Concepts of Chemistry for Engineering
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Lecture 47
Fluorescence Spectroscopy

We have reached the last topic of this part of the course. Earlier, we have talked about molecular orbitals, we have discussed the electronic states, how we define electronic states from electron configurations and spin states. And we have talked about absorption spectroscopy. So, so far, we have learned how to populate an excited state, how to create an excited state.

Today, we are going to ask this question, what happens to the molecule after the excited state has been populated because it cannot remain in the excited state forever. Eventually, it has to come down, it can come down by giving out the excess energy in the form of light like what we see here.

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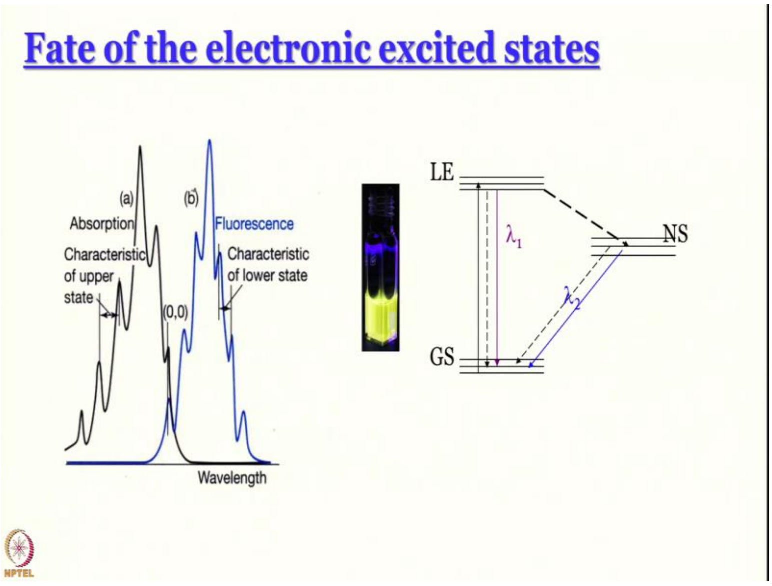

Fate of the electronic excited states

This is a sample that is prepared in our lab which is brightly photoluminescent, we are going to discuss what is the relationship of the fluorescence spectrum with the absorption spectrum. We already have learned that absorption spectrum is expected to have this structured vibronic kind of feature because of participation of higher vibrational levels. But other than giving out light the molecule can also get the excited, giving out the excess energy in the form in some other form.

So, it can just go into the surroundings and increase the entropy or there can be relaxation of some kind, the excited state can either be relaxed by interaction with the solids or sometimes it undergoes what I like to call a reaction in the excited state giving rise to what I like to call a nascent state from the locally excited state that is formed by Franck Condon vertical excitation.

So, these are things that we are going to discuss very, very briefly in this module. Hopefully, this is the last module of this part of the course. First, let us talk about light coming out of these molecules.

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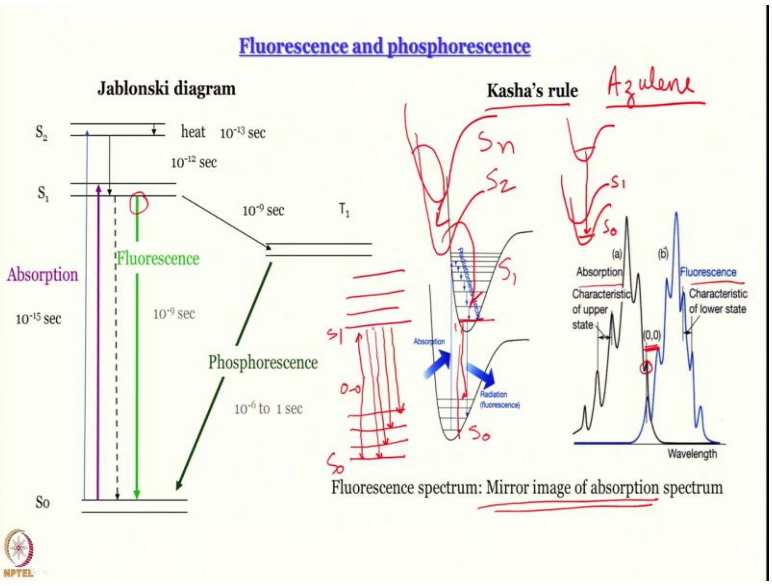

Fluorescence and phosphorescence

Jablonski diagram

Kasha's rule

Azulene

Fluorescence spectrum: Mirror image of absorption spectrum

This energy state diagram showing the transitions is usually called a Jablonski diagram named after the famous fluorescence spectroscopist Jablonski. We have discussed the absorption part already. What I have not said, well, what I have said but not said it in as many words is that this absorption takes place in very, very small timescale, here I have written 10^{-15} second, it is 10^{-18} second, that is why the inter nuclear rearrangement cannot take place during an electronic excitation.

