

Dr. Dalal Alrajeh's Question:

"A.I. nowadays plays an instrumental role in developments in the natural sciences - these have included predicting chemical reactions, discovering protocols for stem cell differentiation and most recently, predicting 3D shapes of proteins (DeepMind, Google).

In the future, could A.I. replace human scientists and why?"

*Answer this question via a feature article, up to 1500 words*

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### **The future of self-driving labs is here**

*Despite the automation of research, AI will never fully replace human scientists*

The term “self-driving labs” sounds like something straight out of science fiction. It conjures images of humanoid robots zooming through a laboratory in a shiny, distant future where scientists no longer exist. But these robotic labs are already a reality – albeit a very different one – for researchers like Alán Aspuru-Guzik.

“It is not your *Terminator*-like robot walking around the lab doing experiments,” he says.

“You want to think more about it as a bunch of pumps that pump chemicals around to certain vessels where they react, are heated up, separated, analysed etcetera.”

Aspuru-Guzik is a professor of chemistry and computer science at the University of Toronto and a pioneer in combining Artificial Intelligence (AI) and robotics to design and discover new materials.

As we speak, his robotic chemistry lab is hard at work. The lab exists within a machine that removes all air so that any new materials are protected against oxidization. Several stationary robotic arms transfer samples and pumps transport a range of chemicals. These robotic platforms feed into a computer that uses unique machine learning techniques to design experiments and find the ideal materials much faster than humans ever could on their own.

### **Man vs. machine**

Aspuru-Guzik is creating a lab where he is less and less involved with the manual process. His ultimate goal would be a fully autonomous lab. His hope is that AI will not replace scientists, but allow them to think more creatively without the same constraints of safety, time or manual labour.

There have already been some great successes with self-driving labs in academia and industry. Discoveries range from [new chemical reactions](#) and drug design to “[sandwich makers](#)” that assemble two-dimensional materials.

Aspuru-Guzik's lab is one of the most tangible examples of AI replacing scientists, but he believes humans will always be behind the machine. To elucidate his thinking, he refers to Argentine writer Jorge Luis Borges' poem "Chess":

God moves the player, he in turn, the piece.  
But what god beyond God begins the round  
of dust and time and sleep and agonies?

The game of chess is a fitting metaphor in more ways than one. AI's defeat of [chess masters and Go champions](#) were major successes in the field. Defeating humans in these complex games has been considered a benchmark for AI reasoning. But how does AI fair in domains where the aim is not to win but to discover?

As with games, it's scientists who are setting the parameters and goals in labs. At the same time, an algorithm can explore ideas that humans might not even imagine. In chess, this could be an unconventional play while with materials discovery it could be an approach that goes against prevailing theories.

"I think it's going to be a combination of the human driving the intuition combined with the machine that's going to be more systematic, but also more naïve," Aspuru-Guzik says.

## **A history of disruption**

AI is hardly the first technology to transform the way we work or how we do science. One of the first examples of a computer arose in Ancient Greece. The Antikythera mechanism was a mechanical calculator used by astronomers to predict eclipses and where stars would be in the sky. This technology helped scientists see the universe in ways they never could with the naked eye.

Therein lies the difference between [enabling and replacing technologies](#) – an important distinction economists have made. Enabling technologies enhance human abilities whereas replacing technologies, as the name suggests, replace the human roles. AI is an interesting case because it has the potential to do both on a wide scale. Replacing is not necessarily a bad outcome so long as new roles can be created and help lift society as a whole, such as the Industrial Revolution.

The challenge that everyone faces now is in how to harness the power of AI across fields to benefit the most people. For policymakers, this question is top of mind with answers ranging from Universal Basic Income to education and skills retraining.

In the research world, integration is also key. Culturally, AI is penetrating our lives from GPS to personal assistants and now that is slowly seeping into labs. Technically, one of the problems is creating a shared language between AI, robotics and other fields like chemistry. Aspuru-Guzik has made a start at addressing the issue with [software](#) that can "translate" between them. On

the most basic level, robotics are becoming cheaper and AI usage more widespread. As these advances combine and converge, Aspuru-Guzik hopes progress in chemistry will advance exponentially.

### **Earth's 12-year deadline**

Humans have already uncovered millions of compounds, but there are at least  $10^{60}$  possible molecular compounds out there. Somewhere in these nearly infinite combinations are recipes for the best solar cells and most energy-efficient batteries. However, time is running out to find materials for a clean future.

The Intergovernmental Panel on Climate Change recently released [a report](#) calling for urgent action to limit global warming to 1.5 degrees Celsius above pre-industrial levels. The deadline to have environmental policies in place is 2030 or face devastating environmental consequences.

Using AI and robotics in combination with new scientific methods could accelerate the rate of materials discovery by a factor of 10. This would speed up the process from 20 years to one or two years, according to [a report](#) co-authored by Aspuru-Guzik as part of the Paris Agreement on climate change.

Aspuru-Guzik's career has spanned many research areas but now he is most focused on working with known reactions and developing more efficient materials for clean energy.

"The world has a deadline of 12 years to find solutions to climate change and therefore I am in engineering mode," he says.

One of the greatest challenges, in his opinion, is not that AI will replace humans but that political problems will divide society.

Aspuru-Guzik has [spoken out](#) about the United States' decision to leave the Paris Agreement as well as the country's shift in politics, especially with the presidential election of Donald Trump. Aspuru-Guzik is a dual citizen of Mexico and the United States who had been living in the U.S. for nearly 20 years before leaving his position as a tenured professor at Harvard University to move to Canada.

"You should never be scared of artificial intelligence," he says.

"You should always be scared of the lack of human intelligence."

(1,076 words)