. And the Fermi level will lie in between them, if HOMO is completely filled and LUMO is by definition unoccupied orbital.

So, it will be empty orbital. In some molecules, HOMO can be half filled in that case, the Fermi level can be assumed to be on the HOMO level. And if the HOMO is completely

filled in that case E F which is the Fermi level of this system can be assumed to be lie exactly midway of LUMO and HOMO.

Apart from that, what we saw was that in these molecular systems we can define ionization potential, electron affinity in order to characterize their electronic structure. So, after this in order to make devices, we also need contacts. And generally, the contacts are bulk contacts. So, in these devices in the molecular devices, we will have a bulk contact, typically a metallic bulk contact.

And this bulk contact has this kind of energy landscape. So, it will have a continuum of energy states as we can see in this picture. And the states up to the Fermi level of this system are completely filled and the states above the Fermi level are completely empty. So, there is this manifold of states, which is a continuum of states and up to Fermi level the states are filled and above Fermi level the states are empty.

So, this is I would say a very simplistic modeling of a bulk metallic bulk contact and when we put a contact in touch with a quantum dot or a molecule, this kind of system or we obtain this kind of system in which, we have a continuum of energy states in touch with discrete energy states and soon after we put these 2 systems in touch with each other they will reach in equilibrium.

Equilibrium means that every process is balanced by the counter process and in that case the Fermi level in the entire system must be uniform. And in order to make this Fermi level uniform across the entire system across this contact molecule system electron transfer takes place. And in these nanostructures in these molecular structures, electron transfer actually corresponds to two things.

And that is a key point here, that is what we need to keep in mind. So, when there is an electron transfer either from the molecule to the contact or vice versa from the contact to the molecule, the number of electrons will change in the molecule. The number of electrons will also change in the contact. But, since contact has a lot of electrons its a bulk contact and that is why, if there is a small change in the number of electrons in the system, it does not actually have any consequence.

But, the molecular system or the quantum dot system is a small system and there are only few electrons in this system and if there is a change in the number of electrons in this

system, it will have it will essentially fill or empty the electronic states in this system, second is charge transfer also happen.

So, when there is an electron movement across this system from the contact to the molecule from the contact to the quantum dot or quantum dot to the contact, in that case two things happen, specially in the quantum dot one is the charge transfer happens because the electrons are charged particles, that is very obvious and second is the number of electrons change in the molecule which means that the states the way the states are filled these states are filled is also changed.

So, in equilibrium, if let us say if there is one electron that comes up here, just by this change in the number this Fermi level will go to the LUMO orbital. So, the Fermi level depends on these two phenomenon, one is the change in the number of electrons in the molecule and second is the change in the charge on the molecule.

So, generally up to now, we have not considered this part which is the change in the Fermi level due to the change in the number of electrons in a system. Generally, it was assumed that, the Fermi level just depends on the electrostatic potential or just depends on the charge on a system. But in nano systems, in nanostructures we need to account for the number of electrons as well or we need to account for the effect of number of electrons on the Fermi level as well.

So, there are two things that we need to consider while understanding the equilibrium one is that, the number of electrons change in the molecule and that also change that will change the Fermi level. Second is the charge will change in the system and that will also change the Fermi level, because the Fermi level depends on the potential energy and the potential energy is given by -q V, where V is the electrostatic potential q is the charge.

So, q times V essentially. If there is a charge rearrangement in that case, the energy is changed and the Fermi level is also changed. And because of this, the first idea because of this because the Fermi level now depends on the number of electrons as well the notion of quantum capacitance comes into picture.

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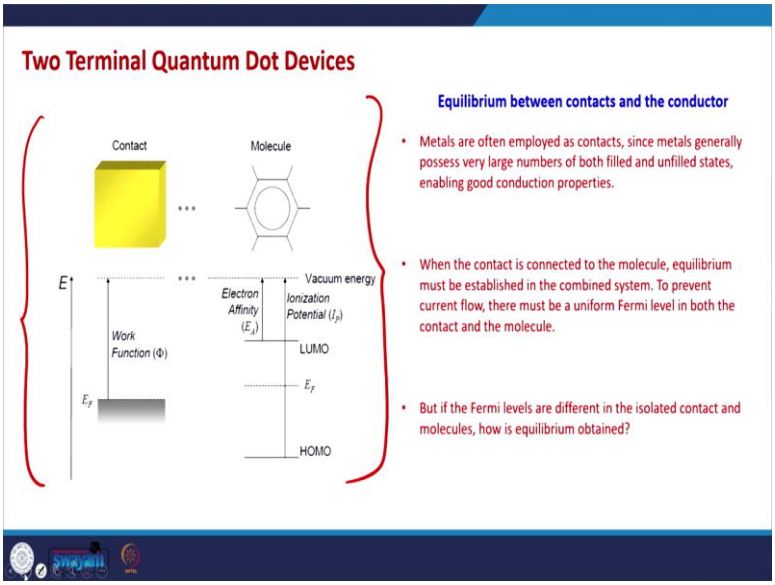

So, that is what, that is where we essentially finished last time and so, this is a two terminal quantum dot device I would say this is the model of that.

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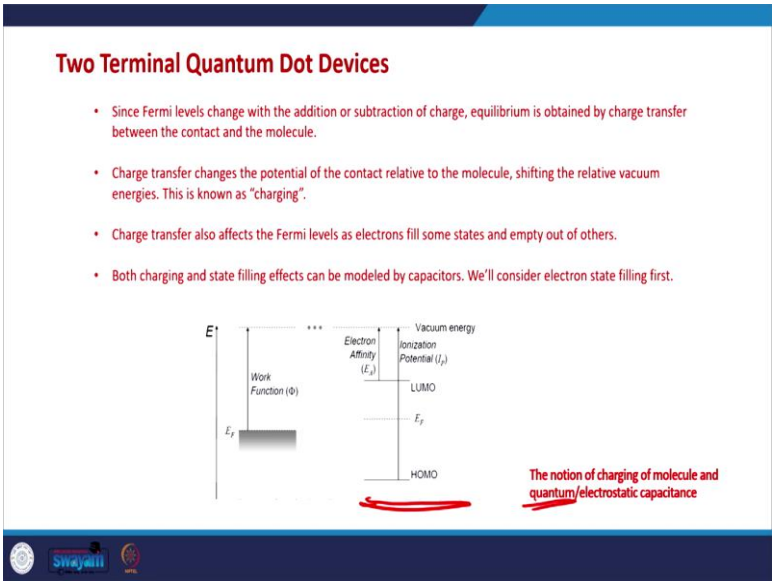

And what we just saw is that there are two phenomenon happen in equilibrium, one is known as the charging of the system, which means the change in the electrostatic charge in the system and second is the state filling. State filling means that by changing the number of electrons in this molecule, the states will be filled or will get emptied and in that case the Fermi level will be changed.

