Professor Shiyu Zhang_ _I Love Making New Molecules_

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SPEAKERS

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S Shiyu Zhang 00:04

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E Eva Dale 00:30

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D David Staley 01:07

My guest today in the ASC Tech Studios is Shiyu Zhang, Assistant Professor in the Department of Chemistry and Biochemistry and a Sustainability Institute Affiliated Faculty Member, the Ohio State University College of the Arts and Sciences. Welcome to Voices, Dr. Zhang.

S Shiyu Zhang 01:22

Thank you very much for having me.

D David Staley 01:24

Well, before we started the interview, before we started recording, you made the statement "I love making new molecules", which I thought was just a terrific statement. And it only occurred to me at that moment, I guess that is what chemists do, isn't it? They... they make molecules. But first of all, tell us what you mean by that, "I love making new molecules"?

S Shiyu Zhang 01:42

Yeah, so like you said, that's exactly what chemists do, right? So, we try to make new molecules, make things that do things, right? So, if I think about all the outstanding problems with sustainability, it basically all requires some form of new chemistry, and how to make these new molecules do different things, have different functions, or just how to make them in an energetically efficient way without producing a lot of waste is just a fascinating question for me.

D David Staley 02:17

So, my chemistry experience is high school chemistry, and I remember I was doing lab work and things like that, but I wasn't actually making molecules there. So, how does a chemist make molecules?

S Shiyu Zhang 02:30

Essentially, it's kind of like cooking, right?

D David Staley 02:33

Like cooking?

S Shiyu Zhang 02:33

Yeah. So you put different ingredients in a flask and you heat things up, you basically watch certain signs that indicate the reaction has completed, and then you take it out and see what you made. A lot of the time you made the stuff you want, and sometimes you get some surprises.

D David Staley 02:54

Tell me about a surprise. What does that look like?

S Shiyu Zhang 02:58

Basically, if you're expecting, like, a solid product, but you end up getting a glue, or you're getting a lot of gas bubbles, like, that's usually saying there's something unexpected has happened. And those sometimes are usually the interesting discoveries, because you make something you didn't expect, and sometimes it has interesting properties that can lead to applications. So, a lot of the very important discoveries - for example, conductive polymers - are made by mistakes, right? So, the student that was doing the research accidentally add one reagents by more than a hundred folds than the requirement, and then ended up getting something that's very shiny like metals. And then the student was smart enough to measure the conductivity of this molecule.

D David Staley 03:47

And when you say conductivity, that means its ability to conduct electricity?

S Shiyu Zhang 03:51

Conduct electricity. Som yes, yes - which is somewhat relevant to what we're going to talk about today, right, so ability of organic molecule to conduct electricity, right. So, this discovery of conductive polymer later lead to Nobel Prize, but essentially just... everything by accident, it's kind of like cooking, right?

D David Staley 03:55

Well, and you say interesting and accident - that's never... or perhaps it is dangerous sometimes in the lab, I'm guessing?

S Shiyu Zhang 04:20

Yeah, yeah, it's definitely important to keep reactions, you know, contained in a safe environment. So, we usually do these, we call it synthesis, in a sort of safe isolated place, we call it a fume hood. And yeah, so that's, yeah.

D David Staley 04:37

You made mention of the research you're doing and it's really, really interesting, and I know you're working on... well you're working on batteries. Let's start with the batteries that we have today, lithium ion batteries - first of all, tell us... tell us what lithium ion batteries are and maybe how they work.

S Shiyu Zhang 04:52

Great, yeah. So, lithium ion battery is essentially an energy storage device, right, so it can be used for storing energy for pretty much everything, like our cell phone, laptop, now electric cars, and even for electric grids that you need to put a lot of energies in, some sort of storage device. On a chemistry level, it's basically made by two electrodes, we call it the negative electrode and the positive electrode, right? So the negative electrode is made by lithium, the positive electrode, usually made by some kind of transition metal, like nickel and cobalt, right. So, it's basically a reversible device, so you can put energy in there and take it out in a very reversible fashion, so, therefore, this is a way to, for us to harness say, energy from renewable sources, such as wind, solar, and things like that into a device and carry it with you, right? So, what do you think about lithium ion battery?

D David Staley 05:51

I think that there's somehow different from the batteries I put in my, you know, cassette recorder or my toys or something like that.

S Shiyu Zhang 05:58

Yeah, yeah. So usually people think about as something that's very sustainable, is going to be this... people think it's a solution for, say, like the CO2 problem.

D David Staley 06:09

Because I can put it in my car, let's say, so I don't use gas or something like that.

