Fall 2025

THE MATERIALS GENOME INITIATIVE

The BRIDGE

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The Bridge publishes articles on engineering research, education, and practice; science and technology policy; and the interface between engineering and technology and society. The intent is to stimulate debate and dialogue both among members of the National Academy of Engineering (NAE) and in the broader community of policymakers, educators, business leaders, and other interested individuals. *The Bridge* relies on its editor in chief, NAE members, and staff to identify potential issue topics and guest editors. Invited guest editors, who have expertise in a given issue's theme, are asked to select authors and topics, and independent experts are enlisted to assess articles for publication. The quarterly has a distribution of about 7,000, including NAE members, members of Congress, agency officials, engineering deans, department heads, and faculty, and interested individuals all over the country and the world. Issues are freely accessible at *www.nae.edu/TheBridge*.

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News and Notes

NATIONAL ACADEMIES *Sciences Engineering Medicine*

The **National Academy of Sciences** was established in 1863 by an Act of Congress, signed by President Lincoln, as a private, nongovernmental institution to advise the nation on issues related to science and technology. Members are elected by their peers for outstanding contributions to research. Dr. Marcia McNutt is president.

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A Word from the NAE Chair

The Critical Role of Leadership in Times of Challenge and Change

James O. Ellis Jr.

I write these words just weeks after assuming the role of Chair of the National Academy of Engineering governing Council, succeeding **Erroll Davis**. On behalf of the entire Academy, I express both our thanks to him for his selfless service and our sincere best wishes for his future health and happiness. Like Erroll, and **Don Winter** before him, I am very grateful for the opportunity to serve as your Chair. I am especially honored to support our new President, Dr. **Tsu-Jae King Liu** as she enthusiastically assumes her leadership role at a pivotal time in the history of the NAE.

In every era, societies, organizations, and institutions face periods of challenge and changes that test not only the strength of systems and organizations but, more importantly, the caliber of their leadership. Whether sparked from economic crises, geopolitical upheavals, technological disruption, pandemics, or internal social transformations, leaders must navigate uncertainty with resolve. Effective leaders provide direction, instill confidence, make difficult decisions, and create the necessary paths to move forward. It is in these defining moments that true leadership emerges—not merely as a position of authority, but as a force for resilience, clarity, and adaptive strength.

Like many of you, I have spent decades in diverse organizations during different and often challenging times. I have also observed countless leaders, myself included. Along the way, I noted constant leadership elements that emerge in times of challenge and change. These are my personal observations. The list is not exhaustive, and they are not dogma or doctrine. I provide them to ignite future conversations as together we navigate the challenges of today and tomorrow.

Leadership as the Anchor in Uncertainty

During challenging times, uncertainty can be paralyzing. It is not the change itself that confounds us but rather the pace and acceleration—in engineering terms—the first and second derivative. People look to their leaders not only for answers but for assurance. The emotional tone set by a leader shapes the morale and behavior of an entire group. Calm, composed, and authentic leaders reduce panic and maintain a sense of purpose even in the most volatile environments. Consider historical figures like Franklin D. Roosevelt during the Great Depression or Winston Churchill during World War II—leaders who were able to inspire hope amid hardship. The example they set and their ability to communicate openly and consistently was as important as the decisions they made.

A strong leader is anchor-providing stability even when the external environment is in flux. This stability is not rooted in stubbornness or denial of the situation, but in an honesty paired with an unwavering commitment to progress. It requires emotional intelligence, empathy and the ability to listen to the concerns of others while charting a path forward. As I often note, real listening is not the same as not talking. One must actively engage to really hear and understand the critical messages amid the cacophony that often comes with rapid change.

Vision and Adaptability

In transformative periods, it is not enough to manage the present; leaders must also prepare for and shape the future. This requires vision—the ability not just to react to change but to see beyond the immediate crisis and reimagine what is possible. A compelling vision acts as a guiding light, offering a destination even when the path to its achievement is unclear. Importantly, this vision must be flexible. Leaders must be willing to revise strategies as new information becomes available or as circumstances evolve. Rigid adherence to outdated plans or organizational structures can lead to failure, while adaptive leadership can enable innovation and resilience and allow us to

capture the opportunities that often come with dramatic and rapid change.

An excellent example of visionary leadership in our recent history is the rapid digital transformation led by CEOs during the COVID-19 pandemic. With physical operations shut down, organizations were forced to pivot overnight to remote work, online services, and virtual collaboration. Leaders who embraced change and adopted new technologies were able to keep their teams functioning and even thrive under novel conditions. This adaptability in the face of challenge was not just about survival, it became a driver of growth. For them, as Thomas Carlyle once observed, "the block of granite that was an obstacle in the pathway of the weak, became a steppingstone in the pathway of the strong."

Decision Making in Complexity

One of the most difficult aspects of leadership during challenges and change is decision making under pressure. Complex problems often involve incomplete information, conflicting interests, demanding risk assessment and no ideal or even obvious solutions. Yet leaders must still make decisions—often quickly and with high stakes in the balance. In such scenarios, effective leaders rely on their core principles and long-term values. They also consult diverse perspectives, weigh the risks as best they can and take responsibility for the outcomes.

Courage is essential here. It is easier to delay or delegate tough calls, but true leaders understand that indecision can be more damaging than a wrong decision. They take ownership, communicate the rationale behind their choices, and learn from the consequences. Importantly, they foster cultures where learning from failure is encouraged, thus allowing organizations to evolve rather than stagnate.

Communication as a Leadership Tool

Clear, consistent, and transparent communication is one of the most powerful tools a leader can wield in turbulent times. Uncertainty breeds rumors, fear, and disengagement. A leader who communicates honestly about challenges, progress, and expectations creates trust. Communication should not be a one-way broadcast, but a dialogue—an opportunity to engage stakeholders, listen to feedback, and respond to concerns.

The tone and content of communication also matter. Leaders must balance realism with optimism. Sugar-coating challenges can erode credibility, while overly negative messaging can crush morale. The best leaders are those who acknowledge the gravity of a situation but also highlight collective strengths, chart paths forward, and exhibit optimism. These leaders show us that, together, we will emerge from the current crisis better and stronger. Simply put, in these times, the role of leaders must be to absorb fear, not create it.

The Human Side of Leadership

While strategy and decision making are critical, leadership during change is ultimately about people. You manage *things*—budgets, programs, schedules—but you lead *people*. Leaders must attend to the emotional and psychological needs of their teams. During crises, individuals may feel anxious, overwhelmed, or demotivated. These are real, human emotions that affect us all; they are not signs of weakness or lack of capability. Leaders who show empathy, provide support, and foster inclusive connection maintain cohesive and engaged workforces. When I used to speak about leadership, I would always highlight the value of compassion and the importance of being self-aware, even when delivering difficult messages. A good leader appreciates the impact of their actions and the importance of sustaining each team member's self-respect.

Servant leadership, a model in which the leader's primary role is to serve the needs of others, can be particularly effective in such contexts. This approach emphasizes humility, compassion, and stewardship. When people feel that their leader genuinely cares about their well-being, loyalty and performance tend to increase.

Building Trust and Integrity

At the Hoover Institution, where I hang my hat these days, the late Secretary George Shultz would often remind us that, in all things involving human beings, "trust is the coin of the realm." Trust is also the currency of leadership, and it is never more valuable than in times of change. Leaders must act with integrity—doing what they say they will do, honoring commitments, and modeling ethical behavior. When trust is broken, especially during a crisis, the damage can be long-lasting and difficult to repair.

Building trust requires consistency, openness, and accountability. Leaders must admit mistakes when they occur, explain their decisions honestly, and remain open to scrutiny. Trust is not built overnight, but it can be eroded instantly. Leaders who protect this trust create environments where collaboration flourishes and where people are willing to take risks in service of a shared mission.

Conclusion

The critical role of leadership in times of challenge and change cannot be overstated. Leadership is not about authority, it is about service, courage, and vision. It is about guiding others through uncertainty with empathy and clarity. Effective leaders inspire confidence, make difficult decisions with integrity, adapt to new realities, and keep people connected to a larger purpose.

As members of the NAE, by definition, you all are leaders. And, as I know you understand all too well, leaders cannot sit on the sidelines. There's an old maritime quotation attributed to Oliver Wendell Holmes that I like:

> Greatness lies not in where we stand but in what direction we are moving. We must sail, sometimes with the wind and sometimes against it, but sail we must and not drift, not lie at anchor.

As the world continues to face complex and unpredictable challenges—climate change, geopolitical tensions, technological disruption, and social discord—the need for capable, ethical, and forward-thinking leadership is more urgent than ever. In these moments, we are reminded that leadership is not just about navigating today's storms but about building vessels strong enough to carry us all to a better future.

Editor in Chief's Note

Transitions

Ronald M. Latanision (NAE) is Neil Armstrong Distinguished Visiting Professor at Purdue University and editor in chief of *The Bridge*.

With this issue we welcome two people to the work of the National Academy of Engineering. **Tsu-Jae King Liu** became the president of the NAE on July 1, 2025. Dr. Liu previously served as dean of the College of Engineering at the University of California, Berkeley. Admiral **James O. Ellis Jr.** USN (retired), the Annenberg Distinguished Visiting Fellow at Stanford University's Hoover Institution is the new chair of the NAE Council.

We also have a change at *The Bridge*. Kyle Gipson, who had been the editor since 2023, accepted a position with the International Council on Clean Transportation (ICCT) in June 2025. I am pleased to report, thanks to the NAE's Director of Outreach and Communications Kristen Koehler, that David Butler has agreed to step in as the interim editor during this transition. David holds bachelor's and master's degrees in electrical engineering with a specialization in biomedical engineering from the University of Rochester. He completed his doctoral work in public policy analysis at Carnegie Mellon University and before coming to Washington, DC, served as a researcher at Harvard's Kennedy School of Government and its School of Public Health. David is the J. Herbert Hollomon Scholar of the NAE and is the director of the Cultural, Ethical, Social, and Environmental Responsibility in Engineering Program. I am especially grateful to him for jumping into the breach on short notice.

One lesson I learned first as an academic and later in the consulting world is that young people move—as they should—to follow opportunities for growth in their field. Such is the case with Kyle. Our loss at the NAE is ICCT's gain, and I am confident he will prosper there, with his skills as a writer and editor on full display. A constant theme in Kyle's interactions with the accomplished authors who contribute to *The Bridge* has been their profuse thanks for his ability to improve and clarify their writing. Kyle is a superb writer and editor, and he combines this talent with a civil and respectful approach to collaboration. I have enjoyed working with him enormously. So, Kyle: I will be watching. Don't forget your roots at the NAE!

