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Introductory Jingle
Connecting for positive change.

Nikoleta
Welcome everyone to the sixth episode of the Battery Caffe, focusing on quantum for batteries. I'm Nikoleta Piperidou from the Clean Energy and Infrastructure Team at Innovate UK KTN hosting today's episode alongside my colleague, Dr. Najwa Sidqi. Hi, Najwa.

Najwa
Hi, Nikoleta. Hi, everyone. Thank you so much Nikoleta for the invitation to the Battery Caffe today and to our speakers for agreeing to join us on this episode dedicated to quantum for batteries. So I'm Najwa Sidqi and I am the Knowledge Transfer Manager in Quantum Technologies at KTN.

Nikoleta
Thank you, Najwa, fantastic. And just a brief intro to the Battery Caffe. It is an initiative of the Cross-Sector Battery Systems Innovation Network, a community founded by Innovate UK KTN and The Faraday Battery Challenge. The Innovation Network aims to open new markets for the battery industry, promote innovation in batteries and help decarbonize a wide range of end users. If you haven't already, please go check out our online platform at ukbatteriesnetwork.org, where you will find lots of useful material and our first five episodes. So today, we're joined by Hallam Davis, Senior Electrochemist at AMTE Power. Hi, Hallam.

Hallam
Hello. It's nice to be here and yeah, I'm Senior Electrochemist at AMTE Power. We work to scale up technologies to produce batteries that are ready for the open market.

Nikoleta
Thank you and Michal Krompiec, Scientific Project Manager at Cambridge Quantum. Hi, Michal.

Michal
Hi, my name is Michal and I'm delighted to be with you today. I am a Scientific Project Manager in the Quantum Chemistry Team at Cambridge Quantum, we develop software for quantum computers and since our merger with Honeywell Quantum Solutions, also quantum computers themselves.

Nikoleta
Thank you very much. So everyone, make yourselves a coffee and join us. So Michal, let's start from the basics. What do we mean by quantum? And what are the key application areas?

Michal

Quantum computing is a fundamentally novel and different type of performing computation by machines. So as you probably know, classical computing relies on Boolean logic and logic gates, so it switches on and off and basic logical operations on them. In contrast to this Quantum computing makes use of interaction between quantum states. So instead of bits that can be zero, or one, we've got qubits, which are two level quantum systems, which can be in a state of 01 or a superposition and they can interact with each other in kind of non-trivial ways. This gives rise to completely new types of logic, new types of operations, which in practice, can run the same algorithm as classical computers can, but the complexity of this algorithm, the cost of performing them can be much, much better. So in certain applications, quantum computation offers even an exponential advantage in terms of speed and memory requirements compared to their classical counterparts. And the main application areas are in optimization in machine learning, in cybersecurity, both in terms of generation of cryptographic keys and in sharing of cryptographic keys and finally, in chemistry, which we'll be talking about today.

Nikoleta
Thank you very much.

Najwa
So, obviously, we just heard Michal on how quantum technologies is a big area of development and it allows us to address several optimization and simulation problems, especially in chemistry, and also for several end users. And the battery sector specifically could be a big use case for quantum technologies, considering the pressing zero agenda, and also the shift for electrical energy and the need for more sustainable processes and materials. Hallam, as an Electrochemist at AMTE Power and being focused on cell technology. Can you give us an overview of the current needs and challenges of the battery sector? And also what could be the biggest opportunities for development?

Hallam
Certainly. So the current needs and challenges are quite diverse. There's quite a large mix of these and that very much ties into what really we're looking to optimise and take advantage of. So there are a lot of issues with not just cell design. So we'll be looking at producing batteries that are lighter weight, that are better optimised, they'll have better cycle lives, better voltage windows and ultimately be safer. But then there's also other things to look at, such as moving into new materials, moving away from materials such as cobalt that are less sustainable and moving, potentially towards new sort of design philosophies, such as sodium materials, as opposed to lithium. All of these will involve an awful lot of design from the ground up. Opportunities to reduce that via things like modelling will allow us to massively reduce the amount of time required, the amount of money required, the amount of experimental steps, as well as potentially highlighting new areas that otherwise we wouldn't be able to identify, if it was a more classical approach to lab based chemistry.

Najwa
Thank you very much. And Michal, as a scientist in a major quantum company and being focused on computational chemistry, besides other chemical optimization topics, how do you see quantum speeding the development of the battery sector? And how can it address some of the industry needs and challenges discussed by Hallam?

Michal
Quantum computing, could in a matter of few years, offer unique opportunities for materials development for batteries. But let's take a step back and first think about what is the role of computation and modelling, specifically computational chemistry, in materials R&D? Well, one thing you can do is to perform modelling, to improve your understanding of the process, so to do kind of basic, fundamental modelling of these processes. But what is probably more interesting is a computation of screening of ideas for new materials, new process conditions, before they are tried in an actual physical lab. So when you come up with say 100 new ideas to try in the lab, you won't be able to try all of them, due to cost reasons, but you can reduce it to maybe a couple of the most promising candidates by performing a virtual experiment on a computer. And now the usefulness of this computation or filter depends on the accuracy of the computational method you use. The workhorse computational methods used in materials science today on the atomistic level, based on density functional theory, which is widely applicable, it's pretty fast but its accuracy is fundamentally capped. On average, the errors in reaction energies or reaction barriers are two to four times higher than what we call the chemical accuracy. So the minimum accuracy required to be able to compare to experiment, on surfaces these errors are at least five times louder than the target accuracy. Now you may be lucky and due to cancellation of errors, your results might be just about correct, but you have to rely on luck. The methods we're developing in the framework of quantum computing are in contrast to DFT systematically improvable so we are always able to put a strict error bound on them and converge them to essentially accurate solutions. Now, it is possible to do this on a classical computer as well but the cost for realistic designed systems would be enormous, due to exponential scaling. So in other words, quantum computing can bring rigour and accuracy into practical computational chemistry, which at the moment is very much juristic. That's it in a nutshell, what quantum computing can do for batteries.

