AI 4 Science Discovery Network+

AI4SD Interview with Professor Aurora Clark
30/11/2021
Online Interview

Michelle Pauli
Michelle Pauli Ltd

28/06/2022

Humans-of-AI4SD:Interview-22

AI4SD Interview with Professor Aurora Clark
Humans-of-AI4SD:Interview-22
28/06/2022
DOI: 10.5258/SOTON/AI3SD0222
Published by University of Southampton

Network: Artificial Intelligence and Augmented Intelligence for Automated Investigations for Scientific Discovery
This Network+ is EPSRC Funded under Grant No: EP/S000356/1

Principal Investigator: *Professor Jeremy Frey*
Co-Investigator: *Professor Mahesan Niranjan*
Network+ Coordinator: *Dr Samantha Kanza*

Contents

1 Interview Details

Title	AI4SD Interview with Dr Al Dossetter
Interviewer	MP: Michelle Pauli - MichellePauli Ltd
Interviewee	AC: Professor Aurora Clark - Washington State University
Interview Location	Online Interview
Dates	30/11/2021

2 Biography

Figure 1: Professor Aurora Clark

Professor Aurora Clark: 'A true interdisciplinary project isn't when one group of people is using the knowledge of another, it's when both groups are intellectually engaged'

Aurora Clark is a Professor of Chemistry at Washington State University. Her research uses both quantum and statistical mechanics to study chemical processes within complex chemical environments, focusing on solution chemistry and liquid interfaces. Of particular interest is bridging the separate communities of applied mathematics with chemistry and materials science by creating algorithms that are well-suited to simulation data and provide new physical insight.

In this Humans of AI4SD interview she discusses breaking down the rules of chemistry, taking an integrated approach to solving problems, the intriguing early history of chemistry and why ECRs should always stay curious.

3 Interview

MP: What's been your path to where you are today?

AC: I'm a professor at Washington State University in the Department of Chemistry. Growing up, I wanted to be a veterinarian, but I fell in love with chemistry as an undergraduate. One of the wonderful things about chemistry that really appealed to me was that you didn't have to do a huge amount of memorisation. Chemistry is lovely because there's a lot of patterns, fundamental rules for which you can derive an understanding.

Although I love learning about experiments and working with experimentalists, I realised during my undergraduate research that I have what experimental chemists would call "very bad hands". After my first explosion and small fire doing synthesis as an undergraduate, I decided it was not really a good path for me; instead I realised I was much better suited for numbers and identifying the patterns and underlying rules in chemistry. I loved data and that's what drew me to computational and theoretical chemistry.

I had two mentors during my PhD at Indiana University. Ernest Davidson is a theorist and Jeffrey Zaleski is an experimentalist. Having two mentors helped to keep me grounded in an interdisciplinary context, because I was forced to be able to talk to people that do a lot of mathematics and physics – people who identify and try to write the rules of chemistry, as well as experimentalists that observe these rules. I continued to have an interdisciplinary mindset after I completed my PhD and moved onto my postdoc at Los Alamos National Laboratory and then when I moved to Washington State as an Assistant Professor. However, when I started my independent career I became very interested in understanding systems that are more complicated and where their behaviour starts to break the rules of what we are taught for ideal systems as undergraduate and graduate students.

MP: What happens when the rules of chemistry break down, and how has that affected your research?

AC: There are a lot of underlying assumptions associated with the rules of chemistry that help us to develop chemical intuition. This is often based on idealised models of how molecules interact with one another, and it leads to very simplified mathematical descriptions. I became really interested in non-ideal systems. What happens when these rules break down?

This led me to pivot my research from some of the gas-phase theoretical quantum mechanical types of simulations I had learned during my PhD and postdoc, to the realm of statistical mechanics. Here we can simulate more realistic chemical environments, with many different molecules and accounting for non-ideality and many-body effects: how the interaction of different numbers of particles influence behaviour. Many tools that we have to analyse simulation data have been somewhat limited, in part because they are based on these concepts of ideality and considering a small number of interactions (like two-body interactions) at a time.

About 10 years ago, we developed an interdisciplinary programme that bridged chemistry with analysis that helped us to discover the correlating relationships and rules in these non-ideal systems. To do that, we've leveraged and expanded on concepts in mathematics and applied mathematics involving graph theory and topology, looking for patterns in the data that reveal these underlying rules. Now we've got a really vigorous, highly interdisciplinary programme in my group. I've got physicists, chemists, material scientists and mathematicians

all working together. It's been incredibly rewarding to have this integrated approach towards understanding these systems.

MP: What are the challenges of an integrated approach? Are differences in your language a primary barrier?