The spring 2024 issue of *The Bridge* on the US metals industry, edited by **Greg Olson** and **Aziz Asphahani**, illustrated how computational materials science and engineering are leading the way in developing metallic materials that meet increasingly advanced design specifications. Computational materials science and engineering form the foundation of the Materials Genome Initiative (MGI), which is the focus of the present issue and is reshaping mate.rials education and practice. In my Editor in Chief's Note accompanying that issue,[1] I described the origins of MGI during President Obama's administration.

In this issue, edited by **Amit Goyal**, the transition to computational materials science and engineering represented by MGI is explored further. Amit, a respected member of the NAE, is the SUNY Empire Innovation Professor and SUNY Distinguished Professor in the State University of New York at Buffalo's Department of Chemical and Biological Engineering. He has assembled a superb group of contributors from government, national laboratories, and academia, all focused on increasing US global competitiveness by significantly accelerating the pace at which advanced materials are discovered, developed, and transitioned into manufactured products.

Amit suggested hosting a webinar after publication to highlight the issue's content—a very good idea that should stimulate interaction among our readers. Planning is under way, and we hope to debut it before the Winter issue appears in December.

Finally, *The Bridge* continues its interview series with a conversation with engineer and author Ainissa Ramirez about her career and her recent book on the iconic engineer, acoustician, and inventor Jim West. I always enjoy these interviews, and this one was no exception.

As always, I welcome your comments. Feel free to reach out to me at rlatanision@alum.mit.edu.

[1] https://www.nae.edu/313365/Editor-in-Chiefs-Note-The-Materials-Genome-Initiative-Grows.

Guest Editor's Note

The Materials Genome Initiative (MGI): Status and Future Outlook

Amit Goyal (NAE) is a SUNY Distinguished Professor and SUNY Empire Innovation Professor at the State University of New York (SUNY) at Buffalo. He is a member of the National Academies' National Materials and Manufacturing Board.

Advanced materials are key to societal development and have been at the center of technological advances since the Stone Age. They are critical to national and economic security, human well-being, and impact diverse sectors including energy, communications, transportation, housing, healthcare, defense, and food packaging. However, discovering new materials with unique and improved intrinsic properties and then manufacturing commercial devices or products that use them typically requires a long, iterative, and expensive developmental cycle that can take several decades.

Taking advantage of recent transformational advances in computing capabilities, theoretical modeling, artificial intelligence and machine learning (AI/ML), and data mining, the Materials Genome Initiative (MGI) was launched by the White House in 2011 to enhance US competitiveness. The goal was to exploit these advances to discover, develop, and commercialize products in a significantly shorter timeframe and at a fraction of the cost (NSTC 2011). The aspirational goals of MGI were to reduce both the discovery and development cycle and the total cost by 50% (NSTC 2011, 2014).

Figure 1a shows the founding conceptual structure of the Materials Innovation Infrastructure (MII), a key component of MGI products (NASEM 2023; NSTC 2014, 2021). It combines experimental tools, digital data, and computational modeling with AI/ML to predict a material's composition and/or how it should be processed to achieve desired physical properties for a given application. Figure 1b depicts the Materials Development Continuum (MDC), the multi-stage, linear process of discovering and developing new materials beginning with discovery and continuing through development, property optimization, systems design and integration, certification, manufacturing, and deployment. And Figure 1c illustrates the MGI paradigm, which promotes integration and iteration across all MDC stages, enabling seamless information flow and greatly accelerating deployment of new materials at reduced costs.

Following the MGI Strategic Plans of 2014 (NSTC 2014) and 2021 (NSTC 2021), the National Academies' consensus report *NSF Efforts to Achieve the Nation's Vision for the Materials Genome Initiative: Designing Materials to Revolutionize and Engineer Our Future (DMREF)* was published in 2023 (NASEM 2023). It provided important recommendations for future DMREF initiatives to increase MGI-related impact. The National Science Foundation (NSF) is one of 19 federal agencies and their associated laboratories engaged at different Technology Readiness Levels (TRLs) in MGI. Others include the Department of Commerce, Department of Defense, Department of Energy, National Institutes of Health, National Aeronautics and Space Administration (NASA), Department of Health and Human Services, and US Geological Survey.

This issue of *The Bridge* presents perspectives from national and global leaders in MGI who are developing strategic plans and policy across federal agencies, as well as

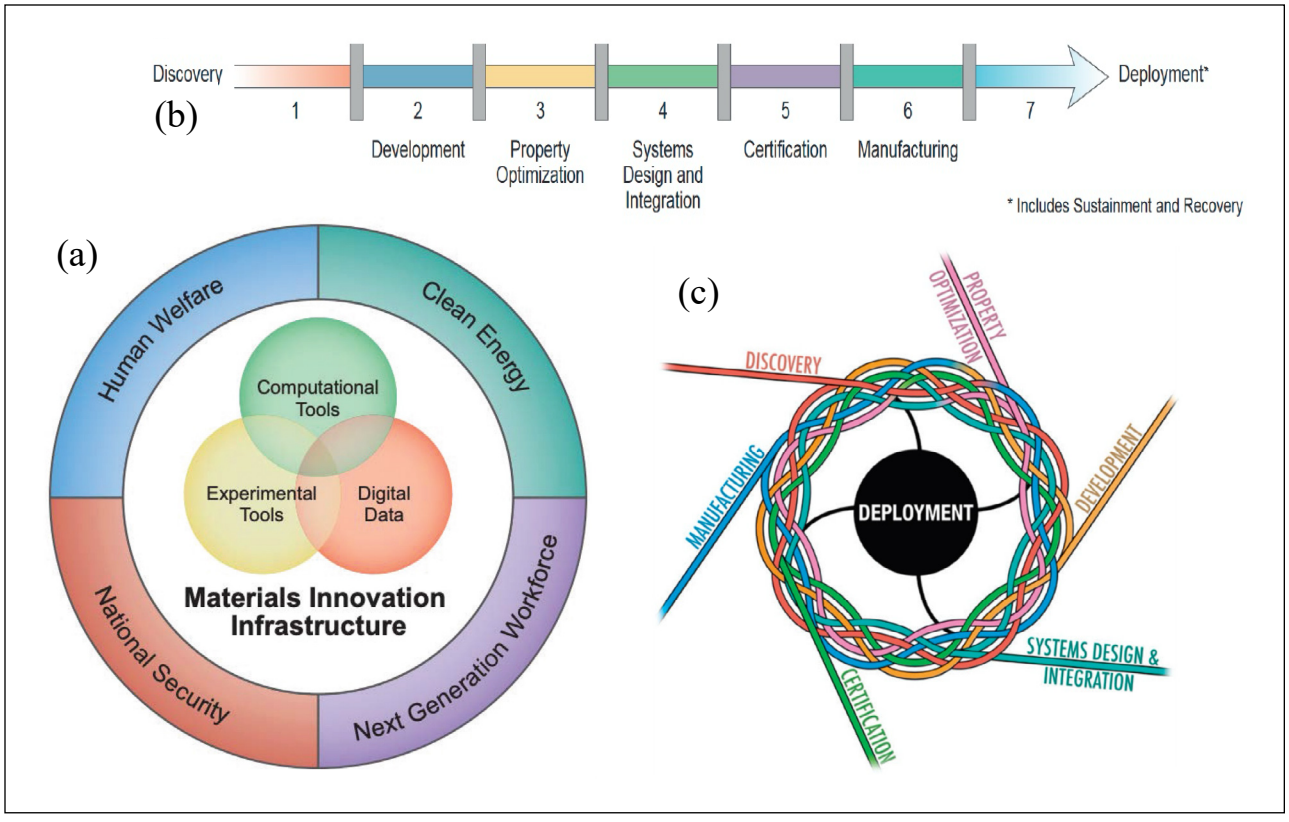

FIGURE 1 (a) The founding conceptual structure of the Materials Innovation Infrastructure (MII), a key component of MGI (NSTC 2014, 2021). (b) Workflow across various stages of the Materials Development Continuum (MDC) from discovery to deployment (NASEM 2023; NSTC 2014, 2021). (c) The MGI paradigm, which integrates and iterates knowledge across the entire MDC with a seamless flow of information, accelerating product development (NASEM 2023; NSTC 2014, 2021).

from research and innovation leaders working in key areas such as autonomous experimentation, self-driving laboratories, advanced microscopy, polymers/plastics, and energy storage. These articles provide state-of-the-art reviews, summarize progress to date, and offer recommendations for future work to fully realize the goals of MGI.

Lisa Friedersdorf (White House Office of Science and Technology Policy) and James Warren (National Institute of Standards and Technology) provide an overview of progress in realizing MGI's goals and outline opportunities for accelerating innovation. They emphasize that AI/ML can generate predictive and surrogate models that may replace physics-based models and simulations. The authors also discuss automated laboratories, autonomous experimentation (AE), and "materials digital twins" to further accelerate materials innovation.

Richard Vaia (Air Force Research Laboratory), Germano Iannacchione (NSF), and Anthony Rollett (Carnegie Mellon University) summarize the path for national leadership toward a data-centric materials revolution. They highlight frameworks such as TRLs and the Manufacturing Readiness Level, Adoption Readiness Level and Materials Maturation Level (MML) frameworks to address the "valleys of death" across the MDC. Vaia and colleagues underscore the importance of collaboration between agencies focused on fundamental and discovery research, mission-driven agencies, national labs, and industry.

Milad Abolhasani (North Carolina State University) reviews global progress in self-driving laboratories (SDLs), which integrate all essential components of MGI by combining AI, AE, and robotics in a closed-loop manner. SDLs can design experiments, synthesize materials, characterize functional properties, and iteratively refine models without human intervention. This capability enables thousands of experiments in rapid succession, converging on optimal solutions. SDLs are thus a critical component in realizing the full potential of MGI.

Figure 2 shows how an SDL operates. Given an end goal, an SDL designs and executes experiments using

materials libraries, synthesizes materials, characterizes them, and iteratively refines results with AI/ML until reaching an optimal solution. Abolhasani provides a summary of recently developed SDLs across various scientific domains and functional areas and involving different synthesis or fabrication techniques. He provides strategic recommendations on how SDLs can be further developed and integrated across various functional areas to fully realize the potential of MGI.

Benji Maruyama (AFRL), Ichiro Takeuchi (University of Maryland), and Jason Hattrick-Simpers (University of Toronto) focus on advances in AE and SDLs applied to materials synthesis techniques such as physical vapor deposition, chemical vapor deposition, and electrochemical deposition, processes essential for producing advanced electrical and electronic materials, including semiconductors, superconductors, ferroelectrics, multiferroics, and quantum materials.

