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Collaborations drive energy storage research

Dr Y. Shirley Meng, Professor of Molecular Engineering at the University of Chicago and Chief Scientist at the Argonne Collaborative Center for Energy Storage Science (ACCESS), discusses her research on energy storage materials and the importance of multidisciplinary collaborations.

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What are the current challenges in improving current energy storage technologies, such as battery systems?

Batteries are very complex systems and it is oftentimes underestimated how complex they are. People tend to forget that, in addition to the three main components (the anode, the cathode, and the electrolyte) that need to be optimized, we also have the current collector and the architecture design to consider. We describe the way that batteries function as a complex living system because they will degrade; some have self-healing powers, and they are very sophisticated systems. Just like the current trend in digital monitoring of human life, we want to ensure that battery researchers are able to design batteries from the bottom (atoms) up and monitor the state of health of the battery from the top down, meaning, from the system level to the molecular level. That requires a digital platform to help us to progress. On one hand, scientists have been trying to build a physics-based model to produce a digital twin of a battery for the past two decades. On the other hand, some researchers are using machine learning and artificial intelligence-based techniques to learn about batteries from a statistical point of view. The two sides are converging in that they are all targeted at making batteries last longer and be safer. Eventually, the goal is to build an infrastructure for the grid of the future that includes mobility and daily life data to build batteries for society based on renewables.

How can computational scientists help to address the most pressing challenges in energy storage?

I believe that one of the biggest breakthroughs that our field has had was the understanding of the salt solvent interface between the electrolyte and electrodes. Where I think computational scientists can help even more is in the electrolyte design and the understanding of that interface. For those aspects, it can sometimes be very difficult to design physical experiments that will separate certain variables, so computational scientists can play a major role in accelerating those studies. The second area that computational scientists can really help is in discovery-based projects, such as identifying new energy storage materials, because experimentalists are limited by how many new materials exist that can be used to build batteries with new chemistry. For example, people have not been able to buy potassium batteries or calcium-based batteries commercially because there are very limited choices for the materials that can be used for energy storage. This becomes challenging because one needs to identify materials that have great performance, but are also widely available, inexpensive and have minimal environmental risks. I did my PhD 25 years ago on how to use first-principles calculations to replace cobalt with more Earth-abundant and sustainable metals in the lithium transition metal oxides. I think that there are a lot of opportunities there for the discovery of new materials that humans have never made before and the exploration of their potential for storing energy.

What are your thoughts on having collaborations between computational scientists and experimentalists for driving materials discovery?

Back in 2000, I — as an experimentalist — decided to join a theory group to learn the computational tools firsthand. Based on my own experience, one of the biggest hurdles in these types of collaboration is that the language we use tends to be different. As in any scientific discipline, we tend to use specialized language that we are familiar with, and computational people and experimental people are no exception. In the computational world, we might refer to experiments in one way, for instance, by talking about the grand canonical ensemble or the canonical ensemble, but experimentalists, who use a different language around experiments, may hear that and think, "what variable am I controlling in the experiment?" because they want to know if they should control the temperature, pressure, the total amount of matter, and so forth. That translation is only possible if experimentalists and computational scientists work together long term. We cannot force cross-fertilizations in the short term: it has to happen organically and people need to appreciate each other's languages and cultures and really know each other in order to spark innovation. The second big hurdle is often related to who gets the credit if something big happens. I have witnessed a lot of setbacks in this kind of collaboration because the computational scientist is the one who comes out with the nucleus of the idea first, but then the implementation and execution by experimentalists adds so much more. For any interdisciplinary collaborative effort, we have to overcome that idea and work as a team because both parts are needed to make progress. Experimental and computational researchers will need to be more goal-oriented and share the credit if something awesome happens.

What are the current challenges with data sharing in the field, particularly between industry and academia?

If the collaborations between computational scientists and experimentalists in academia have a difficulty level of five out of ten, then collaborations between industry and academia have a difficulty level of more than ten out of ten. To give an example, I drive an electric car and I know that my car has a few thousand batteries, but if I ask for the data from my own car, I cannot get it even though I am the owner, because the data does not belong to the customer. This is an extremely difficult task, which will perhaps require industrial leaders and government bodies to come together to decide what data should be put in the public domain for everyone to study. People have different algorithms and different ways of analyzing data, so if an electric car company shared data from the last five years, for instance, and invited talent from all over the world to study that data, there would be a lot of value gained from that. This kind of open-source approach is highly appreciated, if it can happen. At the moment, I am not aware of any companies who are doing that, and I think that is one place where national laboratories could potentially fill the gap. National labs do quite a lot of intensive data testing and they have the resources to get real cell data instead of using small coin cells, so their testing is much closer to what is being used in industry. Last year, NASA shared their battery dataset, and it was widely used by many researchers across the world and contributed to many publications. But I am still waiting for a company that is willing to share their datasets. Companies realize the value of their data and they may want to do the learning themselves, internally, to really capture the economic value of the data, but that could also slow down the progress that could be made instead.

In your opinion, what needs to be done to improve access to affordable, reliable, and sustainable energy?

