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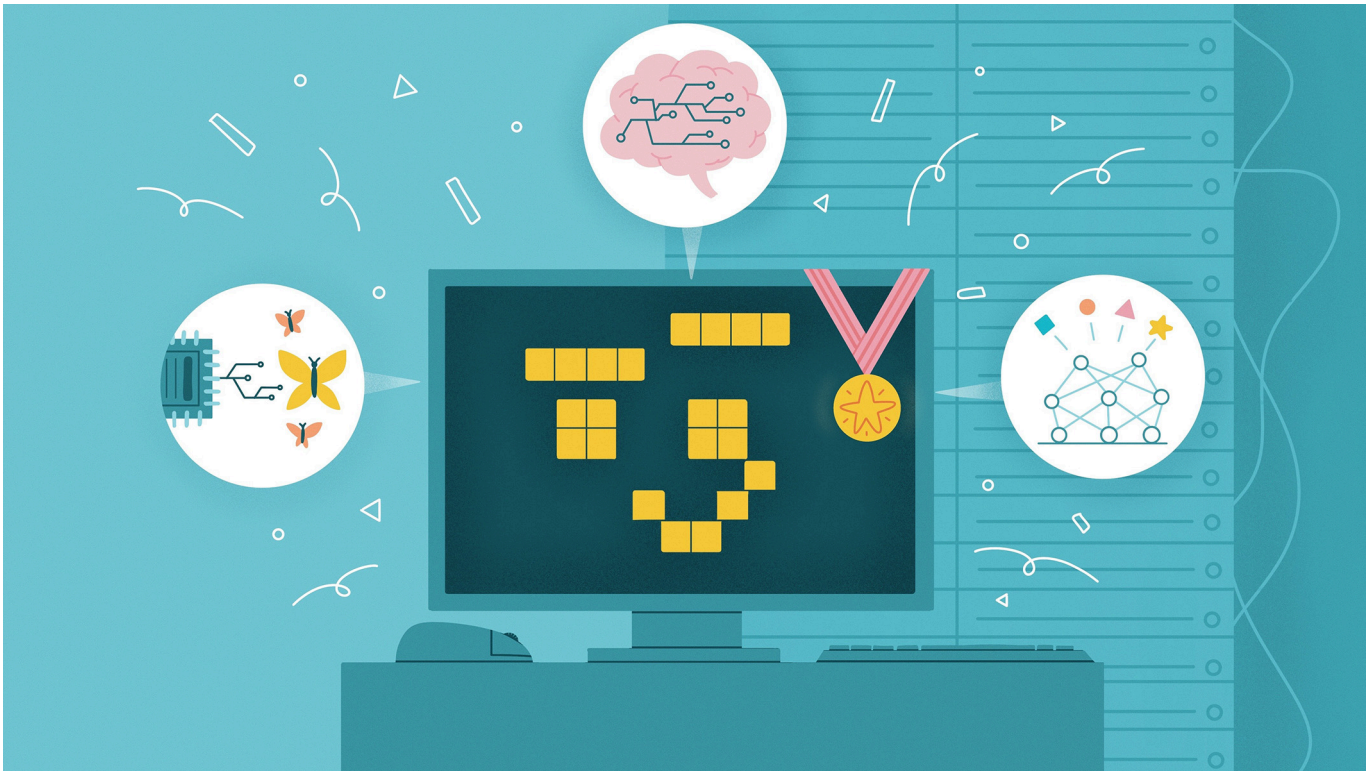

CAN ARTIFICIAL INTELLIGENCE HELP SCIENTISTS DISCOVER MORE, FASTER?

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YOUNG REVIEWERS:

YOURAN
AGE: 14

ZICHEN
AGE: 13

Artificial intelligence (AI) is changing the way scientists make discoveries, helping solve some of the world's biggest challenges faster than ever. By using powerful computer systems, AI can analyze massive amounts of data, uncover patterns, and create solutions that humans might not find on their own. Three recent advancements in AI—deep learning, generative AI, and foundation models—are revolutionizing fields like medicine, energy, and climate science. For example, AI has predicted protein structures in days instead of years, discovered new antibiotics to fight superbugs, and designed better materials for solar panels and electric car batteries. However, AI still faces challenges, like ensuring the data it uses is unbiased, reducing

energy use, and protecting privacy. With careful development and teamwork, AI could help scientists tackle the complex problems we face today by making the future of science faster and smarter.

