CHEN INSTITUTE TIANQIAO & CHRISSY

3D model of a protein generated with the help of AI

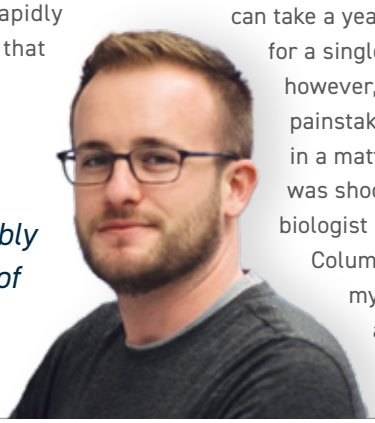
To Turbo-Charge Scientific Discovery, Researchers Are Turning to AI

The Chen Institute & Science Prize for AI-Accelerated Research recognizes researchers pushing back the frontiers of human knowledge.

The first mRNA COVID vaccines saved millions of lives and won their creators the Nobel prize—but there's always room for improvement. At the University of Washington, researchers recently unveiled a next-generation vaccine using a novel protein to give the immune system a more precise target, delivering robust and long-lasting protection with fewer side effects and no need for refrigeration.

The key to that breakthrough? The team's use of advanced software to rapidly engineer novel proteins—a challenge that's been turbocharged by AI tools developed in the last four years.

"There are more ways to make a protein than there are atoms in the universe, so it's an incomprehensibly large space to explore," explains Ian Haydon, head of communications at the University of Washington's Institute for Protein Design. "But using machine learning, we're able to rapidly find useful molecules in that ocean of possibility."



The team's efforts—which could soon yield further novel medications including a multi-year flu vaccine and a gluten-digesting enzyme for celiac patients—are part of a research revolution that erupted in 2020, when Google's DeepMind AI system successfully modeled the way proteins fold. Such modeling requires mapping the simultaneous interactions of over 12,000 atoms, a mind-boggling task that can take a year or more to complete for a single protein. DeepMind, however, was able to generate painstakingly accurate predictions in a matter of minutes. "It was shocking," said structural biologist Mohammed AlQuraishi of Columbia University. "Never in my life had I expected to see a scientific advance so rapid."

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Artificial neural network

Similar AI-enabled breakthroughs are now rippling across the scientific world, driven by the rise of sophisticated computer modeling, deep-learning technologies, and powerful new datasets. From tracing the boundaries of black holes to deciphering the communication of sperm whales or the inner workings of the human brain, AI is driving a Cambrian explosion in scientific discovery, and helping researchers to solve unprecedentedly complex problems, rapidly explore vast datasets—and, in some cases, ask entirely new kinds of research questions.

To accelerate that transformation, the Tianqiao & Chrissy Chen Institute (TCCI) is partnering with *Science* to launch the Chen Institute & Science Prize for AI Accelerated Research—a first-of-its-kind program designed to encourage young researchers to leverage AI in their work. The award recognizes early-career scientists who are using AI to push back the frontiers of human knowledge. Winning essays will be published in the magazine and a total prize pot of $50,000 to support AI-enabled research in the physical and life sciences.

"Artificial intelligence has the potential to break down barriers holding back scientific understanding, and unlock breakthroughs that would otherwise have taken decades to achieve," said TCCI cofounder Chrissy Chen. "Young researchers are uniquely positioned to realize that potential, and we're eager to help them become pioneers in the field of AI-enabled scientific discovery."

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The potential applications for AI technologies are as varied as scientific exploration itself. In some cases, AI can turbocharge experimentation, using automation and robotics to accelerate laboratory processes. (Unlike human lab technicians, robots never stop to take coffee breaks.)

Researchers at the Department of Energy's Lawrence Berkeley National Laboratory, for instance, have developed an automated laboratory, known as A-Lab, that can independently design and test novel material synthesis protocols up to 100 times faster than human researchers. In a single two-week period, the A-Lab created 41 new inorganic materials, helping to fast-track the development of next-generation batteries and solar panels.