Now, excitation can happen to S_1 or S_2 or some other higher singlet state. However, there is something called Kasha's rule that says that in a very small amount of time may be in picoseconds or so, no matter where you excite, if you excite to S_2 or S_3 or S_5 or you excite to a higher level, high vibrational level associated with S_1, the molecule relaxes to the zeroth vibrational level of the S_1 electronic state and that is where it stays for about a nanosecond or so, not one nanosecond in the order of nanoseconds.

So, if light is to be emitted, light can be emitted only from the zeroth vibrational level of S_1 that is Kasha's rule. Light cannot be emitted from S_2, S_2 to S_0 transition is not a radiative transition. Why? Because there is much faster alternative non-radiative relaxation processes that are available for S_2, we have talked about curve crossing in the previous module. So, these S_1, S_2, S_3 these curves usually cross, whereas usually there is a gap between S_0 and S_1. That is why the nonradiative deactivation from S_1 to S_0 is not all that efficient, usually.

And so, the radiative pathway gets a chance. So, what I am trying to say here is this, this is S_0, this is S_1, the higher ones Sn, S_1, S_2, S_3 so on and so forth are usually like this, it is not necessary that the equilibrium bond length would become smaller and smaller, it can be anything, but there is curve crossing. So, even if you excite here, it can come down very easily to S_2 and from S_2 to S_1 and emission takes place from v equal to 0, v equal to 0 of S_1 only. That is the expectation. That is why that is Kasha's rule.

Now see, the downward radiative transition originates here fine, but it can terminate in any of the vibrational levels of S_0. That is why you can have a fluorescence spectrum that looks like this. Once again, it has sort of vibronic structure. So, if you look at the upward and downward transitions, maybe I will draw it separately here. This is S_0, different vibration levels. This is S_1, different vibrational levels.

I just draw this $00^/$ upward transition, $00^/$ upward transition, downward transition begins from $0^/$, so it can come down all the way to 0. So then, this energy difference is the same as the band origin. Remember what is band origin, this $00^/$ energy gap is a band origin.

So, in this diagram, this $00^/$ this is the band origin. Where will the next transition be? It will start from $0^/$ and come to maybe v equal to 1 of S0. Next, we will start from $0^/$ come to v equal to 2 of S0, start from $0^/$ come to v equal to 3 of S_0. So, all these are progressively smaller energy gaps. That is why between absorption and emission, the only two bands that have the same energy are expected to be the $00^/$ or $0^/0$ bands.

The other bands of fluorescence for S_1 to S_0 transition, they occur at lower energies. And the Franck Condon factors are related, Franck Condon factors from 0 to $3^/$ or $0^/$ to 3, they are more or less the same. That is why the fluorescence spectrum is expected to be a mirror image of the absorption spectrum. This is called mirror image rule. Arising out of Kasha's rule, that downward transition originates in $0^/$ level of S_1.

There are exceptions to this rule. Well mirror image rule, we will see what exceptions are there. There is another very notable exception that is called Azulene anomaly. For azulene, what happens is this S_0 and S_1, these two energy levels have a crossover. So, S_1 is non emissive, S_2 is that a little higher energy.

So, the fluorescence originates in S_2, that is why for azulene it is not a mirror image rather the fluorescence spectrum of azulene occurs at a higher energy than the lowest energy transition, electronic transition in the absorption spectrum of azulene. This is called azulene anomaly.

In recent times, this explanation has been debated and other explanations have been provided. But still, this is explanation that is usually provided for azulene anomaly even now. But coming back to more regular situations, this is what one sees for things like sapidine or naphthalene, anthracene, these aromatic hydrocarbons, you get a mirror image spectrum.

Fortunately, it does not hold for many many molecules. Because if it did, then things would be very systematic, very easy and therefore absolutely boring. Fortunately, it does not always happen. Fortunately, post excitation many times excited state, the molecules undergo excited state processes.

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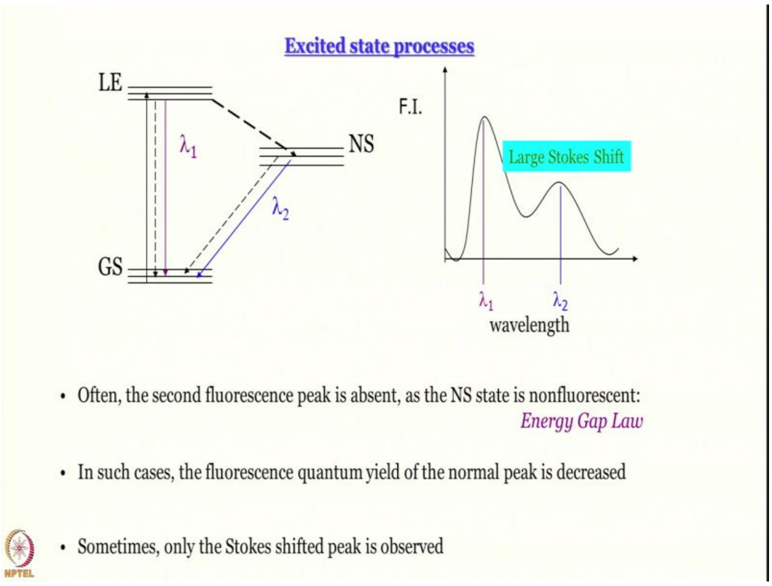