S Shiyu Zhang 06:13

Yeah. But there are actually a lot of problems with lithium ion battery, particular with these two electrodes I was just telling you about. So, it's basically the elements that we have to use to make these electrodes, they're difficult to get, right? So, lithium, cobalt are two biggest problem.

D David Staley 06:32

Difficult - difficult how?

S Shiyu Zhang 06:34

Basically, the source of these metals are restricted to different locations, right? So lithium, I think, based on the trajectory of research is not going to be too big of a problem, because likely in the next couple of decades, we're going to learn how to extract lithium from seawater. But, cobalt... well, in ideal sense, right?

D David Staley 06:56

Okay.

S Shiyu Zhang 06:57

But for, for cobalt, that's going to be a very big problem, right? So right now, there are only a few countries that can produce cobalt, and if you calculate just the amount of cobalt required to to make all the cars electric, it's going to take hundreds of years of mining enough cobalt at a current rate. So... and also, you know, if I've learned anything from this energy, probably in the last century, if there's energy storage media is dependent on the mining process, for example, fossil fuel, right, the price is going to fluctuate a lot, depends on the political situation. So, for example, now, we have very high oil price because of the Russia situation. So, if lithium ion battery become the main source of energy, so the price of cobalt is going to be a big consideration, the price and the source. So, that's where sort of my research comes in - we... hopefully, we don't have to depend on these elements that's very much restricted to the source, so, the supply chains. So, a possible replacement for cobalt is organic molecule. So, this is essentially an organic molecule, like many listeners know, so it's made by carbon, hydrogens, oxygen, sulfur, nitrogen. So, these are very abundant elements that's flowing around the air, it's... it's pretty much everywhere. And they can be easily sourced, so they're not restricted by location, you can easily obtain them in large quantity. So, that's the sustainability argument, and they're also the structural diversity argument. When we're dealing with transition metal, for example, cobalt, there are only a few variants you can make, which means that the research is very restricted to a few candidates. But organic molecule is extremely diverse, so humans are chemical machines made by organic molecules. Likely... so whenever there's a problem in nature, for example, energy storage, likely the biology has already figured out a solution for the same problem; for example, our human eyes, these are organic molecule that's sensing light, right? So it's not made by gallium nitride, but organic polymer that does the same thing. So, that's the structural diversity argument, so, we can essentially just use these five elements and make thousands of variants very easily and test what they do as energy storage media.

D David Staley 09:40

So what's involved in this? In other words, if it were easy to use organic molecules, presumably we would have done it already, so what are the challenges that you face using using organic molecules?

S Shiyu Zhang 09:50

Yeah, that's a great question. So, that's the question we're trying to solve, right? So, you know, the biggest challenge for using organic molecule is they're not as stable as, say, transition metal.

D David Staley 10:02

Stable meaning...?

S Shiyu Zhang 10:03

It basically means the capacity it will face, so basically the amount of energy you can store in a battery will decrease very rapidly. So, this is a common problem as you use the battery throughout, like, different charge and discharge cycles, that capacity will decrease as a function of time. And then, for organic system, this decreases a little bit too fast for practical applications. So, what we're trying to do is to figure out how to tweak the structure of these organic molecule so that they can last a little bit longer when we put them into an energy storage device.

D David Staley 10:44

How do you do that?

S Shiyu Zhang 10:46

So, this is quite a challenging research problem. So we, basically, we will put in two different structural modifications, right, so we basically can take a carbon, for example, change the nitrogen or oxygen and see what it does to the performance, and sometimes the stability increase, sometimes the stability decrease, and that will give us a clue about if we're on the right trajectory, so. And this type of research, we call this a trial and error based study, which is very time consuming, right, it's not a desirable process. So, one of the big goal for my research is coming up with design principles, so basically, coming up with predictable rules, say, like, if you change this one particular atom from carbon to nitrogen at this particular position, then it will be good for the performance, right? So this kind of design rule will help us save a lot of time in a research effort like this.

D David Staley 11:48

When we've been talking about batteries, whether lithium or organic-based, we're talking about powering things like cell phones, automobiles - at what sort of scale could we see these sorts of batteries? In other words, could we have something of the size, I don't know, like an industrial dynamo or something like that?

S Shiyu Zhang 12:07

Yeah, yeah, so that's a great question. So, I think they can really be any scale. So, in our lab, we make things called coin cells, so basically, they look just like a coin that you're putting in your watch or something like that. So, that's the smallest scale, right? Going up, we have pouch cells, so these pouch cells can be put into, say, like electrical cars, and so each electrical car will have about 7000 pouch cells. So, and then from there, you can really just build as large as you want. Sometimes if you want battery for electrical grids, it could be the size of a building or things like that, as long as you have the materials to build the device, yeah.

