AI 4 Science Discovery Network+

AI4SD Interview with Dr Paul Dingwall
22/03/2021
Online Interview

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Humans-of-AI4SD:Interview-19

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Network: Artificial Intelligence and Augmented Intelligence for Automated Investigations for Scientific Discovery

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1 Interview Details

Title	AI4SD Interview with Dr Paul Dingwall
Interviewer	MP: Michelle Pauli - MichellePauli Ltd
Interviewee	PD: Dr Paul Dingwall - Queens University Belfast
Interview Location	Online Interview
Dates	22/03/2021

2 Biography

Figure 1: Dr Paul Dingwall

Dr Paul Dingwall: 'Don't agonise over writing grants - just get it done!'

Paul Dingwall is a Lecturer, School of Chemistry and Chemical Engineering, at Queen's University Belfast

In this Humans of AI4SD interview he discusses data-driven approaches to mechanistic investigation, communicating across disciplines, the lack of progress with AI in synthetic chemistry, and his advice to early career researchers.

3 Interview

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

PD: I'm an early career researcher, three and a half years into my position at Queen's University Belfast. I started my undergraduate degree as a chemical engineer at Imperial College, before I decided to make the jump into chemistry. There was a little too much maths in chemical engineering for me!

There was a particularly good lecturer at Imperial at the time, Donna Blackmond, who was positioned between chemistry and chemical engineering. I liked the work she presented very much, and she had a joint PhD with Alan Armstrong, which had become available. I dropped into the Armstrong group just as Donna left Imperial for Scripps and started a PhD in organic chemistry. I had done about two weeks of organic lab work prior to the PhD, so it was a baptism by fire. I came in as a total outsider, but I learnt a lot while I was there. I also got interested in computational chemistry at that time, particularly density functional theory (DFT), as there wasn't much machine learning back then.

I came out of my PhD to put my fingers in many pies. I did some interesting DFT research at Imperial in Charlotte Williams's group studying polymerisation mechanims for six months. I then moved to UCL for a postdoc in materials chemistry, before moving up to St Andrew's for two years in the Clarke group, investigating mechanisms in hydroformylation and carbonylation catalysis. Then I went down to Cambridge to the Ley group for nine months, where I did some solid flow chemistry, before getting my position at Queen's: a lectureship in physical organic chemistry.

I spent around four and a half years as a postdoc bouncing between shorter positions. People tend to go to one place and stick there, but hopefully I picked up a few different skills moving around. I feel like a bit of a jack-of-all-trades, as opposed to a specialist in one area.

MP: What kind of research are you doing at the moment?

PD: I'm particularly interested in studying reaction mechanisms in homogeneous catalysis, using reaction kinetics to investigate this. That's my bread and butter. On top of that, I am continuing to use DFT to complement these experimental investigations.

What I'd really like to get into is modern data-driven approaches to mechanistic investigation. With traditional approaches, you would monitor a few reactions and use Excel to get initial rate data. But the modern approaches use multivariate analysis and statistical modelling to pull out interesting mechanism details from a homogenous catalysis. If you then include things like machine learning, you go beyond the boundaries of traditional chemistry into system modelling and computer science, and see what new tools they have to offer.

My project with AI4SD is fantastically serendipitous. I'm not an expert in machine learning, but I'm collaborating with Dr Son Mai, in the department of computer science, who is. We met at a Queen's event for early career lecturers and we hit it off. We decided to write a grant together and see where it would go. We essentially married Son's research interest in active learning and cost-effective prediction with mine in homogeneous catalysis and kinetics.

The project is quite interesting because it has a lab component. We're trying to predict kinetic profiles, whereas normally, when you predict a reaction, you'd use a lot of single time point yield data. You can't really do that with kinetics; you have to be there to repeatedly sample reactions and to make a curve over time. We're hoping that the active learning involved will be a particularly cost-effective approach. We're currently waiting for the data to roll in before the computer scientists start to play with it, but it's an iterative approach.

I'm hoping that we'll be able to use this kinetic data to predict reaction mechanisms as well. That would mean we aren't simply able to say, "I predict this set of conditions will give an 80% yield," but we would be able to predict how long it takes to reach that yield and, from the order in each substrate, ideal concentrations as well as the likely reaction mechanism. Practically, this is very useful, for instance if an additive or substrate is zero order, then it won't affect the reaction rate so you know you don't have to add very much and can save on precious or expensive material. It would also hopefully mean being able to scope out the mechanism from an armchair as opposed to being in a lab.

MP: What has surprised you so far in this research?

PD: The only thing which has surprised me is how long it takes to get anything done experimentally, but other than that it's gone remarkably smoothly.

Communication across disciplines with my research partner and me has been relatively easy. He's incredibly interested in the chemistry, and as long as we talk through each point, checking with each other that we understand it in our own words, it works well. When you get the other person to explain it back to you, you can be sure that they understand in the right way. But the differences in our approaches are part of the fun and you learn a lot.

MP: How is AI machine learning changing how we do science?

PD: There's certainly been a lot of hype around AI machine learning and a lot of progress in certain areas. Google's AlphaFold would be the most high-profile recent example. Within synthetic chemistry and physical organic chemistry, there has been very little progress. I'm not entirely sure why this is. Part of the issue is that chemistry is an old, fragmented and siloed field, and it can be difficult for ideas to jump across. There are also some experimental researchers with the mindset of needing to be in the lab.

In the last year, there's been one publication on active learning in the context of synthetic chemistry, but if you look outside of that area, at drug development for example, there's a huge amount of research on active learning. There's just very little within the synthetic community. Hopefully with our project, we'll be able to demonstrate its use, and roll it out a bit more.

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

PD: A good piece of advice I received is that you're your own best postdoc for your first four-to-five years. The good synthetic labs that I've been in have one very experienced postdoc who deals with the daily problems that crop up. It helps to be in the lab as much as possible, to help push things along and solve little problems.

I also found it useful to investigate things myself. Recently, I had an idea for a grant, so I went to the lab to try to synthesise something myself. It was the first time I had done a column in around a year, but I made a compound, I tested it, and the reaction worked. So now I'm in a position where I'm able to write a grant.

Another piece of advice, on the topic of writing grants, is don't agonise over it. Just get it done. I spent far too long writing my first grant, tweaking a sentence here and there. It's better to just get it in and out of the way. It's the idea that counts, not whether what you said on this particular paragraph on page three is perfect. The success of the grant is determined by whether or not it's a good idea. That would have been good to have been told two years ago!