THE WORLD NEEDS FASTER SCIENCE

What do smartphones, vaccines, and solar panels have in common? They are all amazing solutions created through science! Science has always been a powerful tool for understanding the world and solving big problems. The scientific breakthroughs that shape our lives today did not happen overnight—they took years, sometimes decades, of careful research, experimentation, and problem solving.

However, the challenges we face today are becoming more complex. Climate change is speeding up, new diseases are emerging, and "green" solutions are needed to keep the planet healthy as the world's population grows. Will the pace of science be able to keep up? To solve the serious, complicated problems of the modern world, we need a way to speed up scientific processes, so that scientists can make discoveries in months instead of years. But how?

EMERGING TECHNOLOGY: AI FOR SCIENTIFIC DISCOVERY

Artificial intelligence (AI) is a powerful branch of computer science in which computers are designed to perform tasks that typically require human intelligence—like scientific discoveries! AI can help researchers solve problems faster and uncover connections they might not see on their own. This could help scientists to tackle pressing global issues more efficiently, opening up new frontiers of knowledge that were previously beyond our reach.

Three main types of AI are changing the way we do science: **deep learning**, **generative AI**, and **foundation models**. These technologies emerged over time, with deep learning appearing first, followed by generative AI, and most recently, foundation models—each building on the progress of the one before it.

Imagine you are sorting a huge pile of LEGO bricks by color and shape. You start by looking at each brick and putting it in the right pile, but soon you realize that the task is going to take you all day. What if a robot could do it for you, learning from how you sort the first few bricks? That is the idea behind deep learning. Deep learning is a type of AI in which computers use interconnected networks, similar to the network of nerve cells in the human brain, to analyze complex data and recognize patterns. Using deep learning, AI can analyze vast amounts

ARTIFICIAL INTELLIGENCE

A type of computer technology that helps machines think, learn, and solve problems like humans do, such as recognizing faces or predicting the weather.

DEEP LEARNING

A type of AI in which computers learn using connected systems, similar to brain cells, to recognize patterns and make decisions—like identifying animals in photos or detecting diseases in medical images.

GENERATIVE AI

A type of AI that creates new things, like pictures, music, or scientific ideas, by learning from examples and using its knowledge to solve creative problems.

FOUNDATION MODELS

Large computer programs trained on lots of information, like books, the internet or weather data, that can be adapted to solve different problems, such as translating languages or predicting storms.

of data in the blink of an eye, uncovering patterns and solutions that might elude even the most experienced scientists.

You may have already heard about generative AI—maybe you have used it to help you complete a homework assignment, create a picture, or write a story. While deep learning is great at recognizing patterns, generative AI is like a creative artist that makes new things. But in addition to writing a poem or drawing a picture, generative AI could be used for scientific purposes, like helping to design a new molecule for a medicine. Generative AI also learns from existing data—like a library of images or chemical formulas—but unlike deep learning, it uses that knowledge to create something original.

Last, while other AI tools are a bit like screwdrivers—great for one specific job, like tightening screws—foundation models are like Swiss Army knives, equipped to handle many different tasks. These models are trained on enormous collections of data—thousands of books and articles for models that understand and generate language, and weather patterns and climate records for models that predict storms or track global warming—so they "know" a lot about many topics. These models serve as a base upon which more specialized applications are built by individual scientists, much like a foundation supports a building.

If these brief descriptions leave you wanting more details about how artificial intelligence works, check out this Frontiers for Young Minds article, this website, or this one.

TECH TO THE RESCUE

There are many examples of how AI is helping scientists work faster and smarter, changing the way scientific discoveries are made (Figure 1).

AlphaFold is an AI system that predicts the 3D structures of proteins [1]. Proteins are like tiny machines in our bodies—they carry oxygen, fight infections, and help us grow and repair ourselves. Understanding the shapes of proteins is crucial because their structures determine how they work. Before AlphaFold, figuring out a protein's 3D structure could take years of experiments, but now AI can do it in just minutes. This breakthrough uses deep learning. By training on a vast amount of existing protein data—such as information about how proteins are structured and how they fold—AlphaFold "learns" to spot patterns and predict the shapes of proteins with incredible accuracy. Scientists are now using these predictions to design new medicines and understand diseases better than ever before. This breakthrough has been so impactful that the developers of AlphaFold were awarded the Nobel Prize in Chemistry in 2024.