So, the change in the Fermi level, which is required to achieve the equilibrium it depends on two things, one is the state filling and second is the charging, ok. So, yeah, this is the key point here and corresponding to the state filling, we have the notion of quantum capacitance, ok.

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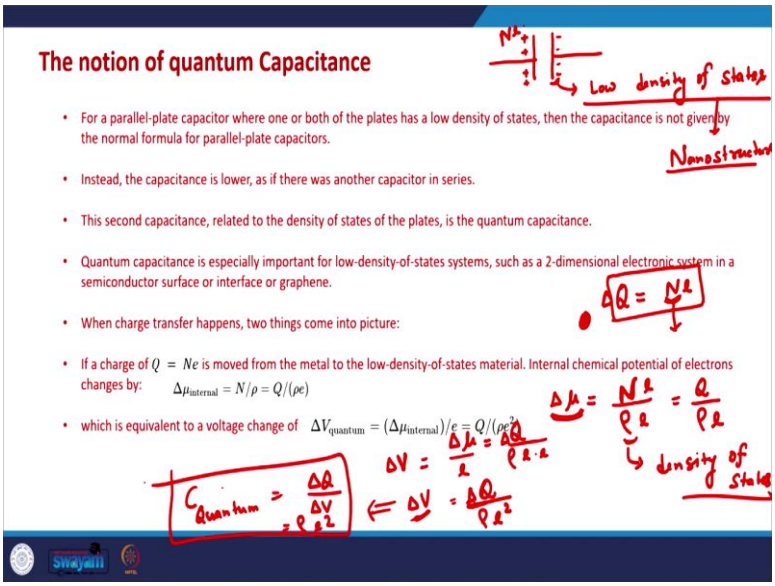

So, the notion of quantum capacitance says that, let us quickly have a look at the notion of the quantum capacitance. So, in a parallel plate capacitor, if let us assume that if one of the plates of the capacitor is a low density of state system. So, in a parallel plate capacitor is if one of the states or one of the plates is, a low density of states which means that the available electronic states are very few on one of the plates or in other words its a nanostructure, its a nano system or it might be a quantum dot as well.

So, if one of the plates is a nanostructure in that case, what happens is if there is change in the charge on one plate, the corresponding change will happen on the other plate as well. And because of this charge transfer, because of this change in the charge on the other plate let us say, that the change in the charges or N number of electrons are transferred or if let us say we put a charge which is N times e.

So, the charge on the big plate is (Ne). So, the similar charge will appear on the other plate on the, this smaller plate on this low density of states plate or the nanostructure plate of the capacitor. So, corresponding to this change, N number of electrons are

transferred or N number of electrons are transferred from the plate or supplied to the plate, depending on the sign of the charge.

If the sign of the charge on the small the nanostructure nanoplate is negative, it means that N number of electrons are transferred; if the sign is positive, N number of electrons are taken away from that plate. So, what it means is that, with this N number of electrons there will be a change in the Fermi level as well. There will be a change in the electronic energy structure and the change in the this chemical potential or the Fermi energy is the number of electrons getting transferred divided by the density of states.

Because, the density of states tells us about the number of electronic states per unit volume per unit energy in a way. So, the change in the chemical energy chemical energy of the system or the chemical potential of the system, will be given by the number of electrons that are getting transferred that are changing on the plate divided by the density of states. So, that will correspond to the energy change in the system.

So, if we multiply by the electronic charge, it will be $Q/(\rho e)$, where ρ is the density of state. Generally, we use g or D for density of states, but ρ is also used for density of density of states at some places. So, please do not confuse it, this is just the density of states of the nano system.

So, the change in the electrochemical potential is Q divided by density of states times e and the corresponding change in the voltage is the change in energy divided by the charge. And please be careful that, we are just considering the change in the potential or change in the Fermi level just due to the change in the number. We are not considering the electrostatic part here, we are just considering the number part here.

So, this change in the Fermi level is equal to the change in the charge divided by density of states times e square, e is the electronic charge. So, if ΔQ charge, let us assume that this is ΔQ, if ΔQ is the charge that is transferred on the nano system this will be ΔQ. So, this so, corresponding to a change in charge ΔQ, there is a change in the voltage ΔV which is not of electrostatics origin.

It is just because of the change in the number. And that is why we can define a capacitance out of it which is essentially known as the Quantum Capacitance of nano systems which is given as ΔQ divided by ΔV and it is density of states times charge

square Q times e. So, that is how this notion of quantum capacitance comes about and as you have seen that it depends on the density of states.

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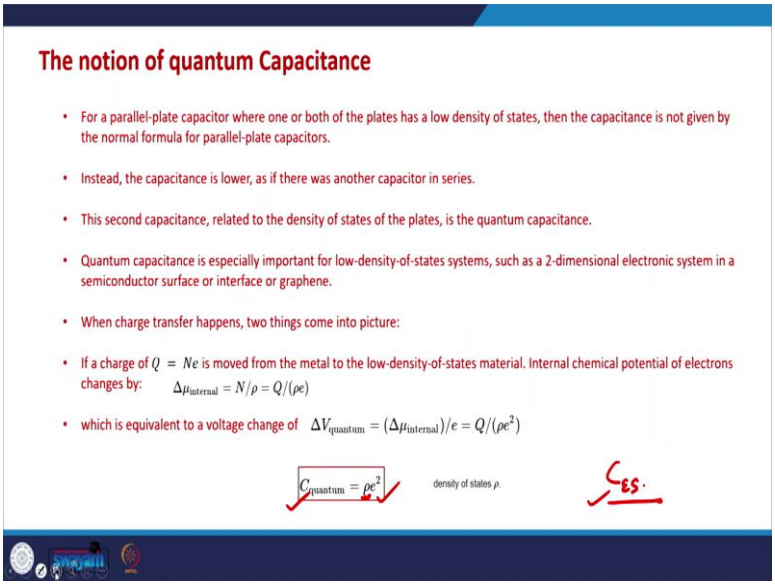

It is directly proportional to the density of states times and it is given as density of states times the charge square, ok. And please be careful that, this quantum capacitance arises because there is there is a change in the Fermi level, just because of the change in the number of electrons.

It does not have electrostatics origin, which is change in the charge brings about the change in the electrostatic potential which changes the potential energy and there is a capacitance corresponding to that which is known as the Electrostatic Capacitance.