Excited state processes

- Often, the second fluorescence peak is absent, as the NS state is nonfluorescent: *Energy Gap Law*
- In such cases, the fluorescence quantum yield of the normal peak is decreased
- Sometimes, only the Stokes shifted peak is observed

We are going to discuss some of the excited state processes in the next few slides, but let us first talk about it in a general manner. Let us say something happens in the after promotion to local excited state. Remember the lifetime is about nanoseconds. The molecule has a little bit of time, nanosecond seems to be a very small time, but it is long enough for the excited state to perform some kind of reaction, there can be a turn or a proton can be liberated or a proton can be taken up, there can be stabilization of this locally excited state by solvation many things can happen.

And that leads to another state which I like to call the nascent state. It forms, from the locally excited state by the excited state phenomenon that is happening. So now see, if the energy gap corresponds to hc/λ_1, between downstate and locally excited state and if the energy gap associated with the nascent state corresponds to wavelength of λ_2, λ_2 is definitely longer than λ_1 because the energy gap for the nascent state is smaller than for the locally excited state.

So, the way it shows up in the fluorescence spectrum is a second emission band which is stokes shifted or redshifted. This is the signature of an excited state process taking place, it can also be a signature for an impurity being present that is a different ball game altogether we will not get into that today, let us say our sample is pure.

So then, if you get not a mirror image, but a big stokes shift, that means it is interesting something is happening. But then, it is not always necessary that you will see dual emission because many times the second fluorescence peak is absent. Because this energy gap as we said earlier between nascent state and ground state is smaller than that of local excited state and ground state.

So, there is something called energy gap law, which correlates the non-radiative rate constant to this energy gap. So, if the energy gap is smaller than the non-radiative rate constant is larger. So non-radiative processes are more favourable usually between the nascent state and the ground state, then between the locally excited state and the ground state. So, that is why very often the second fluorescence peak is not even there.

But then, if excited state process is operative, what happens is there is a population transfer from the locally excited state to the nascent state. So, since the population of the locally excited state is smaller, the intensity of fluorescence of this locally excited band is also smaller than expected, that is how it manifests itself.

And the other end of the spectrum is sometimes this excited state process is so very efficient, that you only see the stokes shifted peak, you do not even see the mirror image peak at all, all you see is one very large stokes shifted peak, all these different scenarios are possible.

That being said, let us think what are the different kinds of excited-state processes that can take place, we are going to discuss one in a little bit of detail. That is the phenomenon of photo acidity and photo basicity. And then we will talk about three others photoisomerization, photoinduced electron transfer, and what is conventionally discussed first intramolecular intersystem crossing. So, we will take them one by one.

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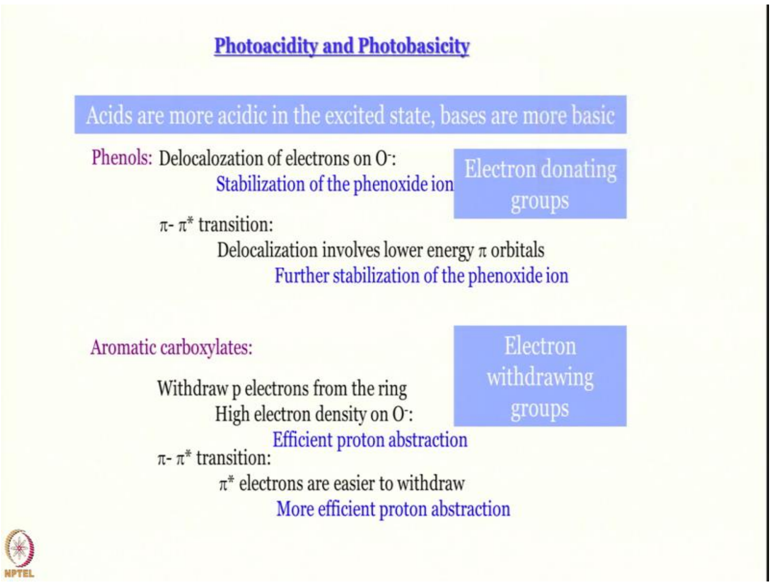

Photoacidity and Photobasicity

Acids are more acidic in the excited state, bases are more basic

Phenols: Delocalozation of electrons on O$^-$:
Stabilization of the phenoxide ion

Electron donating groups

π- π* transition:
Delocalization involves lower energy π orbitals
Further stabilization of the phenoxide ion

Aromatic carboxylates:

Electron withdrawing groups

Withdraw p electrons from the ring
High electron density on O$^-$:
Efficient proton abstraction
π- π* transition:
π* electrons are easier to withdraw
More efficient proton abstraction

The first excited state process that we want to talk about is photo acidity. Now here, this is a line that I love telling students, acids are more acidic in the excited state, bases and more basic, by acid and base I do not mean sodium hydroxide and HCl in reverse order. I mean organic acids, aromatic acids, they have something like phenols, phenols as we know are acidic.