Sergei Kalinin (University of Tennessee, Knoxville, and Pacific Northwest National Laboratory), Steven Spurgeon (National Renewable Energy Laboratory, University of Colorado Boulder, and Colorado School of Mines), and Vinayak Dravid (Northwestern University) review recent advances in autonomous electron microscopy and scanning probe microscopy for AI/ML-enabled physics discovery and materials optimization. They describe the outlook for a transition from human-operated microscopy to autonomous microscopy and then multi-instrument autonomous facilities.

Rigoberto Advincula (University of Tennessee, Knoxville, and Oak Ridge National Laboratory) addresses SDLs for polymers and applications such as plastic recycling. He examines polymer engineering and science, from statistics to digital twins, illustrates the concept with a flow chemistry–based SDL, and considers how SDLs can support a circular economy by enhancing plastics recycling.

Arumugan Manthiram and Tianxing Lai (The University of Texas at Austin) discuss an important functional area, advanced batteries, providing an overview of the status and outlook of different types of batteries and how AI/ML and MGI approaches have affected their development. Batteries are a perfect example of an area where new, environmentally friendly, non-critical materials could be discovered and developed using the MGI paradigm.

In summary, MGI is poised to make a transformative impact on how advanced materials of the future are discovered, designed, developed, and fabricated into devices and products. This transformation is driven by the development of next-generation physics-based models enabled by advances in computing; the creation of surrogate models that provide AI-driven approximations to physics-based models, resulting in materials digital twins; the development of autonomous experimentation tools and self-driving laboratories across different functional areas; the emergence of autonomous and self-driving advanced microscopy tools; and the establishment of mature, consistent data libraries and repositories. Increased research interaction and collaboration among agencies and organizations across TRLs and MMLs is needed to address the risks and "valleys of death" traditionally encountered between discovery, development and scale-up, certification, manufacturing, and deployment. Adequate fed-

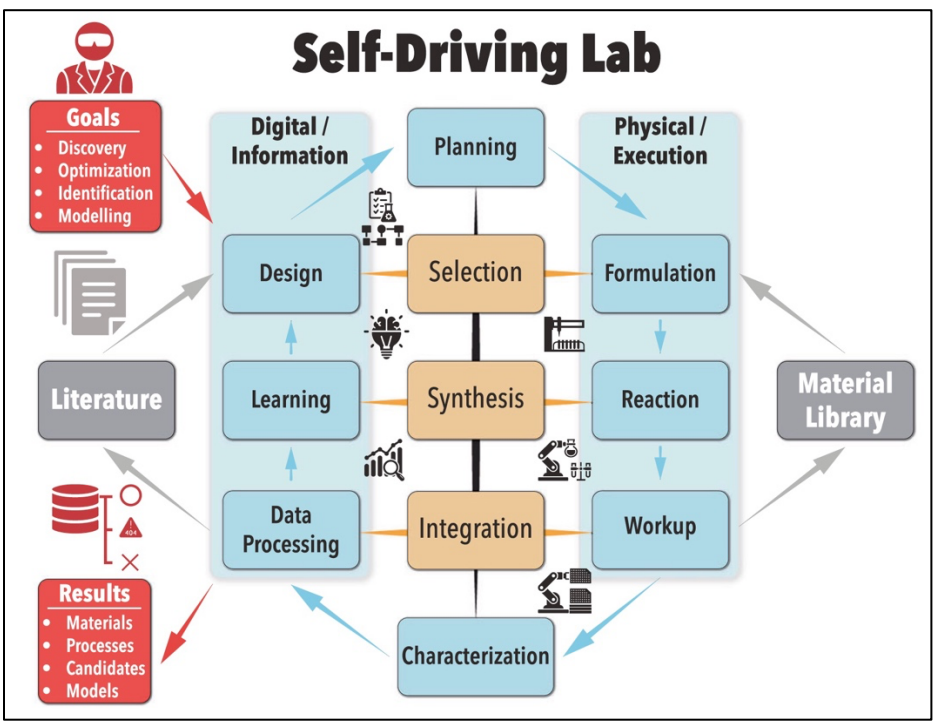

FIGURE 2 Schematic of a self-driving laboratory (SDL) operation (Canty et al. 2025).

eral and industry investments made in partnership with academia must continue to support the further development of the materials innovation infrastructure with a focus on national priorities to ensure US leadership in this critical area of advanced materials that affect national security, economic security, and human well-being.

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I thank the authors of all seven articles in this issue for their contributions and their thoughtful comments on reviewing other articles in this issue. I also acknowledge the following MGI leaders for reviewing articles and providing insightful evaluations: **Kristin Persson** (UC Berkeley and Lawrence Berkeley National Laboratory), William Carter (DOD), **Markus J. Buehler** (MIT), Rampi Ramprasad (Georgia Tech), Venkat Viswanathan (University of Michigan), Scott Miller (NextFlex), Paulette Clancy (Johns Hopkins University), Emmanuel P. Giannelis (Cornell University), and Keith A. Brown (Boston University).

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References

Canty RB, Bennett JA, Brown KA, Buonassisi T, Kalinin SV, Kitchin JR, Maruyama B, Moore RG, Schrier J, Seifrid M, Sun S, Vegge T, Abolhasani M. 2025. Science acceleration and accessibility with self-driving labs. Nature Communications 16:3856.

NASEM [National Academies of Sciences, Engineering, and Medicine]. 2023. NSF Efforts to Achieve the Nation's Vision for the Materials Genome Initiative: Designing Materials to Revolutionize and Engineer Our Future (DMREF). Washington: National Academies Press. Online at https://nap.nationalacademies.org/catalog/26723.

NSTC [National Science and Technology Council]. 2011. Materials Genome Initiative for Global Competitiveness. Online at https://www.mgi.gov/sites/mgi/files/materials_genome_initiative-final.pdf.

NSTC. 2014. Materials Genome Initiative Strategic Plan. A Report by the Subcommittee on the Materials Genome Initiative Committee on Technology. Washington: Executive Office of the President. Online at www.mgi.gov/sites/mgi/files/mgi_strategic_plan_-_dec_2014.pdf.

NSTC. 2021. Materials Genome Initiative Strategic Plan. A Report by the Subcommittee on the Materials Genome Initiative Committee on Technology. Washington: Executive Office of the President. Online at www.mgi.gov/sites/mgi/files/MGI-2021-Strategic-Plan.pdf.

A decade of the Materials Genome Initiative: insights gained and the transformative potential of AI and automation.

Accelerating Materials Innovation: Lessons Learned and Opportunities Ahead

Lisa E. Friedersdorf and
James A. Warren

Lisa E. Friedersdorf

James A. Warren

New materials are the foundation of each generation's ability to enhance prosperity and ensure security. To remain competitive globally, materials research and development (R&D) must be cutting edge, moving the latest innovations from the laboratory to the factory floor—a process that is typically too slow. The Materials Genome Initiative (MGI) was launched more than a decade ago to deploy advanced materials twice as fast and at a fraction of the cost. Here, we review the progress made toward advancing the goals of the MGI and reflect on lessons learned that can inform future efforts.

The MGI was established as an interagency initiative under the National Science and Technology Council (NSTC) of the White House Office of Science and Technology Policy. Initial participants included the Department of Commerce (National Institute of Standards and Technology [NIST]), Department of Defense (DOD), Department of Energy (DOE), National Aeronautics and Space Administration (NASA), and National Science Foundation (NSF) (NSTC 2014). As the initiative evolved, additional participation came from

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the US Patent and Trademark Office, Department of the Interior (US Geological Survey), National Institutes of Health, and US Department of Agriculture (NSTC 2021). The participating agencies have employed both intramural and extramural R&D mechanisms to advance the goals of the MGI.

For example, NIST established the Materials Genome Program, a broad effort to support the MGI through its intramural research portfolio and targeted grants (NIST 2025b). NIST has a century-long tradition of disseminating high-quality data for industry use, so it was natural to focus its efforts on the aspects of the MGI where data played a crucial role. NIST defined three core areas in support of the MGI:

- Data and Model Dissemination
- Data and Model Quality
- Data Driven Materials R&D

Although the second area was a short leap from NIST's traditional role, the first—while seemingly technical and straightforward—proved remarkably challenging, touching on deep incentive structures embedded in the research enterprise. Data dissemination is not something researchers naturally do outside the framework of traditional archival publication. The third area foreshadowed the rise of AI approaches to materials R&D by only a few short years and has since become a central focus of the MGI.

NSF's flagship program to support the MGI, *Designing Materials to Revolutionize and Engineer our Future (DMREF)*, began as a small initiative with partners across NSF and a few federal agencies and launching with 14 projects (NSF 2025a). DMREF has since grown to well over 200 active projects and now includes many NSF divisions as well as collaborative efforts with DOD (Air Force Research Laboratory, Office of Naval Research, Army Research Laboratory; Ground Vehicle Systems Center), DOE, and NIST. DMREF has evolved to address advanced materials needs up the technology readiness ladder and across the entire materials spectrum from biomaterials to quantum materials while incorporating interdisciplinary teams of scientists, mathematicians, software developers, and engineers. These teams share the common goal of advancing materials innovation, while leveraging multiple agency perspectives. The program has been instrumental in translating materials discovery into adoption by fostering the transition from fundamental science to applied research.

NSF also developed and launched the Materials Innovation Platforms (MIP) to establish, at a larger scale, scientific ecosystems that include in-house research scientists, external users, and other contributors who share tools, codes, samples, data, and knowledge to strengthen collaborations and accelerate the discovery and development of new materials (NSF 2025b). These platforms focus on specific materials domains—currently semiconductors and biomaterials—with the goal of creating a self-sustaining engine of materials discovery and development that can operate nimbly and rapidly in these critical areas.

DOD is strategically investing in materials and manufacturing research to ensure the effectiveness and safety of US service members and to advance national defense capabilities across all military domains. A central element of this collaborative effort, which unites the expertise of universities, industries, and the Service Laboratories, is the development of a data-centric materials and manufacturing digital pipeline, along with the workforce to support it. The aim is to enhance the agility of system design, enabling the rapid incorporation of emerging technologies to achieve peak performance against adversary threats while proactively identifying potential material supply risks throughout the acquisition lifecycle. Additionally, this will power affordable sustainment practices that maximize the operational readiness of military forces. Illustrating this effort, the Air Force Research Laboratory is building new research facility capabilities in several key areas. These include autonomous material characterization, fabrication, and synthesis to establish robust data repositories; development of continuously improving processing–structure–performance models using artificial intelligence (AI) and heterogeneous data fusion; robot-human teaming for high-mix, low-volume manufacturing and inspection; and new materials for ultralow-power edge-computing devices.