So, in nano systems while there is a charge transfer, we always need to consider two capacitances one is the quantum capacitance and second is the electrostatic supply electrostatic capacitance.

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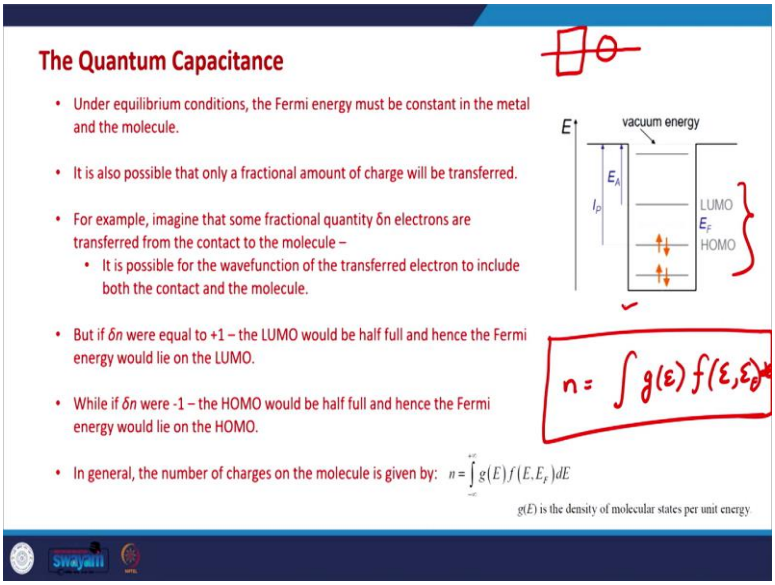

So, let us first just have a look at the quantum capacitance part. So, in a system in a quantum dot metal system, let us say if we have a bulk contact and if we have a quantum dot here.

And when we put both in touch with each other in equilibrium will reach and in order to arrive at the equilibrium the Fermi levels must be aligned, which means, that the Fermi levels must be changed and the Fermi level of the metal does not change because the number of electrons on the metal is extremely high. So, even if there is a change in the number of electrons it will not change.

But the Fermi level of the quantum dot can change, just by changing the number of electrons and it will have two components, one is the change in the Fermi level due to the change in the number of electrons on the quantum dot and second is change in the Fermi level due to the change in the charge on the molecule. So, we are now just considering the change in the Fermi level due to only due to the change in the number of electrons on the quantum dot.

So, let us say, if we put quantum dot in touch with the metal in that case at any point the number of electrons can be given as just the integration of the density of states times the Fermi function of the system. And in equilibrium the Fermi function throughout the entire system will be the same before equilibrium it might be different and that leads to the transfer of electrons across the system, from the contact to the metal from the contact to the quantum dot or quantum dot to the contact.

So, this basic relation holds. And I would also like to sort of remind you, that in nano systems, generally the notion of Fermi level is not rigorously defined, because the number of electrons is not. So, large, but in the last class we saw how do we define the notion of Fermi level in quantum dots and that is defined via LUMO and HOMO energies and their occupancies. If the occupancy changes the Fermi level also changes.

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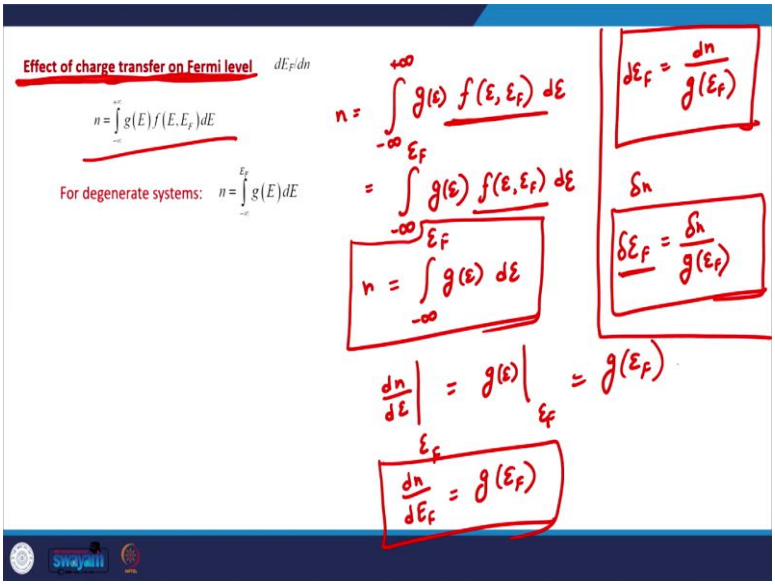

So, with this relationship, what we can see now is that what we are essentially trying to do is we are trying to understand the effect of charge transfer on the Fermi level or how much is the Fermi level changed, when there is an addition of electron in the system. So, with this relationship what we can say is, n is -∞ to ∞ dE.

And generally, the Fermi function is governed by the Fermi function of the contact, where we assume that, the electronic states up to the Fermi level are completely filled and above Fermi level are empty. So, this limit from -∞ to ∞ can be reduced to -∞ to E_F which is the Fermi level of the system in equilibrium.

And the Fermi function is assumed to be 1 below the Fermi energy below the Fermi level. So, this can further be simplified to ∫g(E)dE up to E_F. now, this is a straightforward expression and if we take a derivative of this expression and evaluate at E_F that will give us g(E) at E_F which is the density of states, here g is the density of states at E_F and this becomes the left hand side expression becomes dn divided by dE_F.

So, what we have is this expression. So, what it means is that dE_F is equal to dn divided by $g(E_F)$, ok, which means that if there is a change or there is a transfer of delta n electrons from the contact to the molecule. The change in the Fermi level δE_F will be δn divided by $g(E_F)$, ok.

And that is the change in the Fermi level just because of the change in the number of electrons on the quantum dot or on the molecule. This does not has the electrostatic component yet. It is just the number part, the change in the number of the electrons on the system.