D David Staley 12:51

Should I really be worried about my phone catching fire or my electric car catching fire? I mean, I see... I see this on social media - is that a real concern? And if it is, is this something maybe that an organic-based battery would mitigate?

S Shiyu Zhang 13:06

Yeah, so that was a real concern couple years ago, but I think right now, the technology has matured by a lot compared to just five, ten years ago, and the use of cell phone and electric cars now is actually very safe, yeah. And what is catching fire in the cell phone are the component called the electrolyte, which is an organic liquid that's flowing around inside the cell. So, the material we're using, the electrode material we're using usually are not, not the one that's catching on fire. So in this sense, the development of organic electrode doesn't have a direct impact on the flammability of the cell, yeah.

D David Staley 13:50

When you describe organic-based batteries as being more sustainable, where does that come from? Is it just because the materials are more... are more accessible? Where does the sustainability come from?

S Shiyu Zhang 14:03

So, yes, so essentially, we have to think about if we're going to make a large amount of certain things, where are we going to source the material, right? So, exactly like you said, the source of elements plays a big role, and also, how much resource, how much energy do you need to make the elements into the form that you can't use? And that's also another consideration.

D David Staley 14:29

And what's the difference, what... why is that energy input so much lower?

S Shiyu Zhang 14:34

So right now, we don't know exactly how much energy input we'll need to make a sort of, we call it feedstock compound into a energy storage device, right, so that's still very much ongoing, that part of research. Yeah, so it's difficult to say at this stage, yeah.

D David Staley 14:55

Well, since you're talking about carbon as one of the candidate molecules, are there implications about using, say, the excess carbon in the atmosphere?

S Shiyu Zhang 15:07

Yeah, that's a great question - that would be the dream, right? So, that would be the dream, to essentially capture the carbon from CO2 and eventually make them into an energy storage device, right? So, CO2 is one source of carbon, and it can also be from, say, bio matters, so for example, tree barks, and then flowers. And you can actually find the energy storage material in these solar power matters already, but just figure out a way to convert these biomass to the energy storage compound will be a very interesting direction.

D David Staley 15:45

You say that's the dream; are you optimistic that we can extract carbon for this use?

S Shiyu Zhang 15:51

Yeah, I'm optimistic. There actually already is research that use the molecule directly coming from the plants to do the energy storage. At this stage, not directly from a tree, but they purchased a chemical that can be extracted from the tree and demonstrated that they can also be used as energy storage media in lithium ion battery, so.

D David Staley 16:15

I'm curious to know, well, why did you become a chemist? Why chemistry as opposed to, I don't know, physics or biology or history or something like that? How did you end up as a chemist?

S Shiyu Zhang 16:25

Yeah, so... well, I was a huge chemistry nerd when I was a kid. I loved color change, you know volcano explosions, that kind of stuff. And you know, even now, after work, I will watch YouTube videos of chemistry reactions, which is very cool, right? So these entities are still very fascinating to me. And so as my training progress, I think I started to appreciate more about synthetic chemistry, which is how to make molecules more efficiently, is an extremely important endeavor. So that's where I started focus more on this chemistry or synthetic chemistry direction. Exactly how I get into organic electrode material is because my postdoc training, right? So when I was a postdoc at MIT, it was a very eye-opening experience. So previously, I just make different molecules; they don't do much, but it was interesting to me. When I was doing my postdoc, it appears to me that this kind of skill can actually be applied to very important sustainability issues like the one we talked about today, like energy storage and catalysis, or material design and these kind of topics. So that's why I want to do research in this area, yeah.

D David Staley 17:45

For non-chemists like myself, what would you say has been the biggest change in your field, say, in the last, I don't know, forty, fifty years or so, the biggest, sort of, paradigmatic change?

S Shiyu Zhang 17:57

I think the use of lithium ion battery is definitely, yeah.

D David Staley 18:01

Oh.

S Shiyu Zhang 18:01

So it was, you know, lithium ion battery got a Nobel Prize in 2019, right, so... and I think a lot of the credit has to go to the engineers who optimize the performance of this just by tweaking a little bit of things here and there. But now, the performance of lithium ion battery has reached somewhat of a ceiling, right? So now, we need to go back to the lab and start thinking about designing new materials that are beyond the lithium ion battery paradigm. So then, people started to go back and think more about new chemistry now, because that's potentially the way to break through this hard ceiling of lithium ion battery. So, biggest change, I think, is just how lithium ion battery has been implemented into all of the day to day energy devices, things like that, yeah.

D David Staley 18:55

Sitting here as we're talking about this, I wonder if there's not a Nobel Prize in your future? I certainly would hope that's the case.

