Scaling Materials Discovery with Self-Driving Labs

How to close the gap between AI-guided material design and real-world validation | **Charles Yang**

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This essay is part of The Launch Sequence, a collection of concrete, ambitious ideas to accelerate AI for science and security.

Summary

Materials underpin our national power and prosperity, from the nanoscale silicon transistors powering our computers to the carbon fiber bodies of our airplanes. Innovation in materials will define our ability to maintain our technological edge; the races for hypersonic missiles, new nuclear technologies, and advanced semiconductors all hinge on materials science.

Historically, materials discovery has been a slow and laborious process. But as AI models grow more capable at proposing novel materials, they will offer a flood of promising candidates. The key bottleneck will become experimental testing and validation in the real world. Self-driving labs (robotic systems that automate the process of designing, executing, and analyzing experiments) can close the loop between AI-generated hypotheses and real-world outcomes.

Policymakers should move quickly to scale autonomous experimentation as a core pillar of national AI infrastructure. The White House should direct the Materials Genome Initiative to convene a national self-driving labs consortium to coordinate research agendas, technical roadmaps, and cross-sector investment. Existing appropriations, including recent ARPA-E and CHIPS R&D programs for self-driving labs, should be prioritized and deployed on accelerated timelines. With targeted

support for autonomous experimentation, the US can convert its AI leadership into a compounding flywheel for materials discovery and industrial competitiveness.

Motivation

Materials science sets the pace of technological progress. Advancements in materials have historically been prerequisites for the technologies underpinning US military and economic strength. The following are examples of specific materials innovation that sprung from US scientists and supported national power:

The Material Basis of US Innovation and Power

Decade	Material Innovation	Technology enabled
1950s	Zirconium/Hafnium alloy	Nuclear fuel rod cladding
1960s	Titanium alloys	Airframes for jets
1980s	Radar-absorbing stealth composite	Stealth aircraft like Nighthawk F-117
1990s	Yttrium barium copper oxide (YBCO)	High-temperature superconductors for fusion

Maintaining leadership in materials science will be key to US competitiveness over the next decades, from energy production to manufacturing competitiveness. Discoveries in new materials could unlock new technological capabilities, from high-performance composites in hypersonic vehicles to 2D-materials for next-generation semiconductors. Materials discovery could also offset critical supply chain vulnerabilities (for example, for the rare-earth magnets critical for precision-guided munitions).

The discovery of new materials has historically been a slow, trial-and-error process, taking on average 20 years from lab to deployment. But AI could transform the material discovery process. Over the past few years, AI models have achieved remarkable progress in areas like protein folding and generative chemistry. These same techniques are now being applied to materials science, where AI models can predict the properties of novel compounds and simulate complex material properties. The result is a growing pipeline of promising material candidates. But these digital discoveries cannot be translated into real-world materials without being first validated through experiments.

Self-driving labs bring AI capabilities to the physical world, using machine learning and robotics to automate and dramatically accelerate the process of running experiments, without needing to wait for human input. Early versions of these platforms have proven able to autonomously generate hypotheses, synthesize candidate materials, run experiments, and analyze results — learning from each iteration to optimize the search for novel materials. Unlike traditional labs, which rely on manual processes and human intuition, self-driving labs can execute hundreds of experiments per day, adjusting parameters in real time based on outcomes. This allows them to rapidly explore vast design spaces, compressing years of research into weeks or months.

Several proof-of-concept systems in chemistry and materials science have demonstrated the ability to vastly increase the rate of new material discovery. But scaling these academic pilots to robust and usable national infrastructure offers the chance to transform the pace of materials innovation.

Closing the gap between AI design and physical discovery is now a national imperative. The US leads in foundational AI research and model development, but this edge will only translate into strategic advantage if paired with the ability to rapidly test and iterate in the physical world. Self-driving labs — AI-guided, fully automated experimentation platforms — can bridge this gap. Without investment in autonomous experimentation, traditional scientific experimentation done by humans will not be able to keep up with a deluge of new AI-generated material hypotheses. Now is a critical moment, as AI capabilities start to reach scientific maturity, to begin early investment in deploying autonomous experimentation to ensure the US's lead in developing AI systems translates into real-world materials innovation. Public capital also plays an important bridging role in demonstrating the value of such AI-enabled infrastructure to lead private industry investment in ensuring the US doesn't fall behind in materials discovery.

But US investment today in self-driving labs has lagged those of other countries. Canada has invested over $500 million of public and private funding into self-driving labs. It is only in the past year that the US has taken initial steps towards supporting self-driving labs, through the CHIPS R&D office and Department of Energy's ARPA-E, though the total funding still pales in comparison to the total industry funding for AI models and what other countries have invested in self-driving lab infrastructure. As AI systems mature into powerful engines of scientific reasoning, the US has a narrow window to fuse digital design with physical discovery, converting AI leadership into a flywheel for materials innovation.

Solution

- The White House Office of Science and Technology Policy (OSTP) can coordinate through the interagency Material Genome Institute (MGI) to create a consortium for self-driving labs, bringing together scientific equipment providers, robotics manufacturers, scientists, and AI developers, to develop a roadmap for "Grand Challenges in Autonomous Scientific Discovery." This consortium would mirror consortiums other countries have already formed to coordinate funding and research in self-driving labs. MGI can leverage responses to the recent Request for Information the Department of Energy released on autonomous experimentation to develop this roadmap.
- The Department of Energy (DOE) Office of Science should increase funding support for national labs to invest in autonomous experimentation infrastructure for self-driving labs. While several national labs have preliminary, internal investments into self-driving labs, DOE has not to date provided any specific programmatic funding for national labs to scale this key infrastructure. Allocating an $80 million program for self-driving labs would represent a step change.
- The Trump administration should also work with Congress to pass the bipartisan DOE AI Act, which would support the development of a national AI capability through the DOE and its national labs. DOE's agency focus as a capability building agency, rather than broad exploration, helps bridge the gap between undirected research and pure defense applications. The 17 DOE national labs, which already provide large-scale scientific infrastructure such as hard light sources and supercomputers for the US scientific research base, are well-positioned to build self-driving lab infrastructure at scale to accelerate US scientific discovery.
- Until 6 months ago the US government had not created any scientific funding programs specifically for leveraging self-driving labs. However in the past several months, DOE's ARPA-E created a $40 million program for self-driving labs to discover new chemical catalysts and CHIPS R&D created a $100 million program for self-driving labs to accelerate the discovery of semiconductor

material. The Trump administration should move expeditiously to ensure such funding is allocated towards competitive research teams that are fully leveraging the AI opportunity.

Further resources

- Dean Ball, Accelerating Materials Science with AI and Robotics, 2024.
- Charles Yang, US Progress on Self-Driving Labs in 2024, 2025.
- Charles Yang, A Research Agenda for Advancing Self-Driving Labs, 2024.