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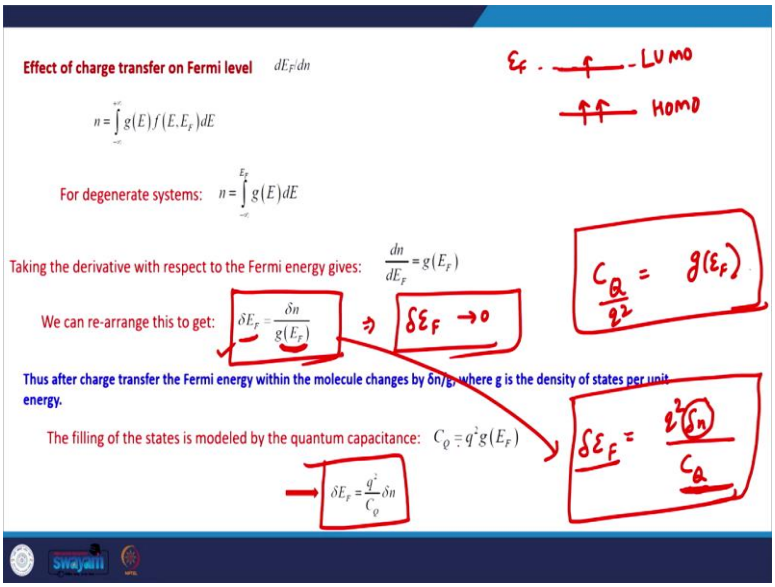

So, that brings this much change in the Fermi level on any system. And as you can see that, the change in the Fermi level is inversely related to the density of states of the system.

So, if the density of states of the system is quite high, in that case, δE_F will tend to 0. And that is exactly the reason that in metals in bulk contacts or in any system where the density of states is quite significant in that case, there is no change in the Fermi level just because of the number of electrons are changing in the system.

But in nano systems, as we had seen that even if we put. so, in this kind of nano system in which we have HOMO completely filled, LUMO completely empty, the Fermi level is in between of LUMO and HOMO. In this case, even if we put 1 electron in LUMO, the

Fermi level now is changed from the mid value to the LUMO value. So, the change in Fermi level is quite apparent in quantum dot system as a as the number of electrons are changed in this system.

So, that is why we need to consider this effect which is related to the quantum capacitance or which is modeled by the quantum capacitance of the system. And, as we had seen that the quantum capacitance is defined as q^2 times the density of states at the Fermi level. So, it means that, this change in the Fermi level now can be this δE_F can be written as δn, $g(E_F)$ it can be written as C_Q divided by q^2.

So, essentially δE_F is $(\delta n/C_Q)$ times q^2. So, this is the change in the Fermi level due to the change in electrons in the quantum dot and this is the relationship between δE_F and quantum capacitance. So, this is known as in a way this is the charging of the or this is the capacitive effect which is which corresponds to. So, capacitance is defined as the change in the potential of a system as the charge at this as the system is charged or discharged.

So, in this case, as we put more number of electrons, the electrochemical potential changes and that is modeled by the quantum capacitance, ok. So, yeah this is an important part this all of us need to keep in mind while dealing with quantum dot systems.

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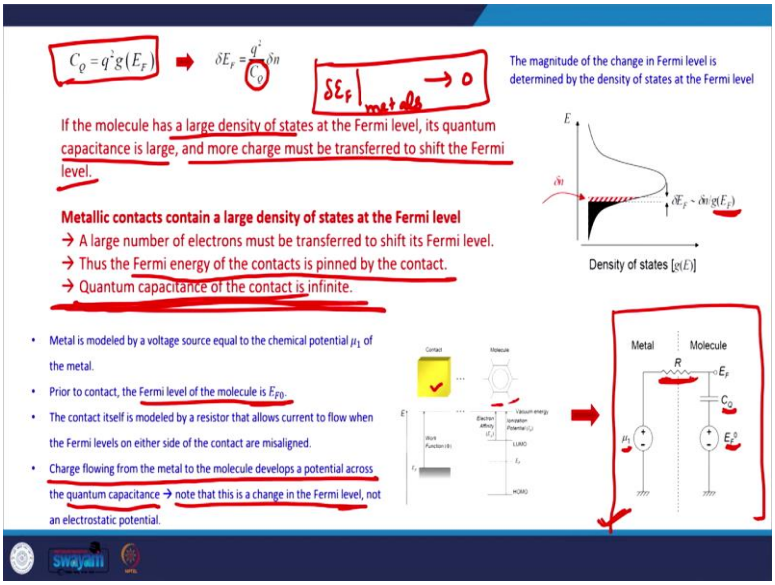

And this is pictorially shown in this way, that as we put more number of electrons Fermi level is altered and it is inversely related to the density of states at the Fermi level, ok. Larger the density of states, the quantum capacitance will be large, because it is directly related to the density of states and more charge must be transferred to shift the Fermi level, ok.

And in metallic contacts, a large number of electrons must be transferred to have this to have this capacitive effect to have this effect of the quantum capacitance. So, that is why the Fermi level of or the Fermi energy of the contacts is pinned actually. Pinned means by changing the number of electrons on the system it does not change.

Because C_Q is extremely high, because the density of states is extremely high in metals. And that is why this δE_F for metals is 0 which is known as the Pinning of the Fermi levels in the contacts. And because of the extremely high density of states, because of the continuum of energy states in the metal, the quantum capacitance is also infinite or tends to infinite which is responsible for this pinning of the Fermi level of the contacts.

So, this effect can be in short or in circuit terms I would say, this junction between a contact and a quantum dot system can be modeled by this simplified circuit. So, this metal is modeled by a voltage source, where the voltage value is the Fermi level of the metal. The molecule is modeled by a voltage source, where the voltage of so the voltage of this voltage source is equal to the Fermi level of the quantum dot without or standalone Fermi level of the quantum dot without any external connections.

Plus, in series we have a capacitor which is the quantum capacitance and the junction between the contact and the molecule is modeled by a resistance. Although, for better or for I would say for more accurate modeling, the junction also needs to be modeled by a capacitance along with the resistance. Because, there is some gap and it the junction is also capacitive because of that its not just the resistive connection, ok.

So, prior to the contact the Fermi level of the molecule is E_F^0 and here we are only considering the this quantum capacitance component we are not considering the electrostatic component, ok. So, please care be careful. So, this circuit is not yet complete. This is just to model the, quantum capacitance of the molecule in a circuit form, ok.

So, this the charging from the metal to the molecule it sort of develops a potential across the molecule and that is modeled by the quantum capacitance. And this is not the electrostatic potential; this is the change in the chemical potential. And the change or the change in the Fermi level, ok. So, I hope things are pretty much clear up to this point.