Other efforts supporting the MGI include the Energy Materials Network, established in 2016 by DOE as a community of practice in state-of-the-art materials R&D specifically aimed at advancing critical energy technologies. The network comprises core consortia focused on different high-impact energy technologies, each leveraging world-class capabilities at DOE's National Laboratories to better integrate all phases of materials R&D, from discovery to scale-up and qualification. It also provides streamlined access to these capabilities for industry and academia to accelerate the energy materials development cycle and enable US manufacturers to deliver innovative, made-in-America products for affordable energy.

Outcomes from these efforts and progress toward the goals of the MGI have been detailed in several publications, including results from the NSF-sponsored workshop "Advancing and Accelerating Materials Innovation: New Frontiers for the Materials Genome Initiative" (de Pablo et al. 2019), "The Materials Genome Initiative and the Metals Industry" (Warren 2024), as well as other papers presented in this issue. Case studies in these publications highlight examples of accelerated deployment of new materials, such as new alloys developed in a fraction of the traditional time for use in a US Navy aircraft and in coins produced by the US Mint. Rather than enumerating additional success stories, this article focuses on identifying key lessons learned that can inform future efforts.

Lessons Learned

The general premise of the MGI is that to accelerate materials discovery, design, manufacture, and deployment—computation, data, and experiment must be brought together in a tightly integrated manner. To enable this integration, the MGI introduced the Materials Innovation Infrastructure (MII), consisting of physical and computational tools and data. Building out the MII allows materials R&D practitioners to design fit-for-purpose materials concurrently with product design, as illustrated above through the efforts of NIST, DOD, DOE, and NSF.

The MGI paradigm was heavily informed by concepts such as Integrated Computational Materials Engineering (ICME). While not all MGI efforts are inherently ICME, it is an excellent example of an "MGI approach" that successfully translates basic scientific research into materials engineering. The concept of ICME has served for about two decades as a useful framework for computational materials design. Although the underlying ideas date back further, a report from the National Research Council crystallized the concept for many in the materials R&D community (NRC 2008). That report also provided practical examples and, perhaps most importantly, a detailed discussion of the return on investment that manufacturers could realize by employing ICME to design fit-for-purpose materials for integration into their products.

MGI approaches can significantly accelerate the development of new materials, but there are some caveats. The greatest successes to date have come in areas where both the theories of the materials and the software to translate those theories into practical engineering decisions are most developed. For example, in metallic systems, the CALPHAD modeling approach (NIST 2025a) has benefited from 50 years of steady improvement and widespread adoption by industry. Another strategy for realizing success with the MGI approach is to start with a system that is already well understood. Thus, for example, if the desired new material is "close" in composition to an existing material, iterative (physics-informed) methods can usually converge with the new system with relative ease.

The general premise of the MGI is that to accelerate materials discovery, design, manufacture, and deployment—computation, data, and experiment must be brought together in a tightly integrated manner.

Substantial challenges remain, though, in realizing all the goals of the MGI. If efforts must stray far from current systems, it becomes a much heavier lift to engage in the materials design required for optimal manufacturing insertion. Similarly, if physics-informed models are unavailable or not mature enough for immediate engineering use, as is often the case in polymer systems, the application of ICME or other integrated modeling efforts is severely constrained. Even in metallic systems, where ICME has had the most success, reliance on existing CALPHAD databases—which offer only limited coverage of possible alloys—means that in many cases the necessary data simply are not available. Acquiring experimental data to fill these gaps remains the critical bottleneck to ICME success.

Another issue impeding wider application of MGI approaches is the set of barriers to entry, including the extensive domain knowledge required, the need for in-house modeling capacity, and the costs involved. For these reasons, small enterprises with limited expertise and resources may find it impossible to undertake a significant ICME campaign. To address these challenges, a major focus of the MGI has been on developing the MII, but progress has been uneven, and much work remains to fully realize this vision.

Finally, even under the best circumstances, the models employed in MGI-style materials design campaigns can be prohibitively slow, requiring clever approximations to achieve speedups. Of course, "clever" here implies that significant domain expertise is still essential for success. Nevertheless, a number of promising new avenues to address this issue are now becoming clear.

Moving beyond the notion of a single investigator who "throws results over the wall" for others to use has been crucial to the success of the MGI.

In addition to the successes and challenges discussed thus far, several other advancements have been precipitated by the MGI. Of particular note is the broad acceptance of more tightly integrated teams as an essential component of the materials R&D enterprise. Moving beyond the notion of a single investigator who "throws results over the wall" for others to use has been crucial to the success of the MGI. Modelers and experimentalists working hand-in-glove to accelerate materials design is now considered best practice under the MGI.

Beyond this significant culture change, the MGI has also focused on many of the issues surrounding software and data publication to build out the MII. Alongside the technical challenges of such publication models, there remain significant cultural and incentive-related impediments. At present, there is little academic or industrial reward for publishing data and software, despite broad recognition of the value of data sharing in principle.

The MGI has maintained close ties with other federal initiatives, including the National Nanotechnology Initiative (NNI). A key example of this intersection was highlighted on the cover of the NNI Supplement to the President's Budget for fiscal year 2018, illustrating the close collaboration of experimentation and computation in nanomaterials (Lin et al. 2017; NSTC 2018). One lesson from the NNI is the importance of research infrastructure. Investigations at the nanoscale were enabled by tools that allowed manipulation of materials at the atomic level, such as scanning tunneling and atomic force microscopy. These breakthroughs have since led to an entire suite of scanning probe techniques.

In the early days of nanoscience, only a few laboratories with these advanced tools were able to conduct research. A key area of NNI investment was the development of user facilities that provided access to the specialized equipment required for nanotechnology R&D. DOE developed user facilities at the National Labs, including the Nanoscale Science Research Centers, and NSF supported a series of networks based in universities, most recently the National Nanotechnology Coordinated Infrastructure (NNCI), which has 16 primary sites and 13 partner organizations providing researchers access to 71 distinct facilities and over 2,200 tools (NNCI 2025).

These user facilities were instrumental in the development of the US nanotechnology community. They are often said to have "democratized" nanoscience, as researchers from smaller colleges and universities, as well as from small businesses, were able to conduct research that would not have been possible at their home institutions. The facilities played an important role across the entire ecosystem, from early-stage research through commercialization, and were pivotal in education and workforce training, with many sites hosting undergraduate students for summer research and other programs.

Materials Innovation Infrastructure

The fabrication and characterization tools available through the NNI user facilities are an important element of the infrastructure required to advance the MGI, but the MII also includes computational tools (models), data, and increasingly, robotics and autonomous systems. To better understand current capabilities, the MGI's interagency working group on Autonomous Materials Innovation Infrastructure (AMII) hosted a June 2024 workshop bringing together experts from government, industry, and academia.

This two-day workshop included a deep dive into existing resources for several materials classes and a discussion of key gaps. Participants identified hundreds of resources and needs, such as the development of automation in experimental hardware for materials synthesis, characterization, testing, and sample exchange; new AI decision methods; standardized data structures and representations; and improved sharing and reproducibility of data and results. The importance of strong industry–university–government collaboration was also emphasized, highlighting models such as public-private partnerships

or consortia as potential vehicles to advance the AMII in the United States. More details are available in the effort's workshop report (MGI 2024).

The biannual MGI Principal Investigator (PI) meeting, which brought together hundreds of researchers funded by several MGI agencies, was another opportunity to build awareness of existing capabilities and identify areas where aligning the MII could help address key challenges. The MGI also hosted industry-focused events embedded in larger gatherings, including the "AI-Accelerated Materials Design and Deployment" town hall (TechConnect 2024) and "The Materials Genome Initiative & Microelectronics: Designing the Next Generation of Materials" workshop at the Electronics Resurgence Initiative (ERI) 2.0 Summit (DARPA 2023). These events, along with a 2025 MGI request for information (Federal Register 2025), have provided valuable insight into the current AMII, key challenges and examples of industry interest in and adoption of MGI approaches.

Opportunities Ahead

For decades, accelerating materials design has depended on our ability to accurately model material behavior. While physics-based models offer powerful insights, their computational cost often limits practical application, especially in fast-paced manufacturing environments. As a result, even the most advanced practitioners rely on approximations and selective use of these models to make informed decisions.

AI is now poised to upend this paradigm. AI can generate predictive models where none previously existed and create "surrogate models" that replace physics-informed simulations with AI-driven approximations. While not exact replicas, these models can operate at speeds many orders of magnitude faster than traditional simulations, making real-time materials design and analysis feasible in ways never before possible. As with all modeling efforts, verification, validation, and uncertainty quantification remain essential to ensure a trustworthy, predictive materials innovation infrastructure.

The integration of AI doesn't stop at modeling. Automation of laboratory processes is enabling high-throughput materials synthesis, which can then be followed by AI-powered characterization techniques that rapidly assess whether a newly developed material possesses the desired properties. If not, AI-driven optimization algorithms can refine the design, automatically specifying the next experimental iteration. This feedback loop is at the heart of autonomous experimentation (AE, or self-driving labs), a transformative technology set to redefine materials research (Stach et al. 2021).

Beyond accelerating innovation, AE addresses a fundamental challenge in materials science: the scarcity of high-quality materials data. Unlike fields such as biology, weather forecasting, and finance, where vast datasets fuel machine learning models, materials R&D has historically struggled with limited and fragmented data. AE can break this bottleneck by generating vast and reliable datasets, laying the foundation for next-generation AI models.

Critically, this revolution extends beyond research labs. AI-driven surrogate models, fueled by AE-generated data, can create "materials digital twins"—fast, accurate computational representations of materials and their behaviors across processing and performance conditions. These digital twins will operate at manufacturing-relevant timescales, enabling seamless integration into the digital thread of production. The result is a direct and unprecedented translation of fundamental materials knowledge from early-stage research to industrial applications, bridging long-standing gaps that have traditionally slowed innovation.

AI-powered materials R&D will propel the field into an era of speed, efficiency, and predictive power unlike anything seen before.

To realize the opportunities ahead, it will be important to leverage the strong community established under the auspices of the MGI to bring together researchers and developers from academia, industry, and government, across disciplines and stages of the technology development continuum. Likewise, it is imperative to build on the foundational tools and methods developed under the MGI—the Materials Innovation Infrastructure—while embracing and adopting new technologies such as AI and AE.

AI-powered materials R&D will propel the field into an era of speed, efficiency, and predictive power unlike anything seen before. The convergence of AI, automation, and materials science is not merely an incremental improvement; it is a revolution poised to redefine how

we discover, design, develop, and deploy the materials of the future.

References

DARPA [Defense Advanced Research Projects Agency]. 2023. Electronics Resurgence Initiative 2.0 Summit, August 22–24, 2023. Seattle. Online at eri-summit.darpa.mil.

de Pablo JJ, Jackson NE, Webb MA, and 17 others. 2019. New frontiers for the materials genome initiative. npj Computational Materials 5:41. Online at https://www.nature.com/articles/s41524-019-0173-4.