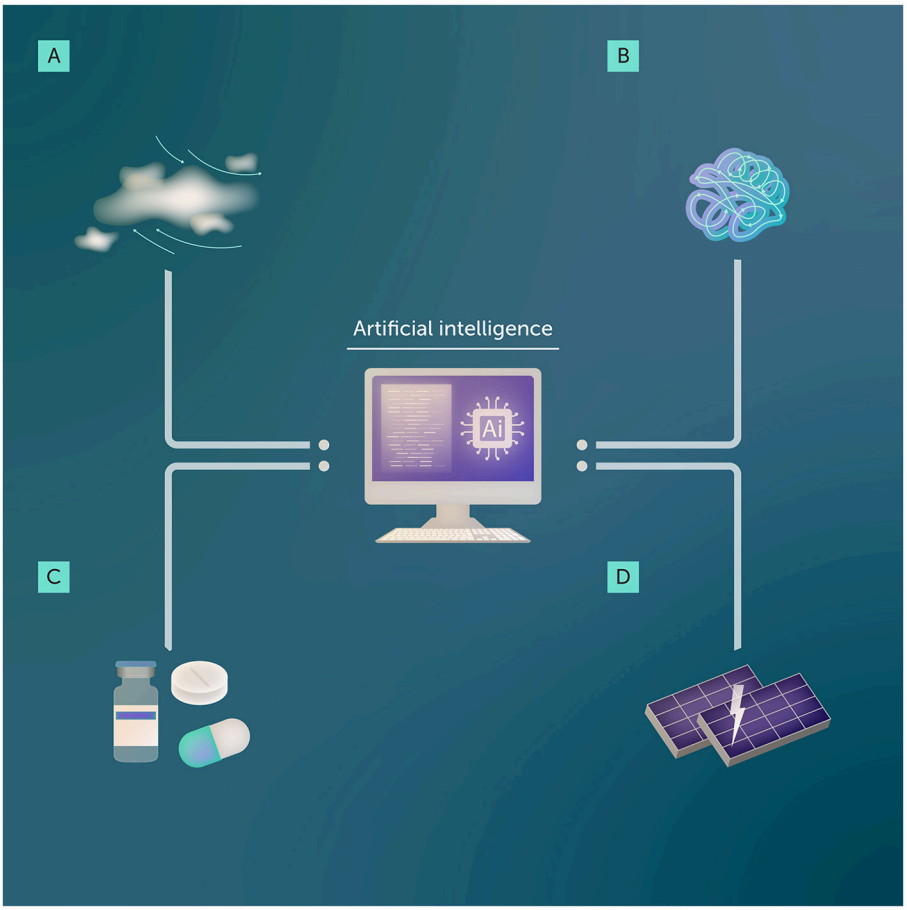

Figure 1

Here are just a few examples of how AI helps scientists work faster and smarter. **(A)** Foundation models trained on vast amounts of weather data can help predict storms and other weather patterns. **(B)** The AlphaFold system, based on deep learning, can predict the structures of proteins in just minutes—a process that used to take years. **(C, D)** Generative AI can suggest potential new materials that scientists might never have thought to test, like novel medicines to treat superbugs and other dangerous diseases, or materials that can improve batteries or make solar panels more efficient at changing sunlight into electricity.

Have you heard about dangerous bacteria, often called "superbugs", that can no longer be killed by the medicines (antibiotics) usually used to treat them? These bacteria are a major health threat all over the world. Developing new antibiotics from scratch can take years of research and testing before the medicines finally become available to patients. Researchers have developed deep learning AI systems that can screen millions of already-existing chemical compounds to see if they might work as antibiotics [2]. In 2020, this AI system discovered a powerful new antibiotic named halicin, capable of killing a wide range of superbugs [3]. This discovery was especially exciting because halicin's structure is different from existing antibiotics, offering a new weapon against antibiotic-resistant bacteria. Deep learning is also used in self-driving cars, to identify pedestrians or stop signs, and in healthcare, to analyze medical scans for early signs of disease.

Discovering new materials—like potential medicines for diseases or materials that could be used to make cheaper or longer-lasting batteries for electric cars—can involve countless experiments to test hundreds or even thousands of chemical combinations. Now, researchers can use generative AI to design materials with specific properties, like conducting electricity efficiently or withstanding

extreme temperatures. Generative AI can suggest promising candidates that scientists might never have thought to test. For example, generative AI helped identify new compounds for Perovskite solar cells—materials used to build next-generation solar panels—by proposing combinations that scientists had not previously considered [4].