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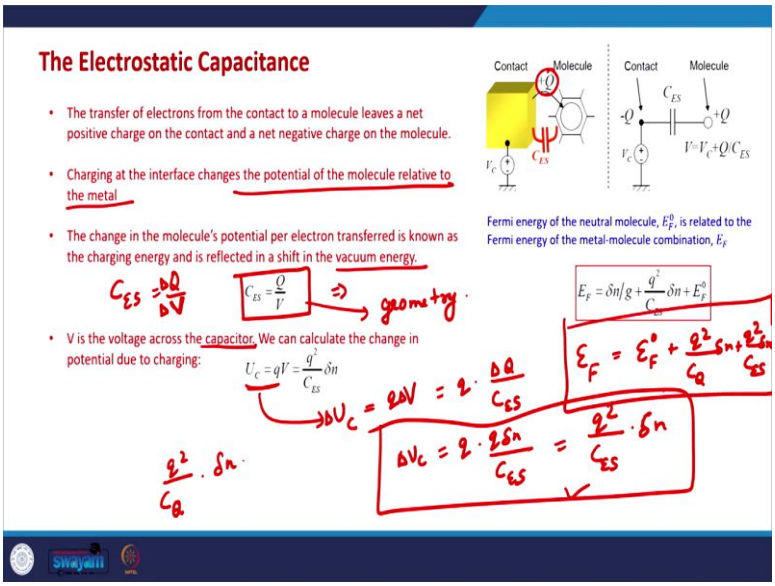

So, now let us consider the electrostatic component as well. So, when there is a transfer of electrons from the contact to the molecule or vice versa from the molecule to the contact, a net positive charge if electrons are getting transferred from the contact to the molecule, the contact will have a net positive charge and the molecule will have a net negative charge, in a way.

And in reverse situation when there is an electron transfer from molecule to the contact the molecule will have positive charge after the transfer and the contact will have a negative charge after the transfer. And this charging at the interface, it changes the potential of the molecule relative to the metal. So, its completely shifts the energy level of the molecule up or down.

This is modeled by the electrostatic capacitance and this is given as the. So, this capacitance also this depends on the geometry as well, depends on the spacing between the contact and the molecule. And this change in the charge on the molecule will change the all the energy levels including the vacuum energy level.

So, if V is the voltage across the capacitor which means, which is the change in the volt electrostatic potential due to the charge transfer, then the or the electrostatic capacitance is defined as the charge divided by the voltage or $\Delta Q/\Delta V$ which is the change in the charge on the molecule, divided by the change in the potential across the electrostatic potential across the molecule.

So, the electrostatic potential energy of the system will be changed by $q\Delta V$ this will be changed by this value where ΔV can be written as $\Delta Q / C_{ES}$ and ΔQ is $q\delta n$ if δn is the number of electrons that are getting transferred. So, it will be $(q^2/ C_{ES}) \delta n$, which is q square divided by the electrostatic capacitance times the change in the number of electrons on the system.

So, that corresponds to the change in the potential energy or change in the electrostatic potential energy of the system ΔU_C, ok. So, if you please remember the previous part, the change in the energy due to the or change in the Fermi level due to the change in the number of electrons is q square divided by the quantum capacitance times δn and this is due to the electrostatic part.

So, the total change will be given by the sum of these two components one is. So, the new Fermi level of the quantum dot system or the molecular system will be the Fermi level without any contact E_F^0 plus the change due to the quantum capacitance plus the change due to the electrostatic capacitance, ok. So, $E_F = E_F^0 + (q^2 \delta n /C_Q) + (q^2 \delta n /C_{ES})$, this is what we need to keep in mind, ok.

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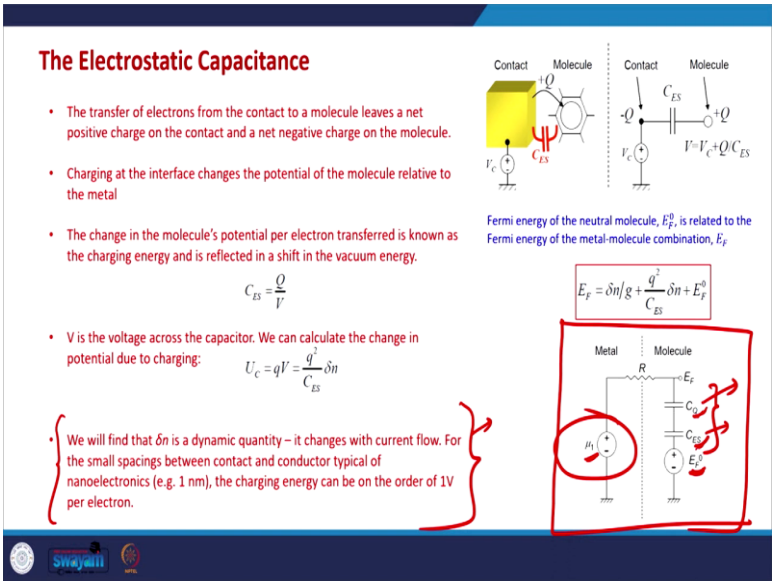

So, this typically gives the order of the magnitude of the voltage or this tells this gives us an estimate of the electrostatic capacitance in nanosystems, ok. So, with this now in this junction between the contact and the molecule contact and this the quantum dot, in addition to the quantum capacitance it also needs to account for the electrostatic capacitance.

And this is the proper modeling of the system when a contact is joint with the molecule. The voltage source, generally these this contact is represented as a voltage source of voltage value μ_1 which is the Fermi level of the metal because, metal can be visualized as a system which is supplying electrons at this potential. So, it can be modeled by a voltage source with voltage μ_1.

Similarly, the molecule can be modeled by a voltage source with voltage E_F^0 which is the Fermi level of the quantum dot without any external connection, along with quantum capacitance and electrostatic capacitance.

So, if there is a charge transfer across this system these quantum capacitance will account for the change in the Fermi level due to the change in the number of electrons and this electrostatic capacitance will account for the change in the Fermi level due to the change in charge or electrostatic potential on the system.

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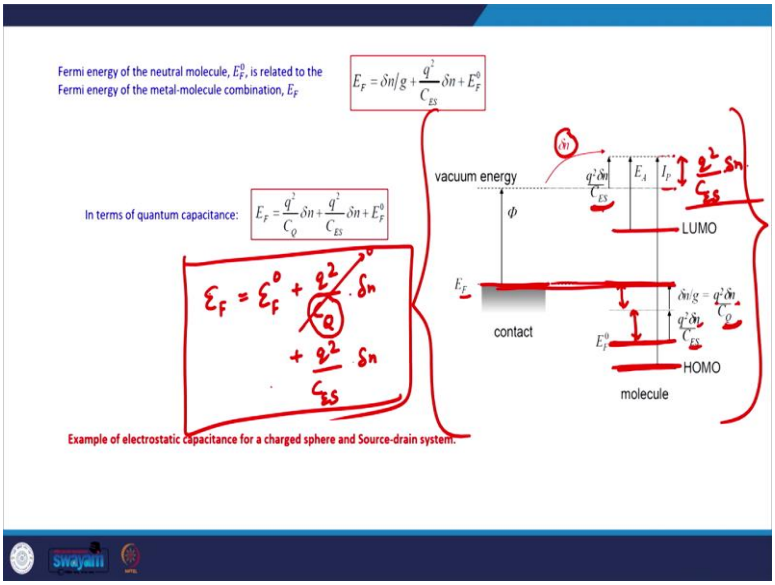

So, this can also be seen in this picture more clearly, this energy diagram energy level diagram of the system. This is the; this is the HOMO orbital, highest occupied molecular orbital of the molecule, this is the LUMO, this is the metallic contact. This the Fermi level of the metal lies here. In equilibrium, the Fermi level of the molecule also needs to come to this level, ok. Earlier it is at this level.

