Big Data robot lab will shape the chemistry of the 21st century

The most complex system in the world around us is life itself, with each cell in your body containing a complex network of molecules and chemical reactions. Chemists have now almost come to the point where they can study and even reconstruct these systems, yet current technology can't fully comprehend its vast complexity. We need a new approach.

According to Radboud University professor Wilhelm Huck, the chemistry of the 21st century is Big Chemistry. He was granted 97 million euros by the Dutch National Growth Fund to shape the Big Chemistry research programme of the Netherlands. We spoke to him about his ground-breaking plans to build a new world-class infrastructure for research into complex molecular systems.

The Netherlands is one of the leading countries when it comes to research into complex molecular systems. It is a direction within chemistry for which Ben Feringa received the Nobel Prize for Chemistry in 2016. The Netherlands considers this an important topic, as evidenced by, among other things, the 30 million euros previously invested in it through a gravity programme. With the Big Chemistry programme, Wilhelm wants to continue in this direction. "The programme will apply artificial intelligence (AI) to learn from the enormous torrent of data that a revolutionary robotic chemistry lab on the Noviotech Campus in Nijmegen will generate. In collaboration with companies and knowledge institutions, such as the Max Planck Institute, we will create a new ecosystem – openly using and sharing data, technologies and knowledge."

To be honest, we never realised there is a connection between data and chemistry.

"What's more: the field of chemistry I'm working in has become so complicated and complex that you can't really get anywhere without the use of AI. Many chemical systems become so complex, that at a certain point humans can no longer put their finger on where exactly a certain characteristic of the system comes from. In a sense, the complexity is getting too much for us. That's where AI comes in as a necessary condition for moving forward."

Why do you need a robot lab to make this happen?

"In order to apply AI, you need enormous amountsof data to feed the self-learning AI programmes. The more data, the better. This means that we have to organise chemistry in such a way that data is produced and stored properly and reliably. The robot lab we're planning to build at the Noviotech Campus in Nijmegen aims to do exactly that. The robot lab will be full of automated, high-throughput systems to provide the torrent of data we use to train the AI systems that can deal with such complex chemical systems."

"WE EXPECT THIS ECOSYSTEM TO CONTRIBUTE ABOUT 400 TO 750 MILLION EUROS TO THE DUTCH GROSS DOMESTIC PRODUCT"

"You have to see the robot lab as one big scientific instrument that all kinds of companies and knowledge institutions can start using. It is an infrastructure that we will make widely available. It is not our intention to, for example, make paint; other companies are better at that. We can help them to make new, better, faster formulations that meet requirements such as sustainability. We might also be working together with scientists who, for example, see possibilities to build a computer with DNA and biomolecules."

A lot of opportunities then, but where are you going to start?

"Well, first things first. We will use the funding we received from the Dutch National Growth Fund. For setting up and building the robot lab. Finding out how you do it, integrating all the components and developing and training the AI. Making sure the AI starts to understand what chemistry actually is, will already be difficult and time-consuming. The next step will be to get together with industrial partners and see which things we can tackle first. We already have contact with companies that specialise in food, soft drinks, medicines, paints and coatings. They all make products based on complicated formulations and processes with many components."

How do companies benefit from the robot lab?

"The companies have a lot of expertise, but they often arrive at new products only through a cumbersome process of trial and error. Right now,

formulating those products is still an art, but we want to turn that into a science-based technology! In most cases, that specific taste is the result of a complex combination of parameters. The AI system can use this knowledge to develop new products faster, better and more reliably. In this way, art becomes a skill.

"THE COMPLEXITY OF CHEMICAL SYSTEMS IS GETTING TOO MUCH FOR US HUMANS, THAT'S WHERE AI COMES IN"

But again, it's important to start simple and develop from there. With the successes, you move on as the basis for new generations of ideas. A robot lab for coatings, a robot lab for formulating shampoo. Modular, by connecting two or three devices per topic first and not twenty right away. With such a simple start – which is already complex enough – you can set up several robot labs for various subjects at the same time, and possibly connect them together later if they prove to be successful."

Connecting several robot labs to each other... How does that work?

"The underlying value, the hidden treasure trove, is the data that is going into the system faster and on a larger scale. The idea is very strong because – like Facebook and Google – anyone can use it. And the more it is used, the better the algorithm is trained, and the more valuable the database becomes. That is actually the core idea: to bundle everything in a central, physical robot lab in Nijmegen.

"WE WILL TRAIN AI TO KNOW WHY BEER TASTES THE WAY IT DOES"

We also want to combine that robot lab with an absolute top scientific institute that can handle such high throughput, AI and complex chemistry. To do so, we want to bring a Max Planck Institute to Nijmegen. The city already has a Max Planck Institute for Psycholinguistics, which might make the arrival of a second institute a little easier."

Are there similar initiatives globally?

"Some academic labs and pharmaceutical companies are also pushing for this approach. Consortia in Canada, the U.S. and China want to move toward automated labs, but they're not that far along yet. So, it's important that we take the lead quickly. The Netherlands has very good prospects of playing a leading role in this field.

If we do it right, this will become a flourishing ecosystem, and in a few years' time you will really have to be in Nijmegen if you want to take part in chemical robotics. A boom of new companies could emerge, not only in chemical analysis and synthesis, but also in building equipment, in training people, in AI, and so on. Once it is up and running, such an ecosystem has a strong pull on all kinds of other sub-activities."

What could be the economic impact of such an ecosystem?

"We expect this ecosystem to contribute about 400 to 750 million euros to the Dutch gross domestic product in the long term. Also, I think the robot lab as a system will already generate money. We have a sort of imec model in mind for this. Imec arose from the University of Leuven with the idea that everything is becoming miniaturised, that electronics are becoming smaller and smaller. That they couldn't do all this themselves and realised that an open system, a network, was needed for this. Eventually, imec developed into a non-profit organisation, where a lot of money is involved. Where industry and science meet, and which has grown into a major global player from which they still benefit enormously in Leuven. That's the model we have in mind as well."

Could this ecosystem and the robot lab eventually help to find the origins of the most complex system we know, life itself?

"We're not working directly on core questions in science like 'how did life come to be'. But what we are setting up now is definitely going to contribute to that in the long run. And more than that. Self-learning AI, with Big Data from the robot lab, will eventually provide answers to problems we can't even think of at the moment. With the money from the Growth Fund, we will establish a brand-new infrastructure for complex molecular systems that is actually impossible to achieve in any other way, and necessary for a different way of doing chemistry. And in the longer term we will also be using this infrastructure for a greener economy, more sustainable production, the fight against environmental problems and scientific issues that we are now only just beginning to scratch."

Video robot lab: the revolution of self-thinking molecular systems