Introduction to Research Prof. Prathap Haridoss Prof. B. Viswanathan Department of Metallurgical & Materials Engineering Department of Chemistry Indian Institute of Technology, Madras

Lecture – 44 Research in Chemistry

Prof. Prathap Haridoss: Hello, it is our pleasure to have with us Prof. B. Viswanathan. He is professor emeritus here in IIT, Madras. He was a faculty here at IIT, Madras for almost 35 years, which is a very long time. Much more than you know the age of most post graduate students. He is the author of numerous books. He is considered very important expert, very well accomplished expert in the areas of catalysis and energy amongst other areas in chemistry. He has contributed in many many ways to the development of science in our country. He serves many important committees which make key decisions on you know what projects should be funded and so on.

He has also served in the United Nations development program committee for looking at funding activities in the area of catalysis and so he is both a national as well as an internationally accepted expert. His areas of research include electro chemistry and catalysis so that covers areas such as fuel cells batteries and hydrogen storage, just to name of few and over 35 years. Numerous students have completed MS and PhD under the guidance of Prof. B. Viswanathan and they hold fairly important positions in many industries, many national organizations and so on. So, it is really our privilege pleasure to have Prof. Viswanathan with us and I am sure the views that he has, that he is going to share with us on research in chemistry would definitely be very beneficial for all of us. So, thank you sir for joining us.

Prof. B. Viswanathan: Thank you.

Prof. Prathap Haridoss: So I would like to start by asking you this, like in engineering, I am sure even in chemistry which has been around for as a recognized field of science for a very long time. Are they still areas that are considered you know old traditional an areas of research in chemistry?

Prof. B. Viswanathan: Yes. There are two areas of chemistry which are old, but still it has a relevance to even today, one of them is synthesis organic chemistry, this synthesis has always associated with organic chemistry, but today it is no longer synthesis in organic chemistry, synthesis of chemicals. Okay therefore, the inorganic chemicals or even industrial chemicals, how they can be economically synthesize and they also produced that is the reason. Second thing is science itself, today has changed its phase. Science in the conventional way we were looking at the basic problems. Today the science has to be delivering materials, material means, for example you take a cell phone it is a material called Glylite resonators, this is simple material pervoskite. Therefore, this type of materials have to be designed and fabricated with a very specific properties, dielectric constant has to be specific value. The temperature coefficient of dielectric constant has to be very very low like that.

This is one of the examples, there are many, many materials even for example, you take through solar cells, solar cells today is based upon silicon solar cells, but silicon being a very important material and also costly. So, the design of new solar materials is coming, silver based solar cells and such things are cheaper than this. In the manufacturing process, cost process silver may be costlier than that, but in the solar cell manufacturing thing it can be cheaper than the silicon solar cells. So, therefore, any any area if you take today chemistry is I will say energy materials and environment. These are the three main areas which are evolving in chemistry, but it does'nt mean that this customer area of synthetic organic chemistry or synthetic inorganic chemistry, they are also still important

For example, in synthetic inorganic chemistry, metal organic frame works which is just like a palace, but only thing is it is a palace in chemicals not a brick and mortal. So, this type of metal organic frame works mesoporous materials, they are all the new generation materials, they have a very great advantages and also utility they can be used in the many industries. For example, today if you take the oil industry it is, if even though oil is the main product and their refined oil is the main product, the conversions are taking place only because of these materials. Previously these zeolites were used now mesoporous solids and this MOFs and (Refer Time: 05:17) they are essentially porous solids are being used. Though why we are using this is if now refining is based upon bottom of the barer, we are not taking the crude which is on the top of the layer because it is when you go to the bottom, the hydro carbons are long thin hydro carbons, therefore they have to be cracked. Previously it was not so long a chain, but previously also long chain, but 30-40 carbon atoms, now 100-200 carbon atoms.

Therefore, the cracking or refining, refining means making the crude oil into those whole products. So, this is requires porous solids of very high porosity, very high poor diameters and their things. These solids have to be fashioned, designed and fabricated. So this is the new generation. In the same way energy conversion and energy storage, these are the two new areas, I will not say new area but newly finding acceptance. Now, the storage is a very important thing, energy conversion is may be possible in where the chemistry, but the storage is a very important problem. The storage must be in such a way that the economy must be equal to the petroleum crude oil or petroleum price. We will simply take fuel price.