And we have a transfer of delta n electrons. This delta n just to remind you delta n can be less than 1 as well. Because, the electronic wave function can exist both on the contact on the quantum dot. So, that in a way is understood as the partial transfer of electrons from the contact to the quantum dot system.

And this delta n can be any number and corresponding to this delta n transfer, there is a change in the Fermi level due to the quantum capacitance which is (q^2 δn /C_Q) which is this value.

And there is another change in the Fermi level due to the electrostatic capacitance which is (q^2 δn /C_{ES}). So, earlier the Fermi level was here, but now because of the because of both quantum capacitance and electrostatic capacitance, the Fermi level will be here; which is just the Fermi level of the metal.

Please, remember this part, that this is the vacuum energy. The change in the vacuum energy is only because of the electrostatic component. Only because of the change in the charge on the system. So, this so, earlier the vacuum energy was here. Now, the vacuum energy has come here and this is just the (q^2 δn /C_{ES}). So, the electrostatic charge or the

this electrostatic capacitance in a way changes the entire energy landscape of the molecule.

This quantum capacitance just changes the Fermi level of the molecule. These are the subtle differences between the 2. So, finally, in terms of the capacitances the new Fermi level or the Fermi level in equilibrium is given as, the Fermi level without any external connection plus q square divided by quantum capacitance delta n plus q square divided by the electrostatic capacitance times delta n : $E_F = E_F^0 + (q^2 \delta n / C_Q) + (q^2 \delta n / C_{ES})$.

So, this is the; this is how the equilibrium is attained in nanosystems in quantum dot systems, ok. And this is different from what we have considered so far because, what we have considered before discussing the quantum dot systems, we considered that the quantum capacitance is extremely high in a way indirectly we assumed that, because the density of states is quite high and that is why this component was negligible in our calculation. But this needs to be taken into account in nanosystems, ok.

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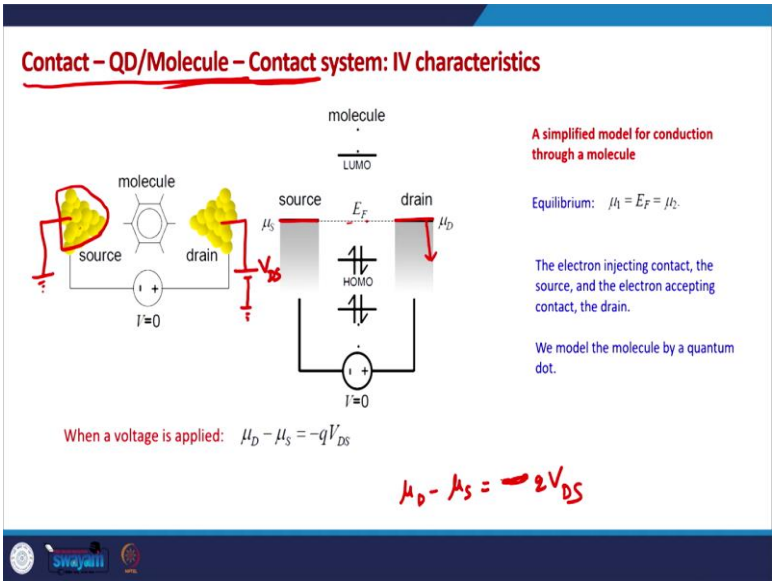

So, now, we have understood how the equilibrium is achieved, when we when a contact or a bulk contact is in touch with a quantum dot or a molecule. Now what we will try to do is, we will try to understand the IV characteristics of Contact Quantum dot Contact System which means that this quantum dot is now in between 2 bulk contact; the source and the drain contacts in a way, ok.

So, when from the discussion that we just had, what we can say is when there is no external voltage in this system, there is no external bias in the system, no external applied voltage in the system, the source contact Fermi level is μ_S let us say, the drain contact Fermi level is μ_D and the Fermi level of the quantum dot is E_F and all of them are uniform, which means all of them are at the same level.

HOMO is below E_F; LUMO is above E_F. HOMO is completely filled in our assumption in our this example and LUMO is completely LUMO is by definition completely empty. If HOMO is half filled, in that case HOMO coincides with the Fermi level as well. But that may change, as we put a metal contact in touch with the quantum dot.

So, this is the situation with no bias, equilibrium which we just discussed and this equilibrium is achieved with two effects one is the effect of the quantum capacitance because of the effect of the quantum capacitance and second is because of the electrostatic capacitance, ok. Now, if we put if we apply a voltage across this system, and by definition generally, we apply a positive voltage on the drain contact generally the source contact is grounded.

Generally, a V_{DS} positive V_{DS} is applied on the drain side. Please do not, confuse these contacts are still bulk contacts. Here they are just showing the connection between the contact and to the molecule by these atoms. Do not confuse it with the, smaller contacts. The contacts are still bulk. This is just showing the connection between the contact and the molecule.

In that case, what will happen is if there is a positive voltage on the drain side, there will be a difference in the Fermi level of the drain and the Fermi level of the source, ok. And if there is positive voltage on the drain side, this will go down. The energy of the this is generally given as q times V_{DS} there is this negative sign is not there, in some conventions it is written like that.