AC: Mathematicians and chemists speak very different languages, but when you work together over time, you can overcome that. The more significant challenge is that, often, mathematicians are actually interested in very different things to chemists. You have to find projects and ask questions that are rewarding to both groups of people. A true interdisciplinary project isn't when one group of people is using the knowledge of another, it's when both groups are intellectually engaged.

MP: Is there anything else that's tricky?

AC: In an ideal world, one would hope that you are able to take the knowledge you learn from your simulations and analyses and turn it into practical impact. You're able to advise a company on how to formulate some new oil, or soap, or new separation strategy, or purification process. That is quite challenging: trying to figure out how to effectively close that research loop so that you can make a difference in the modern world.

One of the things I've noticed about the research culture in the UK, is that it seems like there's a large emphasis on being able to close that loop from research to implementation. In the US that happens somewhat, but you have to actively seek it out, you have to really be proactive. If I project out in my career over the next decade, I think we're going to be focusing a lot more on closing that loop and finding those opportunities to have practical impact. It's all about relationships, network building and learning what's important to people.

MP: What are some examples you have of closing the loop successfully and having that impact?

AC: I've worked with a few different companies on helping them to solve small, very highly targeted problems. I have been a deputy director of an Energy Frontier Research Center funded by the US Department of Energy that's meant to solve a problem that no one group could possibly do. That particular project is associated with the treatment of nuclear waste that is stored in different facilities in the US. There have been successes associated with different processing strategies, but no one person can do that research alone. If you have a big interdisciplinary programme like that, it can make it a little bit easier to create that practical impact than in single investigator projects.

MP: What about your work has surprised you?

AC: One of the biggest surprises is how connected fields are that initially seem very different. I'm actually in the process of writing a book right now, where I've been doing a deep dive to understand how maths and chemistry have influenced each other.

A really beautiful example is how the concept of chemical valence emerged. As chemists, we now take this for granted; it is second nature that we know that carbon likes to have four bonds because of its electronic structure. But before knowledge of atomic orbitals, there was the development of structure theory throughout the 1800s. Although chemists didn't know anything about orbitals or bonding they were gathering information about the relationships

between atomic and molecular weights, which led to the need for tools to determine the number and types of atoms that could be associated with molecules and the arrangement of those atoms. Depicting molecules as graphs, where atoms are vertices and edges are the bonds allowed mathematicians and chemists to work together to enumerate all the different isomers of molecules that could have the same molecular weight – greatly increasing the breadth of early organic chemistry.

So one of the things that surprised me about my research is how intertwined the disciplines are. They've branched out over time, but if you go back in time, there was a tremendous amount of overlap and similarity. I feel like we're in the process of rejoining some of these disciplines a little bit more, and that's been really lovely to try and understand in a more meaningful way.

MP: Where do you think we are right now in relation to open data, and if we're not where we should be, what's stopping it?

AC: It's a complicated problem because data has value when effort is used to create it. You can think about it in the context of someone who designs an instrument to be able to measure something in a new way. A lot of people would say, "Oh, well, if someone designs a new instrument, obviously they're going to have some proprietary access to this instrument for a while." But eventually the expectation is that other people need to be able to make or buy their own instrument and reproduce the measurements. You want that tool to migrate into the broader community — it shouldn't be something that's sequestered away. The use of data is somewhat similar.

In my field, there are people that develop new simulation approaches, for example, that allow them to probe chemical systems that were not available to be looked at before. I respect the amount of effort it takes to be able to create those datasets and recognise that those people have first access to those datasets. But then it needs to be shared with the general chemistry community to allow all of the creativity and perspectives of a broader group of people to learn from that dataset. In the end, the impact of the data is more significant if it is open to the community.

It's an ongoing discussion, but I haven't seen a huge amount of action yet with respect to making data that was originally proprietary openly accessible. I hope that it's something that over the next decade we can collectively start to agree on more. Part of this is also coming from funding agencies that are recognising the opportunities of open data, but there needs to be a plan in place.

MP: What advice would you give to early career researchers in your field?

AC: Every discipline's a little bit different, but in chemistry there is a historical perspective about the way in which you do science that emphasises sticking to the field in which you were trained. There are good reasons for that, but I also think that research is evolving, and it's incredibly important for people to be brave as they consider their own research paths. It's gutsy to try and be interdisciplinary and to do new things. It's scary because it's not necessarily what you were trained to do. But what I appreciate now more than ever is that chemists bring a huge amount of value to the table when they tackle interdisciplinary problems because of their excellent problem-solving skills and because chemistry is "the central science"; our domain expertise is transferrable across many problems. I would really encourage early career researchers to be brave and ask a lot of questions and to be curious

about things that are beyond what they were trained in.

You never lose by being curious. You never lose by trying to put your perspective to a problem that is daunting and out of the box. I would really advocate for the value of curiosity, and engaging with new groups of people, trying to learn from those other groups of people as you progress in your own professional development. I think that advice is good for everybody.