Federal Register. 2025. Notice of request for information (RFI) on autonomous experimentation platforms from Material Genome Initiative. Online at www.federalregister.gov/documents/2025/01/17/2025-01161/notice-of-request-for-information-rfi-on-autonomous-experimentation-platforms-from-material-genome.

Lin H, Lee S, Sun L, Spellings M, Engel M, Glotzer S, Mirkin CA. 2017. Clathrate colloidal crystals. Science 355:931–35. Online at www.science.org/doi/10.1126/science.aal3919.

MGI [Materials Genome Initiative]. 2024. Accelerated Materials Experimentation Enabled by the Autonomous Materials Innovation Infrastructure (AMII). A Workshop Report. Online at www.mgi.gov/sites/mgi/files/MGI_Autonomous_Materials_Innovation_Infrastructure_Workshop_Report.pdf.

NIST [National Institute of Standards and Technology]. 2025a. CALPHAD data informatics. Online at https://www.nist.gov/programs-projects/calphad-data-informatics.

NIST. 2025b. Materials Genome Initiative. Online at www.nist.gov/mgi.

NNCI [National Nanotechnology Coordinated Infrastructure]. 2025. Tools. Online at nnci.net.

NRC [National Research Council]. 2008. Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security. Washington: National Academies Press. Online at https://nap.nationalacademies.org/catalog/12199.

NSF [National Science Foundation]. 2025a. Designing Materials to Revolutionize and Engineer Our Future (DMREF). Online at www.nsf.gov/funding/opportunities/dmref-designing-materials-revolutionize-engineer-our-future.

NSF. 2025b. Materials Innovation Plans (MIP). Online at www.nsf.gov/funding/opportunities/mip-materials-innovation-platforms.

NSTC [National Science and Technology Council]. 2014. Materials Genome Initiative Strategic Plan. Online at www.mgi.gov/sites/mgi/files/mgi_strategic_plan_-_dec_2014.pdf.

NSTC. 2018. The National Nanotechnology Initiative Supplement to the President's 2018 Budget. Online at www.nano.gov/sites/default/files/pub_resource/NNI-FY18-Budget-Supplement.pdf.

NSTC. 2021. Materials Genome Initiative Strategic Plan. Online at www.mgi.gov/sites/mgi/files/MGI-2021-Strategic-Plan.pdf.

Stach E, DeCost B, Kusne AG, Hattrick-Simpers J, Brown KA, Reyes KG, Schrier J, Billinge S, Buonassisi T, Foster I, and 11 others. 2021. Autonomous experimentation systems for materials development: A community perspective. Matter 4(9):2702–26. Online at www.cell.com/matter/fulltext/S2590-2385(21)00306-4.

TechConnect. 2024. Town hall: AI-accelerated materials design and deployment. TechConnect World Innovation Conference & Expo. Online at www.techconnectworld.com/World2024/sym/TCW_Town_Hall.html.

Warren J. 2024. The Materials Genome Initiative and the metals industry. The Bridge 54(910):25–29. Online at www.nae.edu/313309/The-Materials-Genome-Initiative-and-the-Metals-Industry.

Our future depends on making our materials faster, better, and smarter.

Revolutionizing Materials Science and Technology to Secure Our Future

Richard A. Vaia, Germano Iannacchione, and Anthony D. Rollett

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In our pursuit of economic, societal, and defense security through technology, let us not forget that everything is made of something. There is a common saying paraphrased from the writings of the Nobel Laureate Sir George Paget Thomson:

> A civilization is both developed and limited by the materials at its disposal.

We are within a historical time of consequence, a critical period in which decisions and actions will have a lasting, foundational impact. If we are to

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meet this challenge, advanced materials (AdvMat) can and should be reinvented by leveraging today's information technology revolution and re-imaging partnerships between academia, industry, and government. This goal requires a national AdvMat initiative to harness the unique capabilities of all stakeholders ensuring that the modernization of materials science and technology (S&T) anticipates the accelerated rate of change in other sectors—colloquially, *ensuring the right stuff is available to make the future*.

In a time of disruptive change, determining how to close this impedance gap cost-effectively is not only a competitive advantage but also a critical national capability.

This imperative has been answered before. From the Bronze and Iron Ages to the modern era of silicon-based electronics and photonics, breakthroughs in materials have driven societal progress (Miodownik 2014). For instance, the mastery of smelting and alloying technologies led to the production of bronze, iron, and steel. This enabled the development of sophisticated tools for agriculture and the rise of complex civilizations, from the city-states of Ur and Babylon to the later Assyrian and Persian Empires. Similarly, in ancient China, the cultivation of silk—rooted in a deep, albeit empirical understanding of biology and textile manufacturing—fostered economic growth and global cultural influence.

The advent of modern technologies is also witness to the profound impact of AdvMat. Aerospace is an exemplar, where material innovations enabled first powered flight and their lack resulted in tragedy. Charles Taylor's innovative thin-wall casting technique, which significantly strengthened the aluminum crankcase by the formation of Guinier–Preston zones. This reduced the engine's weight making the Wright Brothers' pioneering 1903 flight possible (Gayle and Goodway 1994). In contrast, insufficient understanding of material performance, inspection techniques and manufacturing process controls led to catastrophes, such as the first fatality during powered flight (Howard 1998), or the structural failure of the world's first commercial jet airliner, the original de Havilland DH.106 Comet, due to metal fatigue (FAA n/d). These tragedies highlight that it is more than discovery; a fundamental understanding of materials behavior for reliability and safety is just as important.

The challenges posed by modern technologies catalyzed the formation of the materials science and engineering discipline in the 1960s. Its purpose, conceptualized as the "Materials Tetrahedron" (Deagan et al. 2022), is to understand, manipulate, and employ:

a) the relationships between a material's composition and hierarchical structure;
b) how processing and environment optimizes that composition and structure from the atomic to the macro level; and
c) ultimately using this information to forecast physical properties in service.

The performance required for advanced technology is designed using materials and processes informed by the optimization of properties and attributes like cost, manufacturability and sustainability. The meaning of the term "advanced materials" evolves as new technologies continually expand the boundary of extreme performance. Consequently, the nation that discovers, understands, and utilizes AdvMat is best positioned for prosperity and security in that future "Age."

Today, many nations recognize the pivotal role of AdvMat in future economic growth and prioritize sustained research and development in this area to overtake competitors, such as the ones outlined in the Australian Strategic Policy Institute's Critical Technology Tracker (Leung et al. 2024). The 2024 Nature Index found that eight leading nations in Materials Science research, including China, South Korea, Singapore, Japan, and Russia, dedicate more than 25% of their research articles to this field (Nature Index 2024). Moreover, access to critical elements, minerals, and materials—including their source and refinement—are the foundation of modern supply chains and employed today as a tool for global economic leverage. Whether one considers metals, ceramics, semiconductors, polymers, biomaterials, complex fluids, or a combination of them, the innovation landscape for human health, defense, energy, sustainability, and information depends on an affordable supply of trusted materials that are integrated with engineering design tools and manufacturing processes.

The impact of such investment on future leadership is currently being discussed in academic, economic, futur-

ist, and policy circles. These impacts are driving a revolution in the process of materials research and development (R&D). Traditionally, materials R&D has relied heavily on teams of expert researchers exploring potential applications or applying existing knowledge to solve engineering issues. Even interpolating within a class of materials for a solution can take a decade and hundreds of millions of dollars to mature a promising concept into a reliable, cost-effective solution with certification, databases, standards, and supply chains. Material researchers develop application-driven solutions for entrepreneurs, businesses and engineers who assess their utility when responding to product designers and commercialization requirements. However, this traditional, sequential, 15–20-plus-year process is out of sync with modern 1–3-year design–production cycles. In a time of disruptive change, determining how to close this impedance gap cost-effectively is not only a competitive advantage but also a critical national capability, since *everything is made of something.*

In the United States, the decade-old Materials Genome Initiative (MGI) foresaw the necessity of dealing with this issue, envisioning the deployment of "advanced materials twice as fast and at a fraction of the cost compared to traditional methods" via integration of models, machine learning, robotics, high-performance computing, and automation (MGI 2025). In 2024, the MGI crafted Challenges such as "Point of Care Tissue-Mimetic Materials for Biomedical Devices and Implants" and "Agile Manufacturing of Affordable Multi-Functional Composites" to stimulate a nexus between data-centric materials frameworks and the necessary partnerships along the technology development pathway (MGI 2024).

Numerous professional societies are becoming centers of exchange and community advocacy, such as The Minerals, Metals & Materials Society; The Materials Research Society; and the Materials Research Data Alliance. Examples are also exploding of how these digital approaches are addressing materials challenges early in research (Stach et al. 2021). Similarly, MGI-enabled products are occurring in some industries, such as alloy development at Mercury Marine, Pratt and Whitney, General Electric, Apple, SpaceX, and QuesTek, among others (TMS 2018; Warren 2024). Additionally, use of digital materials concepts, such as digital twins (NASEM 2024a) and data-validated material models, are beginning to occur within the US defense industrial base to accelerate advanced development, prototyping, design and acquisition.