Now, if it is not only fuel price, but fuel for example, if you will take a car it takes 5 to 100 liters of petrol. Therefore, if you are storing the fuel, we should store equivalent to that, so that you will be able to travel 500 kilometers or 600 kilometers at a stretch, instead of the intermediates storage. So, this is a main area of research today in materials for energy storage. In chemistry and physics, these are the two immediate areas. The third thing is in designing this solids or materials we have to now functionalize them, the functionalize say is for example, if you take a solid, there are 10 to power the of 15 sides, out of which only 10 to the power of 12 or 10 to the power of 10 sites will be active of all them; how to make those 10 to the power of 10 as active sites, and how to keep them in the active state. This is a very, very important thing because chemists are always using the molar quantities, molar quantities means 10 to the of 23 molecules.

So, therefore, we can easily analyze them whereas, when you have to analyze 10 to the power of 12 or 10 to the 15, your molar concentrations becomes a nano molar, pico molar or even lower than that. So, the analysis and identification and its structure and all those things are very important area. So this is another important area of research in chemistry, I will say general science. The another development that has happened in the last 10 years is how to predict them? How to apriority you have to design a material or you have to say this is the material has to be designed. So, this is called today is a

theoretical chemistry by you can say computational chemistry whichever way you want modelling chemistry whichever way you want to do that, but computation in chemistry today as taken here a new term which is the called the density functional theory.

Density functional theory takes from the basis okay. For example, why hydrogen is present as h2, that is because of the one s electron of one hydrogen combines with another one s electron of another hydrogen making a covalent bond. Therefore, we will know, now hydrogen cannot exist in the normal conditions as hydrogen atom, but it can exists only hydrogen molecule because the energy of the hydrogen molecule is lower than that of the energy of the hydrogen atom. So, the same way we can now make this thing for materials.

In the olden days the number of atoms in a molecule was very small may be 10-20, may be 100 let us assume, but today for example, you have metal organic frame work there will be thousands of atoms. So, therefore, we have to minimize the energy and predict them. So, this is done by density functional theory or self consistent fuel theory or calculations, but the recent times density functional theory has over run all these other things because of the time involved in the computation and also comprehension by the chemists.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: Because (Refer Time: 10:19) or self-consistent theory requires a tremendous mathematics. This density functional theory is only grass, but there are other approximations, but if this is the highest approximation that is possible today. So, this theory has taken over the thing and many chemistry laboratories are now facing the problem of how to apply these to their materials. So therefore, what has happened here is, in the chemistry if the research has taken a new turn. It is not enough if you are very good synthetic chemists, if it is not enough you can to make use of the tools to analyze them, but you should also be able to predict them.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: So this is that changing situation in chemistry research today.

Prof. Prathap Haridoss: Ok so that's a very I think a lot of detail you have told us about, both I think traditional areas of research and where you know research is heading in chemistry these days. If I go back a little and let say look at the set of students who probably join a chemistry department for an MS degree or a PhD degree and so on, and you have interacted with a lot of them. They come from a variety of different institutions where they would have done, you know bachelors degree, BSc, Bachelor of Science degree, maybe in chemistry and so on and then before they join here for a masters degree or a PhD degree.

So, in general, in their preparation as they come in do you see that there are any specific significant challenges that these students faced when they try to join? I mean when they get into a masters or a PhD degree, are there certain areas that may be their preparations in generals tends to be a little less for which I mean after they joined their required to pick up more maybe more courses or have some more preparation in those areas? Is there some lacuna in terms of you know either theoretical learning that they have or experimental experience that they have in what you have seen?

Prof. B. Viswanathan: Yeah. That is necessary thing especially in the Indian context because as I told you, analysis has to be at the atomic level today. Previously analysis is on the milli molar or micro molar now it is not. We have single atoms have to be identified, so these types of techniques that are available today for example, XPS or UPS or any other technique, we will not go into all the details that is any the analysis must be the probing system also atomic level, the probed system also at atomic level. Therefore, this means this knowledge is not available in Indian universities.

So, therefore, the students who come for research, but they have to use them because if they have to be competitive in research today and publish in very high impact journals or impact is not a correct thing, in high journals then they have to be using these techniques. There is no other way out that. In the same way as I told you theory also is about lacuna here because computing facilities in many universities are not so high. So, they might not have learnt these things. Even if they have learnt they may not be able to use them in the actual sense because the programming is a bugback of many of us because we are not professional programming people.

Now, what has happened is the second thing, that is I would not say the students have become, are they a past students are very brilliant, the present students are not brilliant and this. That is not the criterion, the criterion here is today the diversions for the student is very high compare to the diversion that you and I had, that is why the student is when their attention is diverted then they are not able to concentrate.

Prof. Prathap Haridoss: Attention spans are less.

Prof. B. Viswanathan: Yes.

Prof. Prathap Haridoss: These days relatively generally speaking.

Prof. B. Viswanathan: That is what is reflecting.