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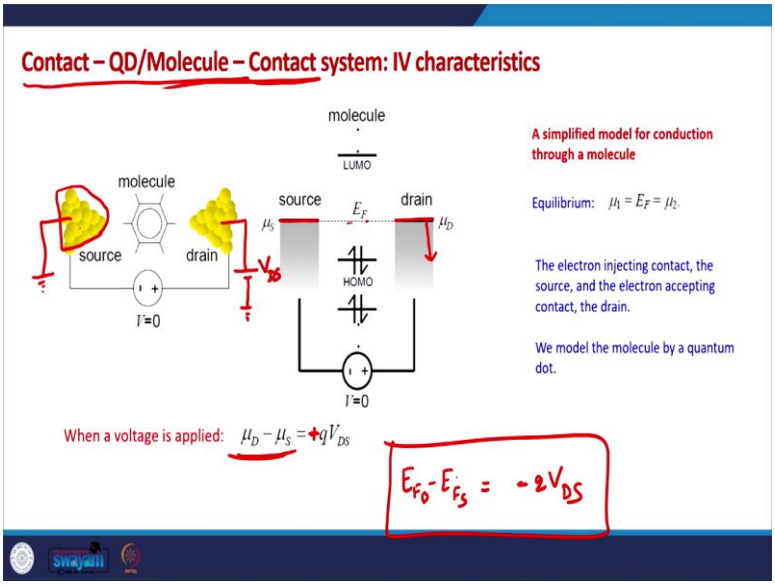

But according to the convention that we have followed, where. So, generally according to these are the potential energies of the contacts, but if we write it in terms of Fermi levels, the Fermi level of the drain E_{FD} and the Fermi level of the source have the difference of q times V_{DS}, $-qV_{DS}$. Yeah, this is this is correct this is correct, sorry, for this. Because the drain Fermi level is now below the source Fermi level, which means E_{FS} is $E_{FD} + qV_{DS}$, yeah.

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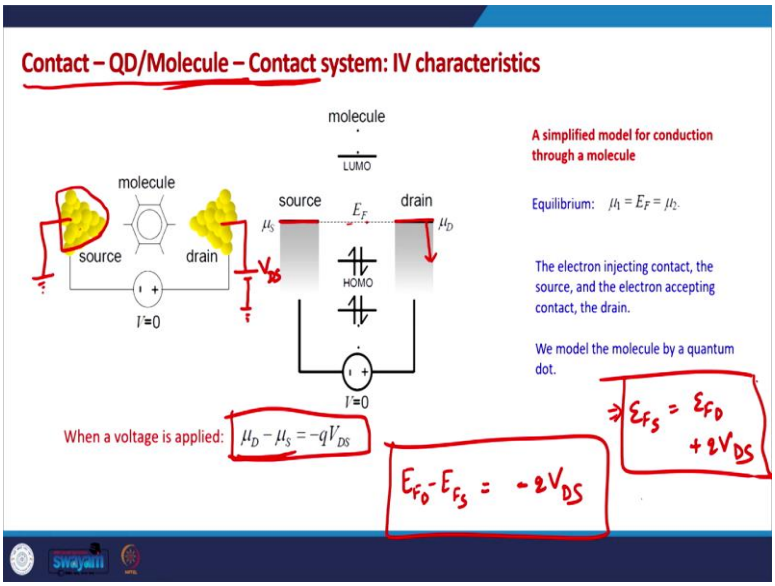

So, this equation is also correct and this is the correct relationship between the source and the drain Fermi levels. But, we need to understand, where this voltage drops. There are two points that we need to understand I would say, one is where is this voltage

dropped. Second is how does this applied bias, change the potential, in the molecular system in this quantum dot system, ok.

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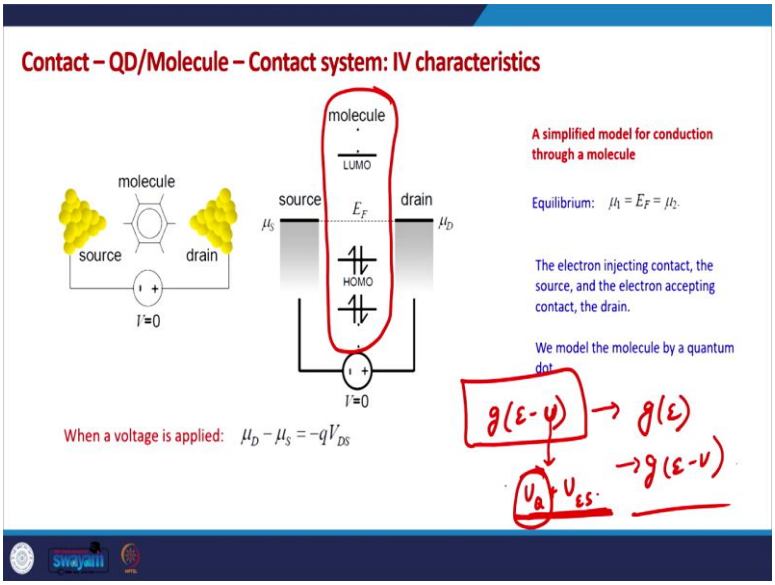

Because, the density of states, depends on the effective potential that is applied on the; on a nanosystem. So, if U is 0 in that case the density of states is just g times E, but if the effective potential which is the summation which has two contributions one because of the quantum capacitance and second because of the electrostatic capacitance.

And this effective potential can be broken down in 2 parts, electrostatic and quantum and if there is this change, it will change the density of states in the system as well. And invariably generally what will happen is, once we apply any positive voltage on the drain, there will be a mismatch in the Fermi levels.

So, the source Fermi level. So, the source will try to bring try to fill all the electronic states in the molecule up to the source Fermi level and the drain will try to fill the electronic states in the molecule up to drain Fermi level.

And in that competition between the source and the drain contacts, there might be a steady state current which means that the number of electrons in the molecule might change.

So, the number if there is a change in the number of electrons in this molecule, it will have two consequences one is the electrostatic potential of the molecule will change and

second is the quantum the contribution because of the quantum capacitance. So, both of these need to be taken into account, while calculating the IV characteristics or while trying to understand this entire system.

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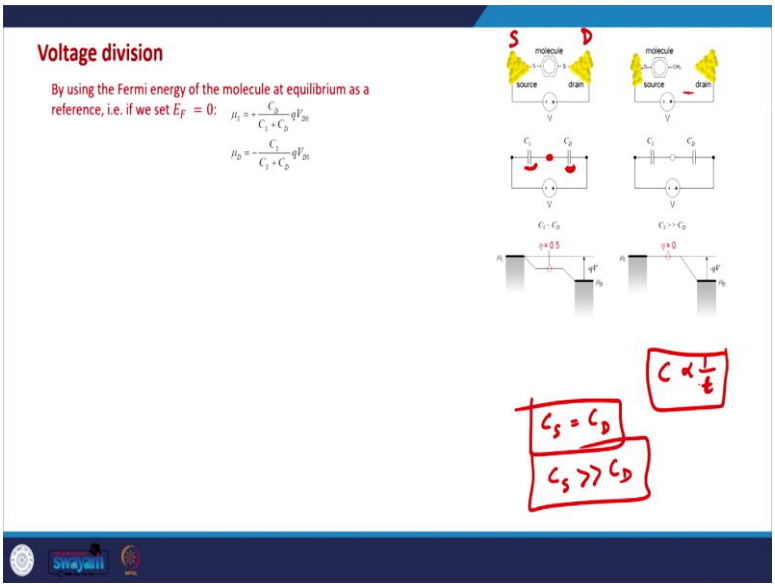

So, first we will try to understand where does the voltage drops in this system. And generally the contacts this is the source contact, this is the drain contact. The contacts are modeled by 2 by the capacitors. So, the source contact is modeled by a source capacitor and the drain contact is modeled by a drain capacitor and this in between we have the quantum dot system.