Why are they acidic? Because as you know, phenoxide ions are stabilized. Now generally, we talk about stabilization by resonance. But now that we have learned molecular orbital theory, we will try to explain this in terms of molecular orbitals themselves. By using MO’s, we can explain that this delocalization of electrons on O$^-$ still takes place. And phenoxide ions is still stabilized, how?

If we think of the π MO’s of benzene, we have had a small introduction to it already. We know that there are three bonding MO’s that are fully filled, and three antibonding MO’s that are unfilled. Many times, we feel that these antibonding MO’s are useless or they are bad, because they are the name anti in it. They have an important role to play in chemistry.

What happens is, if you think of phenol, in phenol, or phenoxide ion rather we have an oxygen atom attached to one of the carbons, and there are some electron cloud on the oxygen. So, if the electron cloud is to be accommodated on the ring, it has to be accommodated in some MO, and that MO would better be vacant. What are the MO’s that are vacant? The antibonding orbitals.

So, these are the ones that are utilized for accommodating the incoming electron cloud from oxygen atom in phenoxide ion, and that is why it is stabilized, that is why phenol is acidic. But I am saying it is more acidic in the excited state. Why is that so? Because you see, if you promote an electron, if there is a pi-pi star transition, then an electron goes from one of these MO’s to up here, let us say this electron is promoted to this MO.

What do I have now? I have a vacancy in this lower-lying, molecular orbital, bonding molecular orbital. So, an incoming electron cloud from oxygen does not have to go here anymore. It can happily reside in the lower energy bonding molecular orbital(MO). That is why, since it is more energetically favorable, the excited state is more acidic.

Similarly, one can explain why aromatic carboxylates are more basic in the excited state. Because these pi star electrons are easier to withdraw, so they can extract the protons more efficiently. This is a phenomenon. Now, there is no reason why you should believe me unless I show you some proof. Let me show you some spectra that demonstrate photo acidity.

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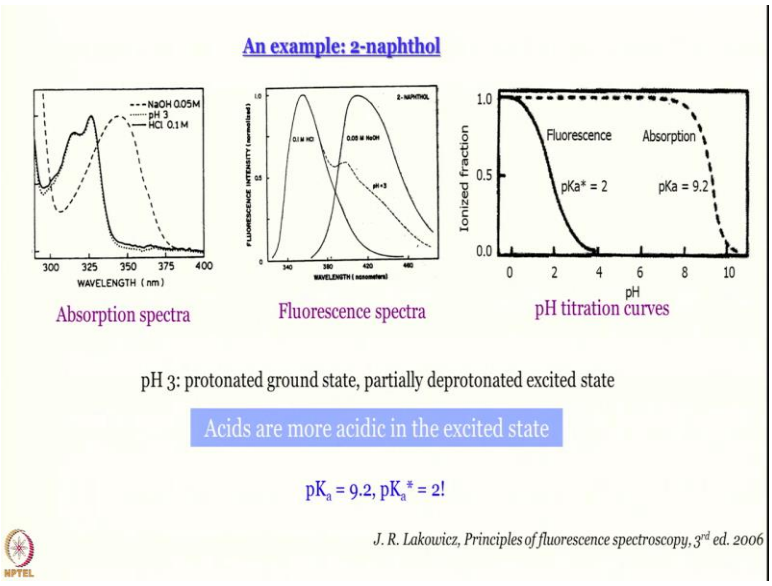

An example: 2-naphthol

Absorption spectra

Fluorescence spectra

pH titration curves

pH 3: protonated ground state, partially deprotonated excited state

Acids are more acidic in the excited state

$pK_a = 9.2, pK_a^* = 2!$

J. R. Lakowicz, Principles of fluorescence spectroscopy, 3rd ed. 2006

And the spectra that we are going to see are of very well-known beta-naphthol. Hopefully, many of you are going to do experiments with beta-naphthol in organic chemistry lab and get your finger stained, same beta-naphthol. See these are the absorption spectra, beta-naphthol at different pH. So, this black line here is the absorption spectrum in the presence of 0.1 molar HCl, very strongly acidic, there is no way beta-naphthol can dissociate at that kind of pH.

So, this blue-shifted spectrum in black, this is the absorption of the naphthol. At pH 3, you hardly even see the spectrum that is drawn in dotted lines, because it is exactly superimposable. What does that say? It says that at pH 3, beta-naphthol exists as beta-naphthol there is no naphtholate.

However, in presence of 0.05 molar NaOH, very strongly alkaline solution, the proton is abstracted. And now, you see this spectrum looks very different. It is redshifted and it is structureless, structureless. This is the characteristic absorption spectrum of the naphtholate ion. What do we learn from here? In the presence of 0.05 molar NaOH, we have naphtholate and no naphthol.

At pH 3, we have naphthol and no naphtholate. If you look at the fluorescence spectrum, let is go in reverse order. Please see the spectrum in presence of 0.05 molar NaOH, it is a redshift spectrum, it is a 420-nanometer strong redshift because the naphtholate ion is stabilized in the polar solvent in solution.