While digital tools such as artificial intelligence (AI) and autonomous self-driving laboratories offer powerful capabilities, accelerating individual steps in research does not automatically translate to an overall acceleration of new technology or their use. The significant time and effort required to overcome the various obstacles along the discovery–development–demonstration–deployment–decommission (D5) life cycle (Figure 1 [Left]) underscore the adage that "the best promise of a new material is often its first report." The ecosystem, acumen, and tools necessary for success at each stage are different. However, the data are interrelated and need to flow both ways, whether via scientific principles or performance

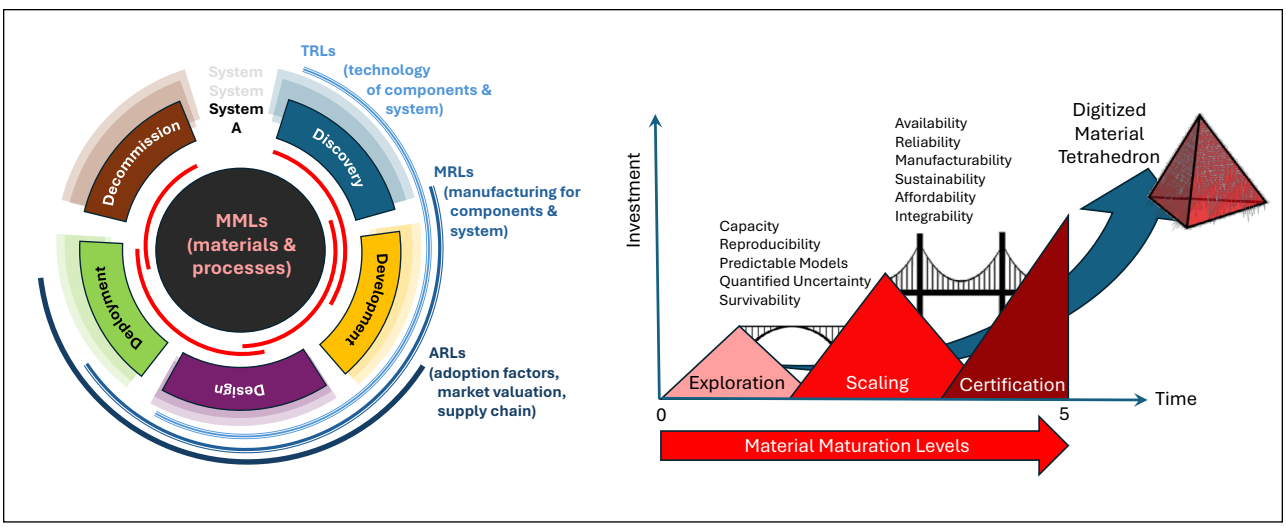

FIGURE 1 System life cycle, risk assessments, and materials maturation. (Left) Risk assessments and levels during the life cycle of systems. (Right) Material maturation valleys.

requirements. For example, to integrate materials innovation into initial design optimization of a component, a digital materials framework must not only facilitate discovery but also provide a foundation for anticipating development and deployment challenges like scale-up, integration, reproducibility, availability, reliability, survivability, manufacturability, and affordability (NRC 2024). Such a framework must be trusted by all communities by empowering their unique processes. Thus, the framework must embrace the convergence of distinct perspectives.

A high MML platform provides increased agility, enhanced predictivity, and improved availability at lower cost to various systems during their life cycle by merging materials knowledge developed for and across various systems.

Framing such a data pipeline is central to translating successful case studies of one material into the broader material S&T discipline. Because investment and engineering decisions are grounded by data, "assessments" and the associated "levels" used for understanding risk along a maturation pathway provide a framework for understanding the role and value of a data pipeline. Figure 1 (Left) summarizes a way in which such risk assessment frameworks help traverse the life cycle of a given system. Most prominent are Technology Readiness Levels (TRLs), developed by NASA in the 1970s, which describe a progression of events that represent systematic reduction of risk during the development of a complex system (Kimmel et al. 2020). Readiness to deploy and meet customer requirements, however, depends on many elements beyond technology integration, including maturity of sub-component technologies, software, manufacturing processes (DOD 2022), markets, and business models (DOE 2024), as well as materials. Each of these elements has spurred complementary frameworks that must be simultaneously addressed for successful system maturation.

Recently, the concept of Material Maturation Levels (MMLs) has been proposed (Rollett et al. 2025). This concept recognizes the strategic advantage of de-risking a new material and its processing as a technology platform that continuously evolves to address the requirements of different systems as well as how these change throughout their life cycle. This contrasts with considering material readiness only within the confines of the requirements of a specific system, where simultaneous discovery and development of a bespoke material solution in parallel with components incurs substantial system-level risk and thus favors the use of existing material solutions. Effectively, material maturation argues for a broader aperture that is informed by, and informs, a set of various systems and their life cycles, as depicted by the numerous MML arcs (red) inside D5 loops for different system concepts (Figure 1 [Left]).

Figure 1 (Right) summarizes the key features of MMLs, emphasizing that curiosity-driven studies, materials discovery, use-inspired R&D, prototyping, manufacturing, and certification cannot be decoupled, but instead their unique acumen and culture must be tied together with two-way bridges so as to yield a successful material technology platform. The process is not linear but ebbs and flows across the bridges embracing push, which imagines orthogonal approaches based on an expanded state of possibility, as much as pull, which solves application-derived requirements with new science, materials, and/or engineering.

A high MML platform provides increased agility, enhanced predictivity, and improved availability at lower cost to various systems during their life cycle by merging materials knowledge developed for and across various systems. A new material technology with a high MML will reduce early system-level risks when it is used by a low TRL concept. Additionally, a digital artifact that reflects the material platform knowledge will allow exploration of a wider system design space, potentially revealing novel architectures that leverage the tailorability of new AdvMat. Since requirements shift during the life cycle, additional MML assessments are important to re-establish risk posture and effective mitigation strategies (such as for repair and sustainment after deployment) or for recycling and disposal during decommissioning. The "Digital Twin of the Materials Tetrahedron" is an example of a construct that could unify materials data across MMLs, affording integration and analysis of vast datasets on materials properties and processing parameters, as well as defining the knowledge deliverables in terms of modern digital engineering and manufacturing tools (Deagen et al. 2022).

Risk Assessments and Levels During the Life Cycle of Systems

As already noted, a system's life cycle may be conceptualized in five stages: *Discovery* (curiosity and use-inspired research to expand the state of the possible), *Development* (demonstration of stable, predictable, and implementable components and the means for integration), *Design* (meet requirements by engineering, optimization, and integration of qualified components for an application), *Deployment* (established means for producibility, fielding, and sustainment of a solution that meets market or customer demand), and *Decommission* (methods of the system's retirement, disposal, or repurposing) (Figure 1 [Left]). The duration of each stage is variable, and there is substantial ebb, flow, and iterations along the path. Each stage is dominated by an ecosystem with different perspectives and motivations, necessitating convergent teams to shepherd the most promising opportunities. Temporal impedance within and between stages nominally underscores success or failure, while using established components is much faster than creating new components. Overall, assessments and their associated levels are common frameworks used for quantifying risks during the process and are critical to determining additional investment. TRLs, MRLs, and Adoption Readiness Levels (ARLs) are examples that help mapping through different stages and provide measures to track gaps, impact, and value. Platform technologies that are foundational throughout the life cycle are the central hub, and are also supported by frameworks, such as MMLs.

Material Maturation Valleys

MMLs provide a framework to identify, assess, and address risks as the valleys are traversed between exploration, scaling, and certification. Materials exploration encompasses early curiosity and use-inspired research to discover new materials, and to understand the limits of their properties via determining their structure–composition–processing correlations, the effect of the environment, and subsequent interdependences. To reduce the ensuing investment risk of scaling, approaches to capacity beyond the lab-scale, demonstrating integration methods, verifying reproducibility, developing predictive models with quantified uncertainties for sets of properties, and quantifying the temporal impact of operational and manufacturing environments (i.e., survivability) must be overcome. These establish a scaled, stable, qualified material technology platform that can be used for development of design methods, prototypes, and fabrication processes that afford integration and tunability. If successful, even greater investment is required to validate manufacturability, reliability, availability, safety, affordability, and supportability, among other factors, in order to realize a certified material solution that conforms to standards, specifications, and a process design kit for use in a component or system. Success for each stage requires a unique acumen and culture, and the bridges require the convergence of these communities. A digital representation of the knowledge developed along this pipeline creates a "Digitized Materials Tetrahedron." This MML deliverable ensures a fully acceptable, trusted material solution by empowering modern digital engineering, production, techno-economic analysis, and support tools across the life cycle. The benefits provided by this digital twin includes earlier evaluation of potential improvement to users by assessing the impact of material tunability on system performance, production costs, or lifetime; sensitivity analysis of changes in suppliers; insight to focus resources on critical path gaps to accelerate development; and rapid response to material failures during deployment with root-cause analysis.

Given all this—the criticality of materials, the opportunities afforded by digital tools and information technology, and a broader aperture for material technology maturation and its impact on future systems—what is missing that limits a market-driven solution? One view is that market forces lack the patience to bring new materials through these frameworks. In this case, the federal government has crucial roles to fulfill. For example, basic science often generates non-excludable knowledge that underpins future innovations but is difficult for firms to fully quantify in terms of benefits to help them with selling new or improved products. Additionally, some critical technology platforms, such as advanced materials and manufacturing processes, require substantial long-term investments in research, development, and workforce education with uncertain returns. Private-sector investment alone would be too risky and impatient in the face of uncertain return on investment. For highly complex technologies, information asymmetry may also hinder innovation, where a lack of comprehensive expertise, facilities, tools, software, training, information access, or partnerships challenge small and medium enterprises to leverage innovations of others and to communicate the value they provide.

In all these cases, the government acts as a broker through leadership, policy, and resources, from facilitating competition to connecting commercial innovation to activities providing a public good such as national defense. Government

resources, expertise, facilities, and policies ensure technological advancements that complement and integrate those of the private sector so that federal procurement delivers the most capable defense systems. For a data-centric materials revolution that empowers all the nation's innovators, these brokerage roles are not just crucial but imperative.

The Impact of the Materials Genome Initiative

The MGI laid the foundation for the materials science and technology revolution by convening 19 federal agencies and their laboratories. As a coalition, the agencies engage stakeholders across materials science and its intersection with various technologies. For example, NSF, the Department of Energy (DOE) Office of Basic Energy Sciences, and DoD's Basic Research Offices (e.g., ARO, ONR, AFOSR) drive curiosity-driven exploration of data-centric methods to accelerate materials discovery. DOE's Office of Energy Efficiency and Renewable Energy, NASA, National Institute of Standards and Technology (NIST), and DoD's laboratories and agencies (e.g., ARL, NRL, AFRL, DARPA, MDA) create public–private communities that address high risk, use-inspired material challenges through grants, contracts, innovation challenges, and partnerships. All of the agencies develop and sustain pre-competitive user facilities that are democratizing materials innovation and demonstrating the impact of artifact intelligence and autonomy. These range from unique collections of synthesis, computation, and fabrication capabilities to one-of-a-kind instrumentation, open-access data banks, and emerging manufacturing technologies. Finally, federal teams are partnering with the private sector to develop policy and regulatory support, ranging from data-sharing policies (National Institutes of Health, NSF, DOE) and championing standards (NIST, DoD). Recent summaries of these activities include an NSF-led assessment of the US infrastructure that is relevant to autonomy-enabled materials R&D (NSF 2024), a National Academies examination of the impact of basic science programs to achieve the MGI vision (NASEM 2023), a report on creating the next generation materials workforce (TMS 2019), and an OSTP assessment of the impact of AI (Hendrix 2024). These reports demonstrate that increased coordination among the federal AdvMat community, and with private institutions, is setting a foundation for a national capability in digitized AdvMat innovation. Such products and forums facilitate communication and awareness between stakeholders and ensure that teams specialize appropriately to maximize leveraging and impact, while minimizing duplication.

Notable examples of efforts to establish a data-centric materials revolution through public–private stakeholder teams are discussed below.

