



TECHNOLOGY FEATURE Technology Report

The AI Scientist: How Machine Learning is Rewriting the Rules of Discovery

Artificial intelligence is not just a path to automation; it is borrowing the other direction into being part of the scientific method itself — from predicting protein structures to designing better batteries.

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Introduction

The scientific method seemed to follow a well-known cadence of observe, hypothesise, experiment and conclude for centuries. That was a human brain that conceptualised it. Sometimes it took years. Sometimes a lifetime. Or it never happened at all.

Next, we had artificial intelligence, and not as a comma but as modular. AI systems today are generating novel hypotheses, creating experiments, and even writing their own research papers. A year or two ago, the main question was whether AI could do science. But the question is this: what happens to human scientists when machines think first?

This is not a distant future. This is already occurring in chemistry, biology, physics, and materials science. And it's compelling a global dialogue on creativity, credit, and what it means to be a discoverer essentially.

“AlphaFold didn’t just predict proteins faster. It solved a 50-year-old problem that thousands of human PhDs could not crack. That changes everything.”

Technology Overview

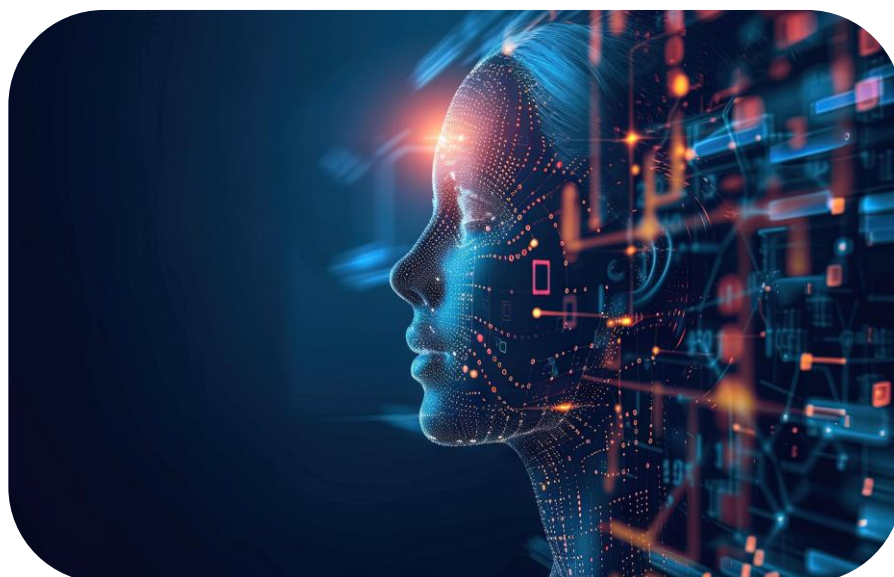
AI for Science is a field of research that has built on two breakthroughs in the last decade. Deep Learning and large-scale biological data. Modern AI learns patterns among vast datasets of millions of protein sequences, thousands of material structures, and decades of climate measurements as opposed to a more conventional algorithm that follows rigid rules.

DeepMind is the most famous example, **AlphaFold**. It predicts the way a chain of amino acids folds into a three-dimensional shape based on a known database of protein structures a result of more than one sombrely called the ‘grand challenge of biology’. Solving it in **2021**, AlphaFold was, on the other hand, as accurate as much as, but too slow and expensive laboratory methods



Graph Neural Networks were recently applied to finding new battery electrolytes, clean hydrogen catalysts, and novel antibiotics. Through training on atomic arrangement-material property relationships, these models can suggest completely novel molecules never seen before.

In simple terms, LLM is being fine-tuned on scientific papers to produce hypotheses. The idea is simple: since **GPT-4** (by the way, prompted scientifically) can read thousands of abstracts, it will offer setup ideas alongside testable research questions that humans would miss.



Key Findings & Impact

Acceleration is Unprecedented.