In 0.1 molar HCl the emission band is at say 350-360 nanometer, it is still redshifted compared to the absorption spectrum, but not so much. So, what we see is that this is the characteristic absorption emission spectrum of beta-naphthol. This one in presence of 0.05 molar NaOH is the characteristic emission band of naphtholate.

What happens at pH 3? In the blue end of the spectrum, higher energy end of the spectrum, short-wavelength range of the spectrum it is superimposable, these are all normalized spectra of course, it is superimposable with the spectrum in presence of 0.1 molar HCl, so beta-naphthol. However, if you go to the red end, the longer wavelength regime, you see there is a shoulder and this shoulder matches the emission spectrum characteristic of naphtholate.

What does this mean? It means that at pH 3 in ground state, there is no anion. However, in excited state anion is there to some extent. So, at pH 3 after excitation, beta-naphthol dissociates to some extent and gives up proton. What is this? This is a demonstration of photo acidity. To understand how profound this effect is, let us have a look at the pH titration curves using absorption and fluorescence spectra.

This is the titration curve using absorption spectrum and you obtain a pKa of 9.2. This is the titration curve using fluorescence spectrum and here you obtain a pKa value in the excited state is called pKa^* of 2. The shift of pKa from 9.2 to 2 is humongous because pH of 9.2

means 10^{-9} molar proton. So, beta-naphthol can give out a proton, only at that low hydrogen ion concentration.

In the excited state however, it can give up a proton even when hydrogen ion concentration is as high as almost 10^{-2}, 10^{-3}, 6-7 orders of magnitude of difference of proton hydrogen ion concentration that is huge, that is how profound the effect of photo acidity can be, it is not a trivial phenomenon.

In fact, it is utilized in many processes to bring about pH jump and it has been utilized in an experiment that was described in a paper that got published in science, two papers actually, 2003 and 2006 by the group of Professor Erik Nibbering from Berlin, where they had established the mechanism of acid-base reaction, a mechanism that we have all learned that cannot be figured out, even that is now illustrated by using a photoacid and using ultrafast lasers. Next, let us quickly talk about three more processes, photoisomerization.

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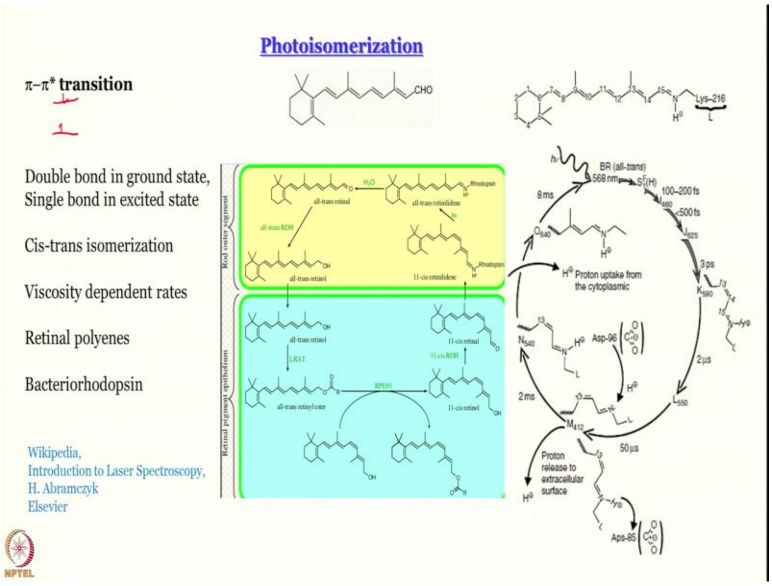

Photoisomerization

π–π* transition

Double bond in ground state,
Single bond in excited state

Cis-trans isomerization

Viscosity dependent rates

Retinal polyenes

Bacteriorhodopsin

Wikipedia,
Introduction to Laser Spectroscopy,
H. Abramczyk
Elsevier

We have talked about π-π^* transition already. When we do a π-π^* transition, what happens this is let us say the pi MO, this is the π^* MO. To start with we have two electrons here. After excitation, I have one electron here one electron here, what is the pi bond order. In the excited state pi bond order is 0, which means what was the double bond in ground state has become a single bond in the excited state.

So, now, as we know, in ground state, we cannot have cis to trans isomerization taking place because it is a double bond is not going to break so easily. However, in the excited state the second bond is gone. Now, cis to trans photoisomerization can take place. This phenomenon is called photoisomerization.

Since we are having rotation of two molecular segments with respect to each other, and many times that we are going to see some structures, these fragments are quite bulky, the rates of photoisomerization which can be determined from fluorescence spectra and time evolution of fluorescence intensities, these rates are usually very strongly dependent on viscosity. So, they can be used to find out for example, what is the viscosity in inside a cell or in the region of a membrane or in a very small volume that you cannot access by anything other than a fluorescent molecule.

And if you think that it is something esoteric, that takes place only in a lab, well think again. Because photoisomerization is something that is going on within me within you within all animals that have eyes all the time. Because retinal polyenes, molecules like these play a very important role in the process of vision of animals, animals with eyes, of course. As you see, this is taken from Wikipedia.