Developing a Data-Centric Materials Research Culture

The Designing Materials to Revolutionize and Engineer our Future (DMREF) initiative is an NSF-wide, multiagency, biannual interdisciplinary teams program that seeks to promote the design, discovery, and development of materials and accelerate their path to deployment. DMREF emphasizes (1) a deep integration of experiments, computation, and theory; (2) the use of accessible digital data across the materials development continuum; and (3) the strengthening of connections among theorists, computational scientists, data scientists, mathematicians, statisticians, and experimentalists. Leveraging AI, autonomy, and automation, researchers not only discover new materials but uncover hidden patterns and predict material behavior with greater accuracy. In addition, multiple federal partners (Departments of the Air Force, Navy, and Army; DOE; NIST) participate through either direct funding or via collaborations with their intermural researchers and facilities. Recently, international partners (United States-Israel Binational Science Foundation; Department of Science and Technology, Government of India; Natural Sciences and Engineering Research Council of Canada; and Deutsche Forschungsgemeinschaft) have been integrated. DMREF exemplifies the power of collaborative and coordinated federal activities as well as connecting public and federal scientists (TMS 2019).

Creating Unique Data-Centric Materials Facilities

Large center-level "aggregators" of significant and unique instrumentation play especially crucial roles in exploring over-the-horizon discovery and de-risking development with industrial participation. Notable efforts at NSF include the Materials Innovation Platforms, Engineering Research Centers, and Industry-University Cooperative Research Centers. DOE supports crucial data and computational infrastructure investments, including the Materials Project, its Computational Materials and Chemical Science programs, and the Energy Materials Network. Joint federal/industry/academic investments in large-scale instrumentation are especially important in transferring data-centric materials practice to industry, such as DOE's Light and Neutron Sources, Cornell's Center for High-Energy X-ray Sciences (CHEXS), the NIST/NCNR Center for High-Resolution Neutron Scattering, and NIST's Materials Data Repository. These efforts dem-

onstrate how to fuse data from disparate experimental and modeling sources and integrate AI, automation, and autonomy into digital workflows for discovery, design, and manufacturing.

Catalyzing Data-Centric Materials Communities for National Priorities

The nation's federal laboratories are vital centers of excellence within the US S&T ecosystem. They attract top scientists and engineers from all disciplines, cultivating global technological leadership for national priorities in economic, energy, health, and defense security. Their unique environments and public–private collaborations result in revolutionary innovations that complement the market by enabling the entire material spectrum, such as high-precision instrumentation, theory and computation methods, first-of-a-kind synthetic approaches, new characterization techniques, and gold-standard reference data. As the public's independent deep-technical experts, the civilian scientists and engineers also play many vital roles by focusing on high-risk material concepts, providing unbiased assessment, and targeting mission-relevant capability gaps to guarantee technological advantages necessary for national strength. Such catalyzing leadership by engineers and scientists at NIST, DoD's service laboratories, and many others, are creating pervasive data-centric tools from material data repositories to autonomy-enabled research platforms for accelerated validation, reducing barriers to entry via open architecture standards, and manufacturing via materials-informed digital twins.

Despite the impact of these federal activities, substantial challenges remain in accelerating materials discovery to market impact and delivering solutions to national priorities. These challenges go beyond deepening the convergence of information sciences with materials discovery and research communities. Rather, they reflect a complex mix of technology, culture, policy, and resources that extend beyond individual segments of the D5 or MML processes. Some examples that necessitate additional federal leadership and partnerships with the private sector follow.

Valuation of Materials Data

Maximal impact of AI is predicated on interoperable data. Notwithstanding the extensive array of current and planned material data bases and automated or autonomy-driven materials R&D facilities, they are generally isolated, geographically and virtually. Interconnectivity, such as via the Cloud, reflects a substantial opportunity to drive exponential growth, but necessitates accessibility to AI-ready and FAIR (Findable, Accessible, Interoperable, and Reusable) compliant data (Brinson et al. 2024). The lack of standardized data formats, application program interfaces, and techniques to measure impact and assess value of data archiving and sharing, encourages data silos and hinder efficient sharing and integration of materials data across all stakeholders, from academia, small businesses, and government to emerging and established supply chains. For example, federal agencies can convene the community to develop and adopt data standards, to validate usage of Large Language Models, and to establish workflow frameworks for research, validation, and certification. Such community practices should balance sharing and accessibility with the protection of intellectual property rights and national security by building on cybersecurity innovations in health, financial, and intelligence communities. These characteristics are foundational to transforming *databases*, where information is archived, into *data banks* where information can be deposited, updated, and retrieved such that the process creates value (Himanen et al. 2019; NASEM 2024b). These and other innovations are necessary for the establishment of viable business models that simultaneously accelerate open innovation, deliver data interoperability, maintain information rights, and provide for the long-term sustainability of the infrastructure, data curation, and software in which a future data-centric AdvMat discipline will be based.

Transferability of Digital Materials Tetrahedra

Another challenge is the compartmentalization of efforts across materials and technology sectors, which not only hampers sharing of successful approaches but fosters niche solutions that lack interoperability through MMLs and across readiness levels. While the pursuit of a universal solution is quixotic, developing strategic plans and roadmaps fosters collaboration among sectors and provides a means to align priorities, eliminate redundancies, and identify gaps to maximize the impact of investments. Such a shift from vertical integration with a few participants to precompetitive partnerships across a common supply chain has occurred historically due to the need for exponentially more complex and costly technologies to meet market demand, such as SEMATECH and other consortiums for microelectronics. The success of an agile vertical with many participants depends on a common vision and shared understanding of gaps, achieved through road-mapping that includes all stakeholders. Knowledge and data sharing of materials and manufacturing processes affords early and evolving analysis of alternatives as well as the abil-

ity to target resources on the challenges most impactful to market needs. This alignment through the discovery–development–deployment arc is especially important to focus discovery on the most impactful problems, as well as fully understand the potential extent of system-level impact of new materials as they ascend the maturity ladder. For such goals, industry must collaboratively define a value proposition balanced across the ecosystem and individual entities, while developing incentive policies for data sharing, streamlining regulatory processes to reduce barriers to new material adoption, and addressing gaps such as access to mid-scale production for validation of emerging materials or enabling the economic viability of solutions requiring only small production runs (NASEM 2025). Examples of such activities in which public–private partnerships are incubating the value of digital materials artifacts in different communities include the Manufacturing USA Institutes (NASEM 2017), MGI's CHIPs for America program on Accelerating Material R&D for Sustainable Semiconductor Materials, and federal approaches to ensure reliable critical materials and minerals (NAE 2024). Other approaches are based on regional networks for innovation and economic development, such as NSF's Regional Innovation Engines and AFRL's Regional Networks. Common across these activities is the need for public funding to not only incentivize partnerships but provide stability as trust is established among the diverse stakeholders. Further success and scalability will require a national conversation of incentives, resources, and culture.

Ensuring the Future Workforce

Finally, an expanded workforce will be necessary to compete globally and employ these data-centric material innovations across the life cycle. A participant must not only be cognizant of information technology and materials science, but thrive in diverse teams that merge materials science, engineering, manufacturing, and digital technologies seamlessly. Not only is an understanding of the complexities of materials required, but also their role and impact on system design, product development, producibility, and profitability. Continuous career learning should also be portable across sectors, enhancing talent flow and providing updated skills to retrain staff. Such a shift in materials education necessitates curriculum and offerings beyond those offered in traditional bachelor's, master's, and doctoral programs. For example, new complementary models for graduate education that embed students in multidisciplinary, team-based cohorts comprised of members with disciplines beyond STEM and embracing internships with industry (established companies or startups), could revolutionize materials innovation. In parallel, a diversity of appropriately sized research funding constructs or grand-challenge prizes that are focused on cross-organization teams will ensure future practitioners have hands-on experiential learning. Technology challenges aligned with national priorities and academic-industry high-risk high-reward projects would provide young materials innovators with experiences at the intersection of basic research and commercialization, serving as steppingstones into US industry. A broader conversation between educators and workforce employers on how we educate the future innovators is imperative if the nation is to stay competitive and transform the potential of a data-centric materials revolution to solutions for economic, societal, and defense security.

Concluding Observations

So, what do we need to do? Materials science and engineering are and will remain crucial to economic and national security. Materials knowledge not only enables emerging technologies and provides differentiators to existing technologies, but also ensures affordable manufacturing, reliability and sustainability. To match the rate of modern technology cycles and deliver discontinuous innovation, the information technology revolution must continue to infuse the entirety of material maturation and adoption pipelines—transforming the "how" of AdvMat so it can continue to deliver as the definition of "advanced" evolves in the future. This goal necessitates a national AdvMat initiative to accelerate the transformation of research culture, facilities, and communities spearheaded by the MGI. Continuing the MGI Challenges' calls to action will provide priority challenges to rally the community to demonstrate cost-effective acceleration of AdvMat solutions with game-changing impact. Federal leadership, investment, and curation of such public–private teams are required to address the complex interplay of technology, culture, policy, and resourcing facing the next challenges of data valuation, interoperability, and workforce. Such efforts, if successful, will build a resilient, responsive, and interconnected materials innovation infrastructure, crucial to securing US leadership in future technology revolutions.

References

Brinson LC, Bartolo LM, Blaiszik B, Elbert D, Foster I, Strachan A, Voorhees P. 2024. Community action on FAIR data will fuel a revolution in materials research. MRS Bulletin 49(1):12–16.

Deagan ME, Brinson LC, Vaia RA, Schadler LS. 2022. The materials tetrahedron has a "digital twin." MRS Bulletin 47(4):379–88.

DoD [Department of Defense]. 2022. Manufacturing Readiness Level (MRL) Deskbook. Washington.

DOE [Department of Energy]. 2024. Adoption readiness levels. Online at https://www.energy.gov/arl/adoption-readiness-levels.

FAA [Federal Aviation Administration]. Lessons learned from the De Havilland DH-106 Comet 1 accident. US Department of Transportation. Online at https://www.faa.gov/lessons_learned/transport_airplane/accidents/G-ALYV.

Gayle FW, Goodway M. 1994. Precipitation hardening in the first aerospace aluminum alloy: The Wright Flyer crankcase. Science 266:1015–17.

Hendrix J. 2024. A conversation with White House Office of Science and Technology Policy Director Arati Prabhakar. TechPolicy Press, June 16. Online at https://www.techpolicy.press/a-conversation-with-white-house-office-of-science-and-technology-policy-director-arati-prabhakar.

Himanen L, Geurts A, Foster AS, Rinke P. 2019. Data-driven materials science: Status, challenges, and perspectives. Advanced Science 6(21):1900808.

Howard F. 1998. Wilbur and Orville: A Biography of the Wright Brothers. Mineola, NY. Dover Publications, 276–77.