Just as it once took researchers like Rosalind Franklin years to piece together what DNA looked like, an AI trained on that data would be able to reckon with the same questions in mere weeks. In drug discovery, AI decreased the timeline of discovering possible candidate molecules for some targets from **3–5 years** to less than **6 months**. Since then, companies such as **Insilico Medicine** have already been attempting to take AI-discovered drugs into human trials.

Reproducibility and Trust Are New Problems.

AI makes predictions, not guarantees. Furthermore, something that seems like the perfect molecule on a computer could be a flop in the actual lab. At worst, certain AI models are "black boxes"; they provide answers with no supporting explanation. If the AI cannot say why it made a suggestion, anyone who wants to be prudent will figure out that anyone, in this case, a human scientist, will take 6 months testing whether or not they should trust the AI. Some early data suggest that as few as **30% to 40%** of AI-generated hypotheses remain standing after experimental validation in some fields.



The Human Role is Shifting – Not Disappearing.

Senior scientists are now thinking more like "research directors," directing the handing off of pieces of a lab to AI systems, rather than being people who do hands-on work in the lab. Quietly, PhD training is evolving as students must now master prompt engineering and data curation in addition to pipettes and microscopes. For one survey of **800 life scientists in 2025**, by contrast, **62%** thought that AI would somehow make their work "more intellectually interesting" by relieving them of the burden of boredom inherent in trial-and-error experiments.

Who Gets Credit for an AI Discovery?

This has sparked an ethical and legal debate, even regarding authorship. But if AI creates a hypothesis, then a human runs the experiment, and another human writes the paper, who invented it? The patent offices are still in the catch-up phase. At present, none of the big patent offices (USPTO, EPO or otherwise) allow an AI to be listed as an inventor. However, human researchers routinely include themselves. Now, some journals want authors to state where AI actually wrote the words.

Global Inequality in AI Science.

Availability of state-of-the-art AI for science is not equitable. Example: MIT, thousands of GPUs per model, how to democratise this. The ability to access computers is also lacking at much smaller universities in countries which are developing. This is enhancing the divide between "AI-enabled" science and "traditional" science. This leads to the same nuanced questions, such as from a researcher in Nairobi or Dhaka, namely, if the question is so smart, why is **Boston** getting its answer via testing **10,000** hypotheses by lunchtime?

What's Next?

AI-Human Collaboration Labs:

Commercially available "self-driving labs" through AI reasoning (robotic experiments) in the coming five years. These systems will create an experiment, execute it, analyse the results, and redesign the next iteration without human intervention. Human scientists will be best at asking the right questions, interpreting unexpected results, and working on high-risk ideas that AI classifies as "below average promise."

Explainable AI for Science:

There is a very large research push to see through the black box of AI models. Attention mapping and concept bottleneck models are some of the techniques that allow scientists to observe the contribution of portions of data to the AI conclusion. This is critical for trust. If we as physicians or pharmacists understand why an AI made a recommendation, we are much more likely to carry out that recommendation or turf it safely.

New Scientific Fields Born from AI:

The discipline of "machine-aided discovery" is already emerging. You can already see research questions that the younger among us are asking, that you could never ask without AI: "Find me all stable folds at 80 °C for protein X", or "design me a material which would have exactly this electric resistance". They are not faster delusions of a prior science. These are what you call new waves of science.

What Humans Keep Exclusively:



AI cannot or never will have its own curiosity in a way that compels a scientist to ask the weird, unfindable question. It also cannot appreciate the special joy of a surprising result contradicting all our models. It cannot pedagogue, mentor, or sway the next generation of researchers. And that may even be unable to put a discovery in its entire human context, the ethical, social or historical one. These remain uniquely human strengths.

About the Author

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References

- [1] Jumper, J. and team (2021). AlphaFold solves protein folding.
- [2] Merchant, A. and team (2023). AI finds new materials fast. Nature Journal.
- [3] Ren, F. and team (2025). How often are AI ideas correct? Nature Machine Intelligence.
- [4] World Intellectual Property Organization (2025). Can AI be an inventor? Global report.
- [5] Nature Editorial Board (2024) New rules: Tell us when you use AI. Nature Journal.