Prof. B. Viswanathan: Now the students are little behind, but otherwise the capacity of the students remains the same.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: Only thing is, they have because today the computer is there and things, they can use computer for learning instead of that they are using it for playing.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: It is one of them, but in chemistry computing usage is only to the limited extent, that is should be improved.

Prof. Prathap Haridoss: So, generally the people have not been using it as much in the computational sense.

Prof. B. Viswanathan: That is one thing; second thing is even such as a search tool. They can use only Google and all those things. That is not enough now because their literature is so high, because even if I were to tell you, I have been recently writing a book on carbon dioxide to fuels in chemicals because we know very well fuels and chemicals can be used to produce carbon dioxide.

Prof. Prathap Haridoss: Reverse process.

Prof. B. Viswanathan: Reverse process, so that means, we are closing the cycle. This literature in the last 10 years is enormous.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: Ok That is how to convert even though we have not succeeded, still succeeded means in the manufacturing level, but we are succeeded level in converting few molecules.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: Few molecules are CO2 into chemicals useful chemicals, but this knowledge must be known to them, then only they will be able take up the challenge and do them. This is only one example, another example is as you have already said is fuel cells. In the case of the fuel cells, the problem does not exist is the electrode; the problem exist is the electrode at that the oxygen reduction, not on the fuel combustion. Therefore, the designing proper oxygen reduction electrode is the question here. Up to now we have been using only platinum based electrodes, but now we can use many other materials one of them is hetero atom nitrogen pass plus sulphur boron substituted carbon materials can be easily used for the oxygen reduction reaction.

It can be comparable, not exceeding the platinum, but it is already comparable with platinum today with respect to time it will be improved, then it will be cheaper electrode and it will become a reality. Second thing as I told you before, the storage; storage also is

a very big issue. For example, super capacitors instead of batteries because battery is weighty substance. So, super capacitor, super capacitor also is a possible means of energy conversion divisor, but only thing is the materials in question.

Now, in the material that we are now using is carbon materials are carbon based materials. We will not go into the details of it, so that we have to innovatively bring out as I told you carbon materials with this is hetero atoms and also structurally they should be made more stabled. A carbon materials are layered materials may be layered materials are possible to use a super capacitors, but chalcogenides, dichalcogenides sulphur containing or phosphorous containing all these things will be in the future will be new super capacitors like that we can go on taking about it in the materials in the catalysis or any field. Therefore, what today is the student research, students should be able to focus on these new materials and since they have been conventionally thought they are not able to think the new materials sense.

Prof. Prathap Haridoss: Ok So, lot more reading up is required to catch up on materials that are more recently being looked at and picked up.

Prof. B. Viswanathan: Yes.

Prof. Prathap Haridoss: Okay So, of course, you already mentioned a lot of examples of where you know, may be there is a direct industry application and certainly you know petroleum industries, one that you were taking about. Generally in MS and PhD degrees, we tend to think of research which is, you know significantly ahead of it is time. So, in this context from MS, PhD kind of research activity that takes place are there where do you see industry interest in this kind of you know in a research program kind of activity.

Prof. B. Viswanathan: Okay in industry, since our center is dealing with refining industry. As I told you, we are today refining industry because refining industry is the major industry in India. Nearly 15 refineries are there and all those things. The refining capacity even though increased, the refining material the crude oil is the bottom of the barer. Therefore, the conversion to useful chemicals is a big problem. Not only useful chemicals even the waste chemicals that come out ok for example, that tar or something

other it is not waste, but it is not a high prized commodity, they can used properly if they can. So, all these involve some kind of a refining process.

The refining process means having a crude oil converting them to the size of the molecule that you want and value added molecules. So, this is called can be isomerization, it can be calculation, it can be addition or whatever chemical reaction that we have studied in general organic chemistry, but it has to be done with this molecules which is a very big molecules.

So, therefore, the industry today insists on this. The same way drug, there drug molecules now you drug molecules for example, you have take a hypertension molecular are something like that as a boots synthesis or whatever it is it all requires 5 to 6 steps. These things can be today with these type of materials, porous materials we can make them in single step.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: EBu propene can be synthesized from basic molecule single in step.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: Today it is produced by 5 steps or 6 steps. So, the cost will come down, cost only is not the criterion the drugs will be easily available.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: Therefore, essentially what it means is that, we have to reorient our research; we cannot succeed in one day. Boot synthesis is known for decades now one, if I were to introduced it in one step everybody will laugh at me, but it is possible. Okay But to economically produce it has to be done. So, like this many things can be done. Okay Prof. Prathap Haridoss: Yes. So, these are the areas that you feel that you know industry itself is directly interested in, a research program that is ongoing.