So, for a little sketchy idea, one can refer to Wikipedia. But actually, these profound decades of research has gone into establishing this. Here, you can see the photoisomerization process taking place in the rod. And there is some chemical reaction that causes the cis to trans photoisomerization in another region. And this is the cycle that generates the impulse which allows us to see. Photoisomerization is an important process in our vision.

In bacteria, things that do not have eyes, they are also photoisomerization has a very important role to play. There instead of retinal polyene, most important kind of molecules is bacteriorhodopsin. So, let us see both are polyenes, so pi-pi star transition can take place. So, what happens in bacteriorhodopsin is that first of all, there is a proton uptake from the cytoplasm. Cytoplasm means inside the cell.

Then in presence of light, and you can see what wavelength of light, 568 nanometer. Very fast processes get initiated 100 to 200 femtosecond, less than 5 picosecond. So, different forms are there. Finally you start from trans or trans bacteriorhodopsin, you get a cis form.

And then there is some longer process that takes place over microsecond, some chemistry happens, there is a participation of some enzyme here and that causes a release of the proton to the extracellular surface and then the original all-trans bacteriorhodopsin that is regenerated. So, what does it do? It initiates a proton pump. This plays a very important role in maintaining pH inside cells.

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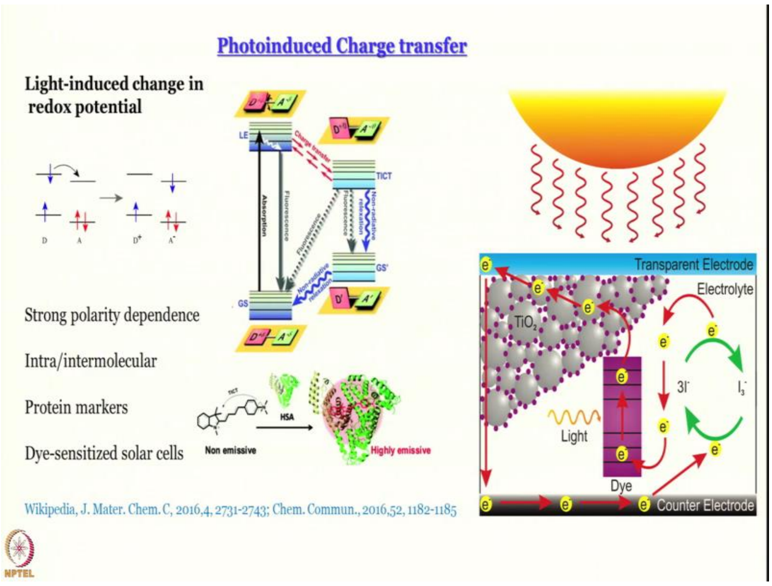

Photoinduced Charge transfer

Light-induced change in redox potential

Strong polarity dependence

Intra/intermolecular

Protein markers

Dye-sensitized solar cells

Wikipedia, J. Mater. Chem. C, 2016,4, 2731-2743; Chem. Commun., 2016,52, 1182-1185

Next, we talk about photoinduced charge transfer, it is photoinduced electron transfer. We have talked about sort of proton transfer earlier in case of photo acidity. This is the other process photoinduced electron transfer. And I ask you to have a look at this here, we are going to use references that are as recent as 2016 in the next slide, we have more recent references.

So, what happens is in excited state the redox potential can be different from the ground state. Let us say we had this donor and acceptor, we had encountered donors and acceptor in case of absorption spectroscopy as well, there was a vacant orbital of the acceptor near a field orbital of the donor, that is how charge transfer took place during absorption and we got the charge transfer band, here it is a little different.

The orbital that is a little lower energy then the filled orbital of donor, that orbital of acceptor is also filled. So, you cannot have an electron transfer from donor(D) to acceptor(A) in the ground state. However, upon promotion of electron to a higher molecular orbital or by promotion of the molecule, donor molecule to higher electronic state, the electron can find a little lower-lying vacant molecular orbital in the acceptor to which it can get transformed.

So effectively, redox potential can be affected by irradiation of light. And when this gets transferred, you have this D becomes D^+ because now it is electron deficient, A becomes A^- because it is electron excess. This is charge transfer post excitation, photoinduced charge transfer, or photoinduced electron transfer. What we are doing here is we are creating a polar or partially ionized at least species.

So, this process is strongly polarity-dependent. It can be intramolecular, can be intramolecular, it can be intermolecular also, like absorption. And we will see examples of both. This is an example of a schematic of intramolecular photoinduced charged transfer, where you have a donor and acceptor coupled together.

This model that is shown here you see there is a T before ICT (TICT), the T is for twist, because the model is that you have donor and acceptor that are coplanar, so electronically couple post electron transfer, they become there is a twist, the planes are at 90 degrees, so they become electronically decoupled. So, the electron cannot go back so easily, back electron transfer is suppressed.