That's the trillion-dollar question! One has to realize that every country is geographically different, so while we are doing energy transitions, each region may need to come up with their own best plan. For instance, in the United States, many people doubt whether we can go 100% renewable without nuclear energy. Just recently, Tesla released their Master Plan Part 3, where they champion for overbuilding renewables by 30% and then using vast amounts of batteries in addition to provide 240 TWh of battery storage. That is just one scenario to think about how we can transition to the grid of the future where renewables provide electricity. I think that reliable and affordable electricity will require a societal level of mindset change towards "this is possible" so that we can think intently about what is practically needed, such as how much investment is needed. If we think back 120 years ago when the previous grid was set up, all the major financiers came in to invest, because there was a societal mindset that electricity could improve the quality of life. That is one of the biggest challenges right now: maybe half of the population is all in and knows that our quality of life in the future relies on access to renewable energies, but I am afraid that there is another group of people that does not agree. My hope is that the younger generations will focus on education so that by the end of the century, humans will realize that we were given a lot of resources by nature — waves, solar, geothermal, and many others — and through those we can make renewable energy possible. I am not worried at all about the technology, because we have so many brilliant people working on it, but I really hope that country leaders will do a better job at the policy level.

What are the challenges in integrating renewable energy technology into the energy grid?

The good news is that the lithium-ion batteries have already created a lot of good examples. There are many hundreds of megawatt hour implementations throughout the world in Australia, California, and Europe, for example. I believe that the sodium field should learn from those lessons to determine what works best and what is still a challenge. To my understanding, a lot of the challenges come from the market structure. For example, the California market structure is different from New York or those in Europe. My prediction is that in Europe we might see a lot more penetration because the market and policy better incentivized renewables. Sodium battery companies should take that into consideration, because there are places where they will have earlier penetration and they may need to work with the local communities to think about how the modern grids will change the market structure. In China, there is a completely nationalized grid, so if the government were to support renewables, they would have a great demonstration project, because they will learn so fast from that implementation and all the data that comes with it. That information could then be used to better approach the global market. In that way, a nationalized grid system is fantastic, but we are still facing quite a lot of challenges in the capitalist markets where it is completely privatized.

Do you think that the current commercially available materials are able to reach our sustainability goals?

The answer is probably no. Tesla's prediction was 240 TWh of battery storage and in my own group, where we work on long-duration storage, we are predicting 400 TWh batteries. By the time we reach 100 TWh, lithium and a lot of metals will become critical materials like crude oil, which we don't want to happen. That is why we are championing sodium, but the global supply chain for sodium is not there yet. Maybe there is a small supply chain available in some areas, but the batteries do not operate as reliably as the lithium batteries, and we are still facing safety problems — there is still a lot of improvements to be made. While we are all hoping to have a new revolutionary technology, we have to recognize the historical trend: revolution does not happen every year. At the same time, we will need to implement the technology into society, so we need people to make revolutionary improvements. However, we cannot choose to pursue one option. Quantum computing is seen as the future of computing, but silicon-based chips keep getting better and breaking expectations. I hope that the same can happen with rechargeable batteries in that we can keep improving the technology we have while searching for the next generation.

In your opinion, do we currently have enough computational resources to support the development of new energy technologies?

The computational power is good, especially with exascale and petascale computing, even though we do consume a lot more electricity with those machines. That is still a challenge that will need to be resolved: how can we store data, run the simulations that we need and keep the system cool in an energy-efficient way? To me, the biggest hurdle seems to be that we have so much data that it becomes wasteful. I think about data in the same way as an energy flow diagram, where we know that 2/3 of energy is wasted as heat (or entropy), and with data I also think that the entropy is too high. In my opinion, we should spend more time organizing data to reduce its entropy and make it clearer what the real essence of that data is and how it benefits the field. Data is knowledge, but going from data to knowledge is a step that is still urgently needed.

What needs to be done to improve battery management algorithms and diagnostics for degradation?

Even though they have been doing a pretty good job, I do not like the current battery management systems (BMSs) and algorithms for the management of health because they are after factors, meaning that when we buy batteries, we don't know anything about its past health history. In the same way that monitoring a person's health would be difficult without knowing their past history, this is a challenge for battery management as well. Myself and many other like-minded scientists would like to create a battery passport, where we know what materials were put into the battery in the very beginning, and that information is digitized. Then, when you buy a battery, it will come with the passport and you have all of the information that is needed to help you manage the system's health. In my research, I have done a lot of destructive testing, but now we are focusing on nondestructive testing so that, after you get the 'birth' passport, like a birth certificate for the battery, you can then record all of the history of the battery operations. Then, when the battery is managed, it should be treated like a health record in that it should always be updated. When the battery finishes the most difficult job in a car, it's like a retirement from that car, then we can use the information from the passport to make more informed decisions about if the battery goes to the grid or if it should be recycled.

The second thing that I would love to see happening is that BMSs were previously designed for graphite-based batteries, but we are now moving towards silicon, lithium metals, solid-state batteries, and many others. BMS researchers will need to be interdisciplinary in working closely with material scientists because new batteries will function differently than previous ones. For instance, with intercalation-based materials, you do not have to worry about the pressure, but in a lot of new non-intercalation materials, there are volume changes, so that needs to be accounted for. At the moment, BMSs are also not utilizing all of the breakthroughs in fiber optics, lasers and other high-end sensing technologies.

Energy materials research highlights the convergence of science and technology, with social science, economics, and policy. How do these different areas inform each other to enable real-world changes?
I always think that, as scientists, we tend to underperform in terms of reaching out to the public. I have experience working with economists and the challenge is, like I mentioned before, that we need to speak a common language, but also a language that non-experts can understand. Collaborations between economists, politicians and battery and energy researchers on actual projects should be encouraged. For example, we could think of the question "if California wants to go 100% renewable, how much money needs to be invested?" That's a design project where the economists and politicians have to work together, and the scientists have to have the technology. We are starting to see the establishment of schools of climate and sustainability, so I am cautiously optimistic that those types of collaboration could happen. I'm hoping that students will be able to be rigorous both on the technical and scientific side, as well as on the economics side, because we have the common goal: we just have to put in the effort.

Interviewed by Kaitlin McCardle