There might be a along with the capacitors there might be a resistor as well, we have just for the simple understanding or I would say for the sake of simplicity we at the moment we have omitted the resistor. So, the coupling between the contacts and the quantum dot is modeled by the capacitors, the source and the drain capacitors.

And this capacitance depends on the distance between the quantum dot and the contact. So, for example, if the source and the drain contacts are symmetric; they are exactly the same in that case, and the distance between the source and the drain contacts and the molecule is the same in that case C_S is equal to C_D. But, let us say if the source is closer to the molecule as compared to the drain as in this case.

In that case the distance between the source and the molecule will be less. And thus, source capacitance will be extra high as compared to the drain capacitance. Because the capacitance is inversely proportional to the distance between the 2 plates in a way, in a parallel plate capacitor depends it is inversely proportional to the distance between the 2 plates.

So, multiple different scenarios can be there and depending on the relative distance between the contacts and the molecule these capacitances are defined. But now, in this system let us say we have applied a voltage V, then, according to the voltage division principle across capacitors, this is the amount of voltage that will drop across the source contact and this is the amount of voltage that will drop across the drain contact. And these depend on the source and drain capacitors contact capacitors.

So, the amount of voltage that drops on the source contact is $+C_D/(C_S + C_D)$ times q V_{DS}. And the voltage dropping across the drain contact is $-C_S/(C_S + C_D)$ times qV_{DS}. The negative sign is there because the molecule is taken as the reference.

Source is if V_{DS} is positive, then source is above μ_S or E_{FS} is above the Fermi level of the system Fermi level of the molecule, in that case there is a positive sign. And because the drain Fermi level is below, there is a negative sign.

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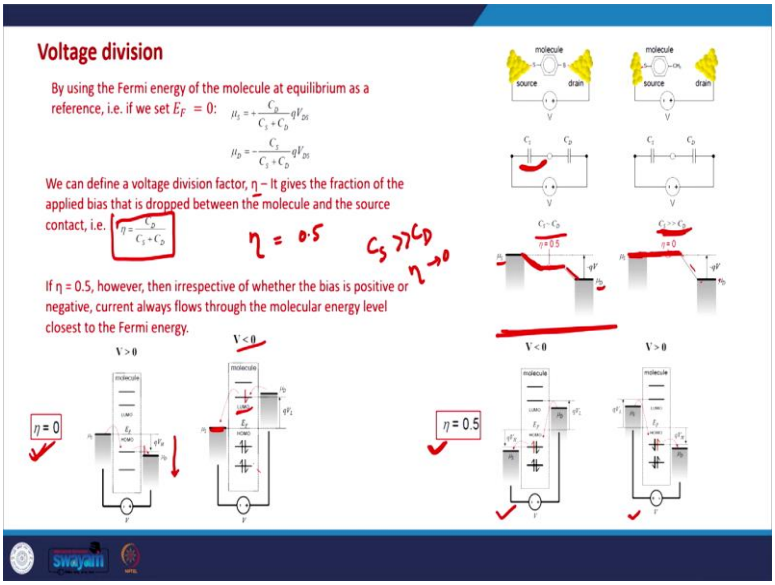

And this can be understood from a voltage division factor, which is here written as η factor. η is defined as $C_D/(C_S + C_D)$ and or in other words it is essentially the voltage that drop across the source contact, source molecule interface, more precisely. If both the capacitors are equal, we have the symmetry contacts in that case eta will be half, which means that half voltage drops across the source molecule interface and half other half drop drops across the molecule drain interface.

And this is the situation that we obtain. So, if there is a applied voltage, μ_S is the source Fermi level, μ_D is the drain Fermi level, E_F the Fermi level of the molecule is this and when η is 1/2 then in that case half of the voltage drops across this interface.

The source molecule interface and the other half drops across the drain molecule interface. In another scenario, if we have the source capacitance extremely large as compared to the drain capacitor which means, that the source contact is quite close to the molecule as compared to the drain contact.

In that case this C_S will be extremely high, η will tend to 0 and in that case, the Fermi level of the molecule and the Fermi level of the source will be almost at the same level. So, the voltage will not drop across the source molecule interface; almost all the voltage will drop across the molecule drain interface. And depending on in both of these scenarios, we can understand the electron transfer across the devices.

So, if the applied voltage is positive, drain Fermi level will be below as compared to the source Fermi level and the electron transfer will happen from the source to the drain side via HOMO in this case. This is the η equal to 0 case, because E_F is still at μ_S level. And if V is negative, the electron transfer will happen through LUMO, because E_F is at the source Fermi level and this is true.

When η is half in that case, E_F does not coincide with the μ_S. In fact, E_F which is the Fermi level of the molecule is between μ_S and μ_D and in that case, the electron transfer happens in this way. So, from the simple logic, we can understand the transfer of electrons in these two scenarios one is η = ½ second is η=0.

Generally, symmetry contacts are considered. So, η = ½ case is generally more I would say is more in use in our modeling. So, I hope you would be able to understand this.

Now, we have understood the voltage division across these 2 interfaces across the source quantum dot interface and the drain quantum dot interface.

The second question that we will deal with is, the change in the potential of the molecule as a voltage is applied which means, electrons will transfer which will change the number of electrons on the quantum dot. So, that we need to understand at the second part and once we have understood that, in then we can calculate the IV characteristics of this system.

So, I hope this is clear up to this point. I will advice all of you to go back and go through it thoroughly. I have written a lot of text on the slides. So, that these things are clear these things are more or less self-contained. So, please go back and study it. And in the next class, which is also the last class of this course, we will discuss the voltage the change in the potential energy of the molecule in steady state, which is the state when there is a constant current in the system.

And we will calculate IV characteristics and then we will have a brief discussion on density functional theory which is the Ab initio method to calculate electronic properties of nanosystems and with that we will finish this course.

So, thank you all, see you in the next class.