This model is very, very strongly contested, though. But what we know for sure is that for molecules like this charge transfer takes place very strongly. And we here have a lower energy excited state, which if it emits, emits in the red, many times it does not emit. These kinds of molecules, where you have intramolecular charge transfer are very often used to sense polarity.

Because in highly polar solvents, you are going to see TICT emission or you are going to see suppression of fluorescence. In media of lower polarity, this TICT state is not going to be favoured. And you can hope to see fluorescence from the locally excited state which will be blue shifted and much stronger. So, this is used to sense proteins.

This here is an example from 2016 of a molecule that undergoes TICT, you can see there is a donor unit here, this n atom is here, that is the donor unit and this is the acceptor unit, there is n^+ when it binds to protein, then it becomes strongly emissive and this emission is because the TICT is suppressed and the emission takes place from locally excited state. There are classes of molecules that more or less, exhibit this phenomenon.

An intermolecular charge transfer is seen in green leaves in photosynthesis and it is emulated in what are called dye-sensitized solar cells. What you can do is you can use sunlight to bring about charge transfer from a dye-molecule to an acceptor, the most commonly used acceptor in this model which is called Grätzel solar cells, named after Grätzel who designed them.

The most commonly used acceptor is TiO2 molecules, TiO2 nanoparticles. So, a suitable dye is excited by sunlight and this dye performs photoinduced charge transfer to TiO2. So, what you have is charge separation. The moment the electron goes to TiO2 it is gone. The dye cannot get it back so easily hopefully.

And now, you can hope to put in electrodes on two sides on one side you need a transparent electrode that is usually obtained by using indium tin oxide ITO. The other side you can use a regular metallic electrode, on this side we have sunlight and then you have charge separation and you can use it as a cell.

Nowadays one can buy kits and make your own dye-sensitized solar cells. Why is it that dye-sensitized solar cells are not so common, why is it that we still use silicon cells? There are issues the biggest issue being stability of the dye, but this is a technology that has kind of the imagination of scientists for about 20 years and it is still going strong. The last example is the one that usually people discuss first and that is of intersystem crossing.

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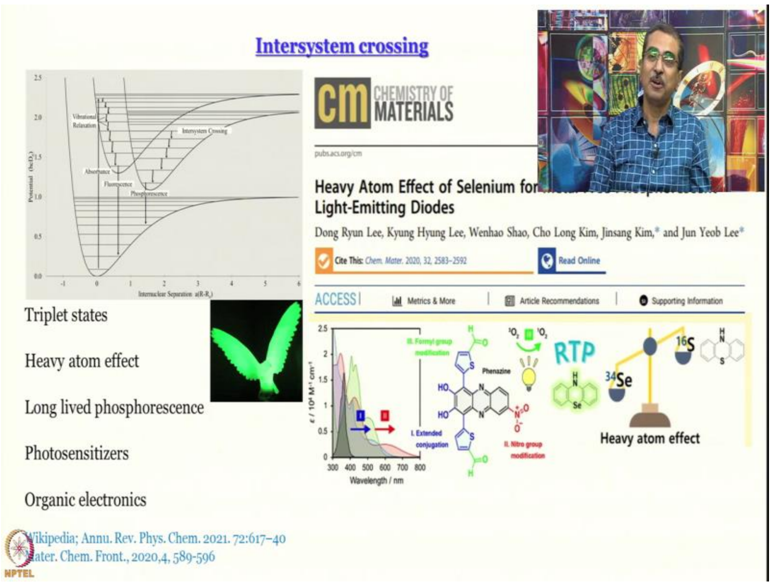

Intersystem crossing

Triplet states

Heavy atom effect

Long lived phosphorescence

Photosensitizers

Organic electronics

Heavy Atom Effect of Selenium for

Light-Emitting Diodes

Dong Ryun Lee, Kyung Hyung Lee, Wenhao Shao, Cho Long Kim, Jinsang Kim,* and Jun Yeob Lee*

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Wikipedia; Annu. Rev. Phys. Chem. 2021. 72:617–40

Mater. Chem. Front., 2020,4, 589-596

Excite to S_1 state, very often it can go over to the triplet state. Remember, T_1 state is lower in energy than singlet state. So, this process is called intersystem crossing, it leads to the population of triplet states as we know by now, singlet to triplet transition is not allowed it has been forbidden, but this via S_1 route can populate the triplet state.

Even higher triplet states can be populated if the energetics are suitable and if you perform an excitation to even higher singlet states. This intersystem crossing is promoted if you have some heavy atom. We will not go into the reason why. This also comes from perturbation theory. What happens is this triplet states are much longer lived, singlet states as we said have lifetime of nanosecond, triplet states have lifetimes of microseconds and milliseconds, sometimes seconds, sometimes even hours.

That is demonstrated in your glow in the dark toys like this. Everybody has seen those I hope, you have a toy when lights are on you do not really think it is any special. But when you turn off the light the toy starts glowing. Why? Because it contains a phosphorescence material which is really really long lived. So, it can glow for a few hours. But phosphorescence is not just useful or rather, triplet states are not just useful for making toys. It can also be used for making medicines.