Foundation models are also starting to play a significant role in science. Instead of starting from scratch, researchers can fine-tune existing foundation models to answer their scientific questions, making breakthroughs faster and more efficient. These models can be adapted for many different problems, from analyzing DNA sequences to predicting weather patterns. A foundation model trained on weather data might help predict storms, but it could also be fine-tuned by other scientists to study climate change or track unusual weather patterns. One group of scientists fine-tuned a language foundation model to read and explain complex chemistry papers, helping researchers quickly understand new discoveries without reading every word [5].

BIG CHALLENGES, BIGGER OPPORTUNITIES

AI and science are working together to make discoveries that once seemed impossible. These discoveries could help solve some of the world's biggest problems, like curing diseases or fighting climate change. But using AI in science is not always easy. One big challenge is giving AI access to all the science of the past—today, most scientific articles are not freely accessible. Open science is a new movement that includes open access publishing and data sharing. Another big challenge is making sure the data AI learns from is fair and complete. If the data is **biased** or missing important information, AI might make mistakes or give results we cannot trust. Scientists are working hard to check and improve AI systems to make them as reliable as possible.

BIASED

Unfair or incomplete, like when information leaves out certain groups or ideas, which can lead to mistakes or unfair results.

Another challenge is that training AI uses a lot of electricity, which can harm the environment by contributing to global warming. Researchers are trying to find ways to make AI systems use less energy, for example by learning from the human brain, see here. Finally, there are important questions about keeping people's private information, like medical records, safe, and deciding who owns the discoveries made by AI. Scientists and government leaders are working together to figure out the best rules for using AI responsibly.

AI has the power to change science and help solve problems like disease, climate change, and more. The world needs faster science—and with the right mix of creativity and care, AI could help shape a better future for all of us.

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YOUNG REVIEWERS

YOURAN, AGE: 14

Hai! My name is Bella, a 14-year-old with an exceptional interest in STEM. My favorite subjects to study are math and science, and I can proudly say that I excel in both. Outside of studying, I play tennis regularly and have a great enthusiasm for it. I have also been playing piano for 8 years. In the future, I hope to explore science and math in greater depth while maintaining my interest in sports and music.

ZICHEN, AGE: 13

I am currently 13 years old. I enjoy reading and playing interscholastic sports. I am curious and like to learn. I am also volunteering in a non-profit organization that helps kids with autism.

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Andrew Maynard is a scientist and author who studies how new technologies affect society. He is a Professor at Arizona State University (ASU) in the School for the Future of Innovation in Society, where he also directs the Risk Innovation Lab. His work focuses on understanding the risks and benefits of emerging technologies like nanotechnology and artificial intelligence. Dr. Maynard has written books such as "Films from the Future" and "Future Rising", exploring the impact of technology on our lives. He also shares his insights through podcasts and articles, helping people understand the complex relationship between technology and society.

SANG YUP LEE

Sang Yup Lee is a scientist who leads research at the Korea Advanced Institute of Science and Technology (KAIST). He studies how to use tiny living things, like bacteria, to make useful products such as fuels and materials. His work helps create eco-friendly alternatives to traditional chemical processes. Dr. Lee has received many awards for his contributions to science and serves on advisory councils to share his expertise.

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Olga Fink is a scientist who leads the Intelligent Maintenance and Operations Systems Laboratory at the Swiss Federal Institute of Technology in Lausanne (EPFL). She uses artificial intelligence to help machines and infrastructure work better and last longer. Before joining EPFL in 2022, she was a professor at ETH Zurich and led the Smart Maintenance research group at the Zurich University of Applied Sciences. Dr. Fink earned her Ph.D. from ETH Zurich and has been recognized as a Young Scientist by the World Economic Forum.

THOMAS HARTUNG

Thomas Hartung has spent more than three decades of his career promoting technologies to replace animal testing. From 2002 to 2008, he led the European Center for the Validation of Alternative Methods (to animal experiments) of the European Commission in Italy, and since 2009 he has led the Centers for Alternatives to Animal Testing in the US and Europe. He is active in many fields of science: he started by studying biochemistry, human medicine, and mathematics/informatics; he initially became a doctor (M.D./Ph.D.), and then a professor of both pharmacology and toxicology. He later expanded his work to include immunology, microbiology, and engineering. Today he holds five professorships at Johns Hopkins University and Georgetown University in the US and at the University of Konstanz in Germany. He is field chief editor of Frontiers in Artificial Intelligence. Aiming to bioengineer brain functions in human organoids, he steers a community of scientists to establish organoid intelligence. *thartung@jhsph.edu