Prof. B. Viswanathan: Yes.

Prof. Prathap Haridoss: And also, similarly if we had research programs in those areas more industry interaction is likely. So, if you look at the students that graduate, I mean let's say masters and PhD students when they graduate, what sort of positions do you see them getting in industry or any other circumstances?

Prof. B. Viswanathan: OK.

Prof. Prathap Haridoss: Of course, in general in general.

Prof. B. Viswanathan: Our center has a peculiar place, but chemistry in general they find the opportunities in chemical industries especially pharmaceutical industries, if he is an organic chemist. He he is a material chemist means a material development, but today India is in a favorable position because all multi nationals have got their head quarters or semi head quarters in India. So, that for example, the shell or Sabey or any anything GM GE or whatever thing even the VPNG they are all here in India and therefore, they have opportunities there are many more. Previously this type of opportunity was not available for India.

Prof. Prathap Haridoss: Indians.

Prof. B. Viswanathan: India, they have to only look for the research positions abroad or employment abroad.

Prof. Prathap Haridoss: In abroad.

Prof. B. Viswanathan: Yeah. Today equivalent employments are possible in India. So, that is not a problem in other as a matter, but chemists I do not see any problem in the next 20-30 years.

Prof. Prathap Haridoss: Okay that's a very heartening piece of information for that thing lot a students who are in chemistry.

Prof. B. Viswanathan: Yeah. If they have that in a necessary inspiration they can easily fit into any of these things.

Prof. Prathap Haridoss: Okay let's say on a more mundane note, how often do you feel I mean when students come and you now get it to a masters or a PhD program, one of the things they are often told that you know classroom learning is one, but you know interacting with peers, interacting with your adviser, interacting with your guide, these are things that actually contribute a lot to their learning process. So, in your experience what would you recommend as you know how often student should be meeting their guides or how that process should go?

Prof. B. Viswanathan: Okay This is one of the main issues of Indian education itself. I am sorry to tell this, but it is a fact for example, if you our learning in class room, teacher or the professor will come and give lectures and he may not be having time to establish that crossed their barrier of that, it reached to a lecturer to the student. This is the students, also is inhibited to ask questions are raise doubts. So, this is a very big ballot

So, what I suggest is instead of giving lectures and courses, courses should be interactive, more interactive as a matter about questions can be on both sides. The teacher also can ask questions instead of delivering the lecture. See previously what was bothering and lecturing process is covering the syllabus. Now covering the syllabus is not at all the criterion okay. How you have comprehended this syllabus is the question because that is what you are going to make use of in your career. Therefore, the classroom means in your lecturer hour of 60 minutes, there should be 60 questions across.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: It can be across between both of them, that is one thing that has to come in India in Indian education. This is not at all.

Prof. Prathap Haridoss: This is a under played, this is quite bit a under played, but what about you know as a student guide interaction I mean.

Prof. B. Viswanathan: The guide should be available on all the time.

Prof. Prathap Haridoss: All the time. OK.

Prof. B. Viswanathan: That is.

Prof. Prathap Haridoss: Easy accessibility of guide is a very important.

Prof. B. Viswanathan: And that also he should treat the students equally.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: Because he should not put him in a fearful situation.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: Or respectful, in both the situation.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: That respect should be only inherent. It should not be shown outside.

Prof. Prathap Haridoss: So, that makes the interaction more effective.

Prof. B. Viswanathan: The students should be able to tell him what is inhibitive to him.

Prof. Prathap Haridoss: Sure.

Prof. B. Viswanathan: That is, in Indian situation, this 'guru-shishya' situation is really that is what is the shishya is capable of asking anything to the guru, guru also is capable of asking the shishya anything that is somehow in between this, disappear.

Prof. Prathap Haridoss: OK. So, that is something that is worth.

Prof. B. Viswanathan: Yes.

Prof. Prathap Haridoss: So also in a similar., sort of in a related sense there are different ways in which people measure, you know how students have performed in, you know research activities in commonly we refer to just publications, over and above publications are there other ways in which you look at students to measure you know how much they have evolved as a researcher.

Prof. B. Viswanathan: Okay this is one thing that in our center, that we are practicing for example for example I will tell you one example then you will and also this example is well known for example, when ammonia synthesis was proposed by Fritz Haber, his boss Ernest, Ernest equation, Ernest put thermodynamics and said it is impossible. So, you cannot work on this, but in spite of it Haber worked on it and got the ammonia synthesis with a BSF, that is not the criteria. If ammonia synthesis where not to be there, world population will be one-half or one-third, because it has provided the food for all the people, that is why world population has increased.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: Now, the question is the same question only we asked, CO2 to chemicals is not thermodynamically possible.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: So, for example, this is the way we came to this CO2 problem. If Haber could do ammonia synthesis, why cannot we do carbon dioxide to chemicals?

