AI 4 Science Discovery Network+

AI4SD Interview with Dr Olexandr Isayev
01/12/2021
Online Interview

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Humans-of-AI4SD:Interview-39

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Interviewee	OI: Dr Olexandr Isayev - Carnegie Mellon University
Interview Location	Online Interview
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2 Biography

Figure 1: Dr Olexandr Isayev

Olexandr Isayev: 'We're seeing the next evolution in how we do science – and it's liberating'

Olexandr Isayev is an Assistant Professor at the Department of Chemistry at Carnegie Mellon University. In 2008, Olexandr received his PhD in computational chemistry. He was Postdoctoral Research Fellow at Case Western Reserve University and a scientist at the government research lab. During 2016-2019 he was on faculty at UNC Eshelman School of Pharmacy, the University of North Carolina at Chapel Hill.

In this Humans of AI4SD interview he discusses developing the next generation of computational chemistry methods, the challenges and rewards of multidisciplinary projects, how AI is changing science and the importance of cultural change for open science.

3 Interview

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

OI: I grew up in the late Soviet Union, in Ukraine. I was a very nerdy boy. I was always disassembling things and mixing liquids, which left my parents very unhappy! There was an occasional explosion, which would get me into trouble at school. But eventually this passion, and an interest in science fiction books, helped to steer me towards the scientific career I'm in now.

I've always had a fascination with computers and I started programming at an early age, making primitive games. Alongside the chemistry experiments, I guess that is what led me to computational chemistry. Now, I'm actually looking at learning robots — as a child I could never have dreamed I would end up doing this.

I completed my undergrad in Ukraine but, in the 1990s, things in the ex-Soviet Union were very bad, so a scientific career wasn't viable. So I looked to the US to apply for PhDs, and I was successful. It's now been 20 years since I left Ukraine. I'm very much proud of my home country still, but I now feel Ukrainian-American.

MP: What kind of research are you working on currently?

OI: My laboratory is at Carnegie Mellon University (CMU) in Pittsburgh, Pennsylvania. Although by training I'm a hardcore quantum mechanics and computational person, for the past seven or so years I have worked at the intersection between chemistry, machine learning and AI. CMU is at the forefront of the next AI machine learning revolution, helping to amalgamate technologies and taking chemistry forward.

We have a few different projects at the moment. One of the big directions involves developing the next generation of computational chemistry methods. Whereas quantum mechanics and force fields have traditionally been used, they have their limitations. Now, data-driven technology and algorithms help to make these methods faster and more accurate. We also use these methods to help national projects on the application side. For example, with drug discovery, we developed molecules that would attach to certain proteins. We work with medicinal chemists to computationally design or to screen molecules for certain experiments.

The next generation of experiments are actually driven by a robotic system, by automation. We develop the algorithms, we orchestrate and script them, so they are able to do automatic pipetting, mixing and learning reactions. So there are a few big directions our research is going in!

MP: What kinds of challenges are you finding in the research?

OI: There is always a challenge when you interface with multiple disciplines; people speak different languages, and these gaps must be bridged. As a computational person you might think a lot about algorithmic functions, but then a person from the lab would think about something completely different, and understanding is needed here between the languages.

You cannot overestimate how important it is to listen. This is the most important skill I have learned. Listening well also helps me to be a mentor and to educate my students. It's very rare that we work in isolation, so this practice helps. As a scientist changing countries and

moving to different jobs, working in both industrial, academic and governmental lab settings, that range of experience helps.

You also need to be able to explain the subject. Teaching ourselves not to use the jargon and the specialised language, but to explain complex phenomena in simple language in a way that people understand. It also helps if students do outreach too. If, for example, PhD students speak at schools and museums, this practice of interacting with 'normal' people helps.

I think there's a moral obligation for us as scientists to benefit society, especially because it's mostly paid for by the state, with public money. One of our missions is to educate the public, especially during the pandemic when a lot of people have become sceptical about public health. There are a lot of misconceptions in relation to both chemistry and AI. Typically, the response you get about chemistry is that it's all bad, people saying nonsense like they don't want chemistry in their food. With AI, people's opinions are generally shaped by movies, people think of Terminator. But because there's now a constant stream of media, there is a lot of misinformation circulating. It can be hard to challenge these misconceptions.

MP: Away from the misconceptions about it, how is AI changing how we do science?

OI: It's been a really fascinating time, and I think we're seeing the next evolution in how we do science. Just as in the Industrial Revolution, something similar is happening in the sciences. We now have smart machines, automation, and algorithms running these machines, which are getting rid of tedious work and manual labour. Say, for example, you used to do farming completely manually and can only do a certain amount of square acres of land per day; with tractors and other machines, that work became much more efficient. This kind of process translates on a practical level to how much more efficient we are in running experiments and synthesising molecules and materials.

On a more conceptual level, machine learning and AI algorithms allow us to do science more efficiently. Our human brains are not perfect — we cannot grasp a lot of information and typically we have difficulties understanding multidimensional problems. With a science experiment, there are a lot of different things to control: how you mix, what you mix, how you heat, how much time to wait, what's in it. There are so many variables to control, but the algorithms of machine learning are extremely efficient in controlling them. If made well, these algorithms have less bias and can also be run 24/7. This can help us to transform how science is done.

Eventually, there will be ways that humans can be augmented with algorithms. It's very futuristic right now, but we are already seeing it in certain limited tasks. Still, I don't believe that humans will be replaced by robots. What will happen is that humans will be liberated from boring, manual tasks. In organic chemistry, for example, if you want to optimise the conditions of reaction, you have to spend long hours in the lab and try multiple things. If this manual task is outsourced, imagine the opportunities that would give the creative sides of your brain. You can do more productive work instead of wasting your time on repetitive and tedious tasks. It's already beginning to lift humans to the next level of what we can do.

MP: What has surprised you in your work?

OI: What's surprised me is the creativity in how things have been adapted from computer sciences and applied to chemistry, physics, and biology. Some real magic has happened at the

interface between the fields, when one group has a solution to another's problem, and an interesting, unexpected result has taken place. I'm so happy to see these transformations.

MP: Do you think this interdisciplinarity should filter down into education?

OI: Absolutely. In the US, our chemistry curricula is extremely classic. It's a controversial subject, but I genuinely think that in the 21st century, everyone should be able to code, as a skill it's a must. Most chemists need to know the basis of statistics and data analysis, because even if you don't do machine learning, you're always dealing with data. The standard curricula need to be refreshed, and programming needs to be there in school. When I was around 10, we had a kind of coding club, which taught me these things. This education should be far more widespread in the school system.

MP: How do you see the current state of play with open science?

OI: Open science is crucial. We have a lot of problems with reproducibility in the field, with some claims being very hard to verify. It's a little better in the physical sciences, but in medicine, biomedical, and the social sciences, it's a dire situation. I advocate for open science, and most of our data is available from GitHub. I try to lead by example.

Several colleagues and I published our opinion in Nature Chemistry about machine learning and chemistry, in which we essentially came up with a checklist of how to make open, reproducible science. This has to happen on the sides of both the scientists and the publishers. The top publishers and funding agencies can mandate, but when things happen from the top, they may backfire. For example, Plan S in Europe: it had good intentions but it was executed badly. From the bottom up, the key is education and cultural change. Sometimes people are afraid of competition or embarrassment about others judging the quality of your code. Making this cultural change requires the collective effort of many stakeholders.

MP: What advice would you have for early career researchers?

OI: Steve Jobs once said, "Stay hungry, stay foolish," and I think that's good advice. This kind of curiosity certainly helped me, but also persistence and tenacity, because being a scientist is hard in many ways.