And here I asked you to look at what we are looking at the references, the references are from 2020 and 2021. So, here this is an example of a molecule which undergoes facile crossover to the triplet state. And then what it can do is oxygen, if you remember from your class 11 12, oxygen has a triplet ground state. So, it can photosensitize oxygen and produce excited state oxygen, which is singlet.

So, singlet oxygen is called reactive oxygen species, very strongly reactive it wants to kill anything, react with anything that is around. You might have heard that people want to have antioxidants in their diet, that is to take care of this reactive oxygen species so that they do not kill your cells in the skin and you look younger. So, here what is done is that intentionally singlet oxygen is produced by photosensitization, taking help of a dye that undergoes efficient intersystem crossing to the triplet state.

So, the singlet oxygen that is produced can kill, so suppose you do it inside a cell, this can be useful in killing the cell. Why would you want to kill a cell? You want to kill a cell if it is associated with the disease, cancer for example. This photosensitization is utilized in what is called anti-cancer photodynamic therapy, where you use this kind of molecules to produce singlet oxygen and selectively kill tumour tissues and not healthy tissues.

There is a limited success in this modality but, again, there is something in the works. And it is not only medicine, this photosensitization is useful in devices as well. Organic Electronics is the order of the day, that is why these papers are published in 2020 and 2021. Here is an example of a paper that got published only last year, where we have a molecule, where due to heavy atom effect, so what they have compared is similar molecule one with sulphur, one with selenium.

Since selenium is heavier, there is stronger intersystem crossing and from there one can get room-temperature phosphorescence. What is the benefit of room temperature phosphorescence? If you now make a light-emitting diode out of it, you have got a diode which does not have inorganic materials, it is made completely of organic material. That is the promise in organic electronics.

We have discussed some excited state phenomena, we have got a very sketchy idea of what happens, what is the fate of the excited states, this part of the discussion is complete. And that brings us to the end of my part of this course.

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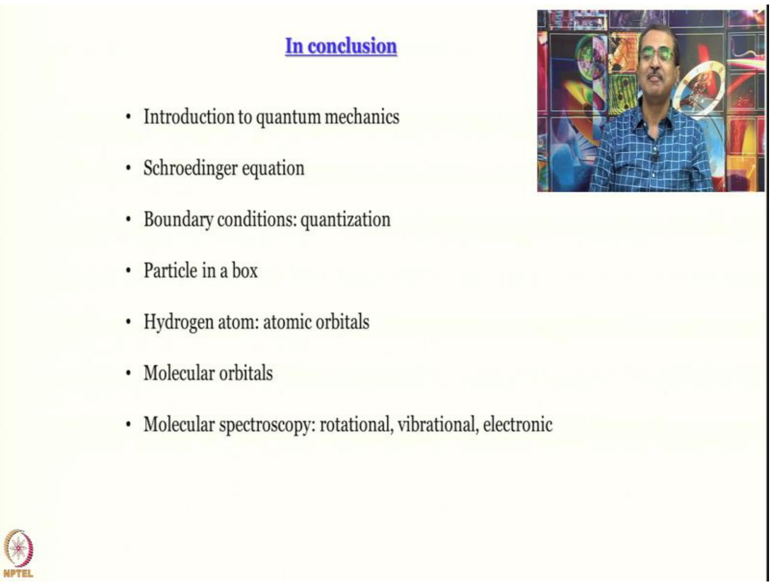

In conclusion

- Introduction to quantum mechanics
- Schroedinger equation
- Boundary conditions: quantization
- Particle in a box
- Hydrogen atom: atomic orbitals
- Molecular orbitals
- Molecular spectroscopy: rotational, vibrational, electronic

To conclude, we have been introduced to quantum mechanics and we advise that we have not even seen the tip of the iceberg in this course, we have learned Schrödinger equation, we have learned how quantization comes in as a result of imposition of boundary conditions, we have taken examples of particle in a box, from hydrogen atom, we have learned about atomic orbitals.

And for the rest of our lives, we will never say that orbitals are regions of space where probability of finding the electron is maximum, we will say an orbital is an acceptable one-electron wave function of an atom. Similarly, we know what molecular orbitals are. Finally, we have talked about quantum mechanics in action. We have talked about rotational, vibrational, electronic spectroscopy, once again, not even the tip of the iceberg.

I hope that this discussion will enthuse many of you to study these topics, and perhaps utilize them in future. For the rest of the course, my colleagues are going to take up from here and introduce you to the fascinating world of organic and inorganic chemistry, that is an ancient field of science but is ever-evolving, always new field as well.

And as you learn, and I hope as you have got some hint here as well, is that there is no boundary. Even if you are an electrical engineer or I dare say even computer engineer, you can take lessons from chemistry, you can do something new in the field of chemistry. With this background, and with the background that you are going to generate in your field of study.

Research today is interdisciplinary; industry today is interdisciplinary. So, with that message, I bid you, goodbye. Thank you very much, thanks to all the NPTEL staff who have helped very patiently in recording these lectures. And let me wish you all the best not only for this course, not only for your college study but for whatever it is that you do for the rest of your life. Goodbye.