Prof. Prathap Haridoss: Chemicals. OK.

Prof. B. Viswanathan: So, this type of questions we asked the students and make them interested in the research because these researchers will not provide or give results immediately. So, they should not get discouraged.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: They should be willing to face problems. So, like this today the students should be motivated for this is only one example, many examples are there. For example, super capacitors as I told you, the hetero atom substitution in carbon materials is now known, but when we started 20 years back nobody even thought that nitrogen can be substituted in carbon.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: Because nitrogen is a 5 valence, carbon is 4 valence.

Prof. Prathap Haridoss: valence. OK.

Prof. B. Viswanathan: So, such a solid state material is not possible. Even now many solid state chemistry will not agree with that.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: But those types of things are possible. So, one can unconventionally think.

Prof. Prathap Haridoss: So, you are looking for unconventional thought processors.

Prof. B. Viswanathan: Yes.

Prof. Prathap Haridoss: To

Prof. B. Viswanathan: Or induce those processes.

Prof. Prathap Haridoss: Induce those processes and that gives us the sense that they are actually thinking different from you know being you know put into a stream line and then they are therefore, that is something that they are learning as a research processes that was a very interesting insight on you know how they have to think outside of whatever parameters they are conventionally told about and then that helps them grow as researchers. So, I would like to conclude this discussion by asking you this, I am sure there are lot of students out there, who are considering, you know advance degrees in chemistry masters degree or a PhD degree. So, what are your words of advice to these kinds of aspiring students for aspiring for higher degrees in chemistry?

Prof. B. Viswanathan: Okay Chemistry is generally considered as a substrate design, physics ethics and physics is more basic than chemistry like that is what if the people think, but as I told you, the students should have first thing is that he has analytical skills, have to come to atomic skill, not the molar or milli molar or micro molar it has to come to atomic skill. Now when we it is coming to the atomic scale the probes also have to change for example, electro chemistry it can now do nano skill, but what we want is peco scale or femto scale, 10 to the power of 12 or 10 to the power of minus 15 molar concentrations. Now, the students should have dynamism in taking up that such challenge such thing that is the first thing. Second thing is if the chemists are always afraid of mathematics, now today mathematics is only, even today or everything mathematics is only a language for non mathematicians.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: Mathematics is pure mathematics, mathematics for mathematicians, but for all others it is only a language. If I want to say 4, I can say 2 plus 2 is 4. So, therefore, that is how it has to be. So, therefore, we should all.

Prof. Prathap Haridoss: Embrace it.

Prof. B. Viswanathan: Embrace mathematics as a language for the other scientists. If they do that then they will be able to perform. As I told you DFD or HR (Refer Time: 30:56) even self consistent it will become easy, but unfortunately our quantum mechanics is people who teach it for the chemists, they immediately go to $\frac{a}{a}$ second order differential equation and solution of them and all those things since it of the emphasizing the physical significance of the solutions.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: So therefore, this type of things they should not take it too much. They should look for the analytical solutions of the mathematical expressions.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: Then they will be able to perform well. So, I don't think the chemistry or even physics or even natural sciences or physical science is a challenging job. It is a very entertaining and interesting job.

Prof. Prathap Haridoss: OK.

Prof. B. Viswanathan: So, that students should feel.

Prof. Prathap Haridoss: Comfortable.

Prof. B. Viswanathan: Engineering is one of them, I am not denying that.

Prof. Prathap Haridoss: Sure. Sure.

Prof. B. Viswanathan: Because you are doing it to hands on, the same thing can be done which example of you MOF metal organic frame work is building in the molecules instead of making a building with brick and mortar. So, like that porous solids also is building a material only. So, therefore, the chemistry generally, science can be more interesting than what it is today.

Prof. Prathap Haridoss: Or what it is may be perceived to be, may be people perceive more challenges than the immediately recognize the interested in it.

Prof. B. Viswanathan: Yes.

Prof. Prathap Haridoss: And so an aspiring student, I think if they learnt to distinguish that and you know put away their fear and embrace it in a more you know whole hearted way they probably will be more comfortably fit into masters or a PhD degree. Thank you very much Prof. Vishwanathan.

Prof. B. Viswanathan: Thank you.

Prof. Prathap Haridoss: It is a pleasure, that we could have you. It is a privilege that we will have you in this discussion.

Prof. B. Viswanathan: Thank you very much.