Najwa
This is really great to hear Michal, about what quantum can do in quantum computing, specifically in simulation and what it can do for the area of battery development, whether it's materials or processes and providing more accuracy. Nikoleta at Innovate UK KTN we also addressed that specific topic of quantum for batteries and delivered a couple of activities on this topic. So, what were the key findings from these activities and could you point us to some material we can be looking at?

Nikoleta
Thank you very much Najwa. Yes. You may recall, we tested the water with a brief session on quantum for batteries back in September, that was part of Quantum Tech Live and we saw that the audience was really engaged. We found loads of common ground and we thought, okay, let's do something more. So back in February, we ran a technical webinar, just over an hour long, exploring the topic in detail. So you can listen back to the recording, it's on the KTN website. If you check on Quantum for Batteries KTN, you should easily find the link and listen back to the recording. But some of the key findings were, well, the obvious one, quantum technology in batteries has a huge potential for the future, so that was the main key learning from both sessions. And then we talked a little bit about quantum simulation just now and how it can drastically reduce error and experiments. The other point with that was quantum sensors, and how they offer a great degree for better detection than regular sensors and how it can be commercialised. So, we had some excellent insights from CDO-Squared. So if you haven't heard of them, look them up online, they're doing some

great work in this space. Thank you very much Najwa. And back to you Michal, are you able to tell us a little bit more about the projects you have been involved in, in chemical simulation that may be relevant to the battery sector?

Michal
Of course, I'd been more than happy to. So about two years ago, we did a project for Nippon Steel on simulation of two types of crystal structures of iron, BCC and SCC iron cells. And we are able to calculate the correlation energy of the three electrons with pretty good accuracy, good enough to reproduce the experimental difference in cohesive energies between these two. So this was a first demonstration of a correlated electronic structure calculation of a solid, on the quantum computer. So the relevance to electrochemistry is that all of electrochemistry happens on an electrode surface, which is at least as difficult as these iron crystals, as we did to model. Another project I can tell you about is actually still ongoing with TotalEnergies. This is about modelling of carbon capture in metal organic frameworks. So here we are looking into the dissociation curves of a small molecule, which is carbon dioxide, onto an absorbing site. So again, the relevance to electrochemistry is that we're looking at the fundamentals of the absorption process. And finally, at the moment, we are running a project on the mechanism of the oxygen reduction reaction on two different electric catalysts. So this is of great importance for fuel cells.

Najwa
I think these are really amazing examples you just gave Michal, on electrochemistry and obviously, we can hear that these are quite industrial projects with the likes of Nippon Steel and Total. And I guess back to Hallam, we would also love to know about your current projects and what you've been recently working on. So if you would like to give us an overview of your current projects and if any of these actually involve quantum technology?

Hallam
Yeah, so a lot of what our company is doing at the moment is scaling up some of our future products and getting ready for sort of full scale commercialization. Relevant to quantum technologies, we have an ongoing project where we plan to investigate and optimise our battery ageing processes. Generally battery ageing processes are historical and unoptimized, they tend to be passed down from research institutions, from people in the know without ever having spent too much time truly, truly optimising the process. This generally means that once a battery has been made fresh, it will have to undergo some conditioning steps. These can take a very long time, upwards of weeks, under various temperatures. This allows the internals of the batteries to fully form their SEI layers that allow them to reach a good state of health. Unfortunately, this is time consuming and it's expensive. There isn't really, currently a very useful way of monitoring the progress of this SEI formation, this ageing process, it is associated with a very small discharge current but that's very, very small, it's not very easy to measure. If it was to be measured, we'd also have to have every single cell that's being aged, physically connected and disconnected from battery testing equipment, which would be expensive in cabling, it would be time consuming, it would be tedious and it would also involve handling the cells, which is generally something that is to be avoided. What we are working on is an opportunity to use quantum sensors to monitor the very, very small discharged currents, we can see that we should be able to see the tiny magnetic fields associated with these discharge currents, which are associated with the ageing reactions taking place to monitor their progress. This

should allow us to do large batch testing with multiple tests over time throughout the ageing process, so we can start to develop a sort of a bespoke to each product ageing process that cuts down on time involved, cut down on heating costs, it can cut down on manpower and it can result in a cheaper and safer and hopefully better product for the end-user.

Nikoleta
Thank you very much, Hallam and thank you to our brilliant guests. Thank you all for listening. We hope you enjoyed this discussion as much as we did. Don't forget to visit our online hub at ukbatteriesnetwork.org and register to receive our news and updates and participate in the networking hub of the website. Our next episode will focus on battery recycling and reuse. An area we've been working on over the past few months and we look forward to sharing this work with all of you. So thank you and bye for now.

Outro Jingle
Connecting for positive change.