S Shiyu Zhang 19:02

Thank you.

D David Staley 19:04

We've been talking about sustainability and I introduced you as an Affiliated Faculty Member of the Sustainability Institute, and I wonder if you could just tell us a little bit about the institute, the Sustainability Institute here?

S Shiyu Zhang 19:14

Yeah, so it's really a great environment to bring together faculties from different departments, from different colleges, and sometimes we're thinking about the same issue, but we have different approach, right? So one really helpful things from these, the Sustainability Institute does is these SI grants. So, faculties can come together and write a short two page proposal and get some fundings to explore a new idea, right. And that's something I took advantage of a couple years ago in collaboration with another faculty, Joe Paulson, in the chemical engineering department. So, we essentially were talking about... I was telling him how time consuming it was to do my line of research, because my grad student will make 30 and 40 molecules and turn out only one or two of them actually does what they're supposed to do, right? So this, you know, while two works, we're very happy about it, but the other 35, 38, we just throw them away. So, we're talking about how we can actually use the other 35 data point more efficiently, and that's how we come together and come up with this machine learning approach to efficiently use the poor data point to come up with design principles. And these are all because of the Sustainability Institute to give us a platform to communicate.

D David Staley 20:43

And I'm going to ask you more about that research in a moment, but you mentioned that Professor Paulson is a chemical engineer, and as we've been talking, I was thinking myself, well, if you're making molecules, it almost sounds like you're an engineer of some kind. What's the difference between what you do and what a chemical engineer does?

S Shiyu Zhang 20:59

So yeah, it's kind of strange, right? So we're chemists and chemical engineers, we are in the same building, but we're actually different colleges, right, so we're in Arts and Science, they're in the engineering college. So, I think... it's kind of hard to say what exactly the difference is, but I think we are more interested in the developing new chemical reactions, right, so how to make this molecule in a more efficient way, how to produce it with less amount of energy. But chemical engineers, you might... in my opinion, they think about how to take a reaction that's working and scale this up to a practical level, or optimize this process of producing a new molecule, yeah.

D David Staley 21:44

Are you thinking about practical applications in your work? I mean, you must, since you're talking about batteries, this must be guiding your research in some way.

S Shiyu Zhang 21:52

Exactly. So, you know, it's interesting to see the molecule we made can be put into a coin cell, and this is probably the most applied research I've done in my career. So, we keep in mind about the performance of the compound, right? We want it to last for a long time, we want it to be able to store a lot of energies, so all of these are keeping the application in mind. Another aspect is the charging rate of the molecule - how do we design molecule with specific features so that it can be charged, say, within an hour or within ten minutes or even a couple of seconds? Yeah.

D David Staley 22:32

Well, you started down this path, but tell us what's next for your research.

S

Shiyu Zhang 22:37

So I'm very excited with this direction of applying machine learning to material discovery. So, this collaboration with Professor Joe Paulson...so in this collaboration, we try to develop a machine learning algorithm to predict the performance of a particular organic molecule just based on the structure. So, the idea is to have some sort of structural input, give it to the computer, and the computer can tell us what's the likelihood of success. So, we have some interesting preliminary results suggesting that this idea might work, but right now, it can put us in the correct ballpark, right? So some of them, the algorithm will tell us it's absolutely no, some of them will be a maybe, some of them will be probably as a good choice, right? So as long as it can give us a general idea of if this molecule is going to work or not, then it will already save us a lot of time.

D

David Staley 23:41

So, your lab features... well, yourself, and postdocs and graduate students and undergraduates - do you envision your lab to soon have artificial intelligence as a team member?

S

Shiyu Zhang 23:53

Yeah, it's already part of the team member, but it's not as fancy as it sounds. So, machine learning is just essentially a fancy way to looking for trends that's not very intuitive for us, right? So it will basically just look a little bit deeper into this data points than what we can, but essentially is a fancy way to look for trends.

D

David Staley 24:20

Who's writing the program, who's writing the algorithm?

S

Shiyu Zhang 24:23

That would be Professor Paulson, yeah, yeah. So he's an expert in this field here, looking into all sorts of different problems, like how to apply machine learnings to different problem and this collaboration is one way to use the algorithm to solve a chemistry problem.

D

David Staley 24:41

But no one is suggesting that this will replace chemists, that chemists will be replaced by algorithms anytime soon?

S

Shiyu Zhang 24:48

Hopefully not. Hopefully, we'll still have a job in couple of years.

Hopefully not. Hopefully, we'll still have a job in couple of years.

D David Staley 24:53

Shiyu Zhang. Thank you.

S Shiyu Zhang 24:55

Thank you very much.

E Eva Dale 24:57

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