ARTIFICIAL INTELLIGENCE

DeepMind predicts millions of new materials

AI-powered discovery could lead to revolutions in electronics, batteries, and solar cells

By **Robert F. Service**

The materials cookbook has suddenly grown tens of times longer. Modern technologies, from electronics to airplanes, draw on just 20,000 inorganic materials, largely discovered through trial and error; scientists have predicted but not made tens of thousands more. This week, however, researchers report that with a new artificial intelligence (AI), they have predicted the ingredients and properties of another 2.2 million materials. In a companion study, a separate team has shown that such predicted materials can be made efficiently, again with the help of AI.

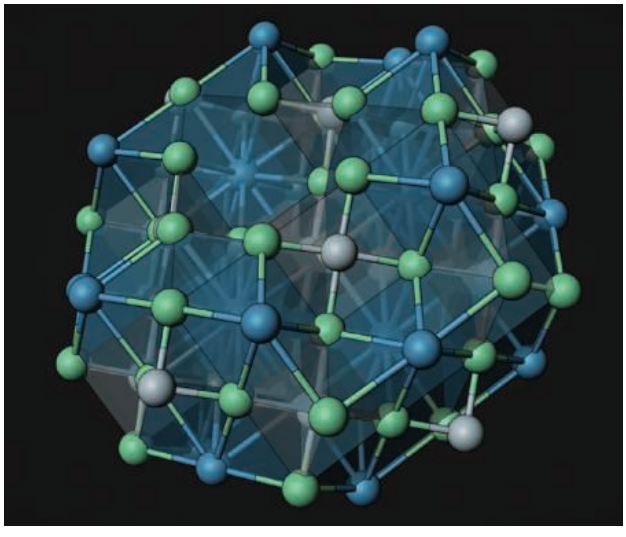
Together, researchers say, the reports foreshadow a new age of materials science, when AI programs and robots will power the search for the makings of novel batteries, superconductors, and catalysts. "It's very impressive," says Andrew Rosen, a computational materials scientist at Princeton University.

The predictions, published in *Nature*, are another coup for the AI innovators at DeepMind, an offshoot of Google. Last month, they described an AI algorithm that runs on laptops and can predict the weather as accurately as large, supercomputer-driven models (*Science*, 17 November, p. 748). Prior to that DeepMind developed AlphaFold, an AI that's able to predict the 3D shape of hundreds of millions of different proteins from their amino acid sequence alone (*Science*, 30 July 2021, p. 478). The new work, Rosen says, "is the AlphaFold equivalent for materials science."

Like previous DeepMind achievements, this one trained an AI with extensive data. The researchers started with the Materials Project, a database of all known and predicted inorganic crystals. That database includes not only each material's crystal structure, but also properties such as its electronic structure, magnetic behavior, and hardness. Over the past decade, Materials Project teams have fed data on the 20,000 known inorganic crystals into pattern-matching machine learning algorithms to predict another 28,000 inorganic crystals that should be stable.

For their current work, DeepMind researchers, led by Dogus Cubuk, who heads materials discovery for the company, used the data on those 48,000 known and predicted compounds—as well as information from other related databases—to train an "active learning" AI model. Dubbed GNoME (for Graph Networks for Materials Exploration), the AI can spot patterns beyond those in the original training data. It made an initial round of predictions of possible new stable crystals and calculated their properties; the team then added the results to the training data and repeated the cycle.

After several such rounds, GNoME wound up with predictions for the 2.2 million new compounds. The calculated "formation energy"—a measure of stability—for 381,000 of them suggested that if researchers could synthesize them, they should be stable and not decompose into other structures.



Barium (blue), niobium (white), and oxygen (green) form a novel material.

IMAGE: MATERIALS PROJECT/BERKELEY LAB

Among the finds are layered materials like those used in battery electrodes. Whereas the Materials Project identified 1000 such compounds, GNoME predicted 52,000, including 528 lithium-ion conductors, a kind of material critical to today's best batteries. Cubuk also notes that in contrast to previous predicted crystals, which mostly combined two, three, or four elements, many of DeepMind's predicted structures contain five and even six elements. "This is really exciting," says Alexander Ganose, a materials chemist at Imperial College London. "It is enabling materials discovery across a much wider composition range. We might be able to find the materials of the future in this data set."

The next step is actually synthesizing the materials, traditionally a process of trial and error that can take months or years for a single compound. "Predicting something is nice," says Janine George, a computational materials scientist at the Federal Institute for Materials Research and Testing in Berlin. "But making it is really great."

External benchmarks suggest GNoME's success rate at predicting stable structures reaches 80%, up from the 50% achieved by previous algorithms. And the DeepMind researchers note that independent experimenters have already made 736 of the predicted materials, verifying their stability. Cubuk says even materials not certain to be stable might be extremely long lasting, just as diamond survives 1 billion years or more before decomposing into graphite.

A different kind of AI might help synthesize more of GNoME's predictions, another paper this week in *Nature* suggests. Researchers at Lawrence Berkeley National Laboratory, led by materials scientist Gerbrand Ceder, recently built an AI-driven robotics lab to make predicted new materials (*Science*, 21 April, p. 230). Now, he and his colleagues report that this setup quickly learned to refine recipes for synthesizing new compounds predicted by the Materials Project algorithm. In 17 days, the robots successfully synthesized 41 materials out of 58 they attempted.

DeepMind researchers say they will immediately release data on the 381,000 compounds predicted to be stable and make the code for its AI publicly available. They may ultimately release all 2.2 million recipes. But Ganose, for one, does not want to wait. Studying the whole panoply could help scientists better determine what allows some compounds to be stable whereas other are less so. "If this is locked away that's a real loss to science," Ganose says. Cubuk, however, notes that with almost 10 times more targets to aim for than ever before, materials scientists already have plenty to keep their test kitchens busy. ■

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