"Our vision is using AI to discover the materials of the future," said Yan Zeng, a staff scientist leading the project.

In other areas, researchers are studying AI itself as a way to drive their research in important new directions. At Caltech, neuroscientist Dr. Daniel Wagenaar studies the underlying mechanics of artificial neural networks to better understand the processes at work in organic brains. That's valuable because researchers can "lift the lid" on AI models, gaining deeper insights than is possible with flesh-and-blood subjects. "AI is a game-changer, because we can test and quantify artificial neural networks in ways that just aren't possible with animal or human brains," Dr. Wagenaar explains.

By quantifying the information hierarchies that emerge as AI models classify images, for instance, Dr. Wagenaar's team can make novel predictions about visual processing pathways in mammalian brains. "By comparing natural and artificial intelligences, we're able to understand the brain in a whole new way," Dr. Wagenaar says.

Berkeley Lab researcher Yan Zeng looks over the starting point at A-Lab. The new lab combines automation and artificial intelligence to speed up materials science discovery.
Credits: Marilyn Sargent/Berkeley Lab

Other researchers believe that AI could fundamentally change the process of scientific discovery, giving scientists powerful new ways to generate hypotheses and ask fruitful research questions. At the University of Chicago's Knowledge Lab, sociologist James Evans uses machine learning to study the social dynamics underpinning new discoveries. By using AI to map connections between researchers—in the lab, at conferences, or as they move between institutions—it's now possible to predict with surprising accuracy when and by whom new breakthroughs will be made.

Crucially, Dr. Evans says, that makes it possible to identify neglected research spaces: areas where breakthroughs *should* be happening, but where researchers aren't yet sharing insights or asking the right questions. "Our AI models can make plausible predictions about the spaces that we aren't currently exploring," he says. "That's likely to be one of the most powerful uses of AI—compensating for human blind spots and biases and driving discovery by pushing us in entirely new directions."

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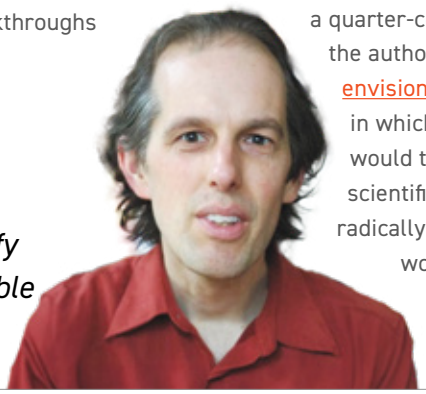

Writing in *Nature* almost a quarter-century ago, the author Ted Chiang envisioned a world in which AI systems would transform scientific discovery so radically that humans would effectively be left behind, unable to fully

comprehend the findings of their digital successors. We're a long way from that point, Dr. Evans says—but there's no question that AI has the potential to open new frontiers of scientific inquiry beyond anything we can currently imagine. "The big question is what AI-enabled discovery will look like 20 or 30 years from now," he says. "The future is going to be interesting—and complicated—as we begin to figure these things out."

That's exactly why we need smart, mindful, and forward-looking researchers to start thinking carefully about how best to incorporate AI into their research, adds TCCI cofounder Tianqiao Chen. "From the workings of the human mind to the secrets of the cosmos, AI is pushing back the boundaries of human knowledge," he says. "We need more researchers to engage with these technologies—and we're proud to support the young scientists who are leading the way on this incredible journey."

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About the Tianqiao and Chrissy Chen Institute The Tianqiao and Chrissy Chen Institute (TCCI®) was created in 2016 by Tianqiao Chen and his wife Chrissy Luo, the founders of Shanda Group, with a US $1 billion commitment to help advance brain science. The organization's vision is to improve the human experience by understanding how our brains perceive, learn, and interact with the world.