Kimmel WM, Beauchamp PM, Frerking MA, Kline TR, Vassigh KK, Willard DE, Johnson MA, Trenkle TG. 2020. Technology Readiness Assessment Best Practices Guide. NASA [National Aeronautics and Space Administration]. Washington.

Leung JW, Robin SR, Cave D. 2024. ASPI's two-decade critical technology tracker: The rewards of long-term research investment. ASPI [Austrian Strategic Policy Institute].

MGI [Materials Genome Initiative]. 2024. 2024 Materials Genome Initiative (MGI) Challenges. Online at https://www.mgi.gov/2024-materials-genome-initiative-mgi-challenges.

MGI. 2025. Materials Genome Initiative. Online at https://www.mgi.gov.

Miodownik M. 2014. Stuff Matters: Exploring the Marvelous Materials That Shape Our Man-Made World. Houghton Mifflin Harcourt.

NAE [National Academy of Engineering]. 2024. Critical materials. The Bridge 54(2).

NASA [National Aeronautics and Space Administration]. 2020. Technology Readiness Assessment Best Practices Guide. SP-20205003605. Washington.

NASEM [National Academies of Sciences, Engineering, and Medicine]. 2017. Securing Advanced Manufacturing in the United States: The Role of Manufacturing USA: Proceedings of a Workshop. Washington: National Academies Press.

NASEM. 2023. NSF Efforts to Achieve the Nation's Vision for the Materials Genome Initiative: Designing Materials to Revolutionize and Engineer Our Future (DMREF). Washington: National Academies Press.

NASEM. 2024a. Foundational Research Gaps and Future Directions for Digital Twins. Washington: National Academies Press.

NASEM. 2024b. Options for a National Plan for Smart Manufacturing. Washington: National Academies Press.

NASEM. 2025. Mid-Scale Manufacturing and Characterization Capacity for Department of Defense Critical Materials Supply Challenges, Part 1: Proceedings of a Workshop—in Brief. Washington: National Academies Press. Online at https://nap.nationalacademies.org/catalog/29117/mid-scale-manufacturing-and-characterization-capacity-for-department-of-defense-critical-materials-supply-challenges-part-1.

Nature Index. 2024. Online at https://www.nature.com/collections/hjggcijhdf.

NRC [National Research Council]. 2004. Accelerating Technology Transition: Bridging the Valley of Death for Materials and Processes in Defense Systems. Washington: National Academies Press. Online at https://doi.org/10.17226/11108.

NSF [National Science Foundation]. 2024. Accelerated Materials Experimentation Enabled by the Autonomous Materials Innovation Infrastructure (AMII): A Workshop Report. Alexandria, VA.

Rollett AD, Brinkley MK, Dimotakis P, Graham S, Pugliano V. 2025. Materials maturity levels: A systematic approach to evaluating materials development. Integrating Materials and Manufacturing Innovation. Online at https://doi.org/10.1007/s40192-025-00413-6.

Stach E, DeCost B, Kusne AG, Hattrick-Simpers J, Brown KA, Reyes KG, Schrier J, Billinge S, Buonassisi T, Foster I, and 11 others. 2021. Autonomous experimental systems for materials development: A community perspective. Matter 4(9):2702–26.

TMS [The Minerals, Metals & Materials Society] on behalf of MForesight: Alliance for Manufacturing Foresight. 2018. Harnessing Materials Innovations to Support Next Generation Manufacturing Technologies. TMS. Pittsburgh.

TMS. 2019. Creating the Next-Generation Materials Genome Initiative Workforce. Pittsburgh. Online at https://www.tms.org/portal/portal/Publications/Studies/MGIworkforce/MGIworkforce.aspx?hkey=830f10ad-47c7-4ea8-8563-1bba0c8ae586.

Warren J. 2024. The Materials Genome Initiative and the metals industry. The Bridge 54(1):25–29.

Self-driving labs promise to turn the Materials Genome Initiative's bold vision into reality.

Accelerating the Materials Genome Initiative with Self-Driving Labs

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The Materials Genome Initiative (MGI), launched in 2011, set a national goal to discover, manufacture, and deploy new materials at twice the speed and half the cost of the status quo (MGI n.d.). While substantial progress has been made through computational methods and curated data infrastructures, experimental bottlenecks persist. Self-Driving Laboratories (SDLs) offer a transformative pathway to overcome this limitation. SDLs integrate robotics, artificial intelligence, autonomous experimentation, and digital provenance in a closed-loop system capable of rapid hypothesis generation, execution, and refinement in a closed-loop fashion. This article explores how SDLs can activate each layer of the MGI, from foundational data generation to workforce development, and presents a 10-year roadmap for integrating SDLs into a national Autonomous Materials Innovation Infrastructure.

Introduction: From Genome to Genius

The Human Genome Project redefined biology through coordinated, large-scale data generation, leading to breakthroughs in medicine and genetics (Watson 1990). MGI extends this model to materials science, aiming to reduce discovery timelines through the integration of computation, data, and experiment (de Pablo et al. 2019). However, despite theoretical and simulation advances, a critical barrier remains: empirical validation. Physical experimentation still relies on

manual procedures, limited throughput, and fragmented infrastructure, hampering the pace of materials innovation.

SDLs can close this gap. By combining programmable hardware with artificial intelligence (AI)-driven decision engines, SDLs create autonomous platforms capable of performing thousands of experiments with little or no human intervention (Abolhasani and Kumacheva 2023) (see Figure 1A). SDLs redefine experimentation as a continuous, data-rich, adaptive process (Delgado-Licona et al. 2025). They are not replacements for human intuition but instead serve as powerful robotic collaborators that can test and iterate on ideas far beyond what is practical in conventional settings (Canty et al. 2025).

The implications of SDLs are profound. For example, a national network of SDLs continuously generating validated datasets for new battery chemistries, semiconductor heterostructures, or polymer formulations could reduce time-to-solution by 100× to 1,000× times compared to the status quo. These platforms could rapidly identify promising candidates, validate theoretical predictions, and flag anomalous behaviors worthy of deeper study (Bennett et al. 2024; Boiko et al. 2023; Dai et al. 2024; Epps et al. 2020; Koscher et al. 2023; MacLeod et al. 2020; Slattery et al. 2024; Snapp et al. 2024; Steiner et al. 2019; Szymanski et al. 2023; Volk et al. 2023). More than just tools, SDLs become infrastructure—an autonomous experimental layer in the materials research ecosystem.

SDLs represent the missing experimental pillar of the MGI vision. Their integration would not only accelerate discovery but also enhance reproducibility, access, and resilience. By converting experimentation into a programmable, scalable infrastructure, SDLs can become essential assets in achieving the MGI's objectives. This article outlines how SDLs complement MGI's strategic pillars, demonstrates how they can be deployed at scale, and explores how their widespread adoption can transform both how and who conducts materials science.

The Materials Genome Initiative: Vision and Strategic Evolution

Since its inception, the MGI has driven coordination across federal agencies, national laboratories, academia, and industry. Early successes were primarily computational. Initiatives such as The Materials Project (Jain et al. 2013), Open Quantum Materials Database (OQMD) (Kirklin 2015), and the Automatic FLOW for Materials Discovery database (Curtarolo et al. 2012) provided researchers with instant access to millions of calculated material properties. These resources allowed researchers to screen candidate materials virtually, reducing the time and cost of identifying promising materials with intriguing properties.

Despite these achievements, the experimental layer of MGI remains underdeveloped. Data generation is often manual, idiosyncratic, and difficult to scale. Experimental metadata are inconsistently recorded, making reproducibility and cross-laboratory validation challenging. More fundamentally, the speed at which computational models improve outpaces our ability to generate corresponding experimental datasets. This misalignment limits the feedback loop between computation and experimentation that is central to MGI's vision.

By combining programmable hardware with artificial intelligence (AI)-driven decision engines, SDLs create autonomous platforms capable of performing thousands of experiments with little or no human intervention.

The 2021 and 2024 MGI strategic documents explicitly recognize this gap (MGI n.d.). Both reports call for autonomous systems that can generate high-quality, reproducible data in a scalable and shareable format. This includes automated synthesis as well as characterization and integration of AI to design, interpret, and adapt experiments. The term "Autonomous Materials Innovation Infrastructure" emerged as a framework to conceptualize this vision (MGI 2024a). SDLs are uniquely positioned to operationalize this mandate. By strengthening all three foundational pillars of MGI—computation, data infrastructure, and experimentation—SDLs provide an integrated environment where theory, simulation, and empirical validation converge.

Furthermore, SDLs directly address high-priority 2024 MGI Challenge Areas (MGI 2024b) such as decarbonization, semiconductor manufacturing, and critical mineral recovery by enabling rapid, reproducible testing and optimization. With their closed-loop learning and real-time adaptability, SDLs bring us closer to a truly predictive materials science ecosystem.

The Architecture and Algorithms of Self-Driving Labs

At a technical level, an SDL consists of five interlocking layers (see Figure 1):

Actuation Layer: Robotic systems that perform physical tasks such as dispensing, heating, mixing, and characterizing materials;

Sensing Layer: Sensors and analytical instruments that capture real-time data on process and product properties;

Control Layer: The software that orchestrates experimental sequences, ensuring synchronization, safety, and precision;

Autonomy Layer: AI agents that plan experiments (decision making), interpret results, and update experimental strategies (model refinement); and

Data Layer: Infrastructure for storing, managing, and sharing data, including metadata, uncertainty estimates, and provenance.

The *autonomy layer* distinguishes SDLs from traditional automation. Rather than executing a fixed set of experiments, an SDL interprets results and decides what to do next. This is crucial for navigating complex, nonlinear, or poorly understood materials spaces. For instance, in optimizing catalytic activity, an SDL may shift focus from composition to temperature as more is learned about the system, mimicking a human researcher's strategy. Algorithms such as Bayesian optimization and reinforcement learning allow SDLs to efficiently navigate complex, multidimensional design spaces (Abolhasani and Kumacheva 2023). Large language models further enhance SDLs by translating user intent from scientific literature or natural language prompts into structured experimental constraints (Boiko et al. 2023; Ruan et al. 2024).

Recent advances in AI have further enhanced the autonomy layer of SDLs. Multi-objective optimization frameworks can balance trade-offs between conflicting goals such as cost, toxicity, and performance. Uncertainty-aware models ensure that the SDL explores areas where predictions are weak, reducing bias. Large language models can parse scientific literature and translate user intent into experimental constraints. These developments expand the capabilities of SDLs, making them not only faster but smarter.

An exemplary SDL—an autonomous multiproperty-driven molecular discovery (AMMD) platform—is illustrated in Figure 2. This SDL unites generative design, retrosyn-

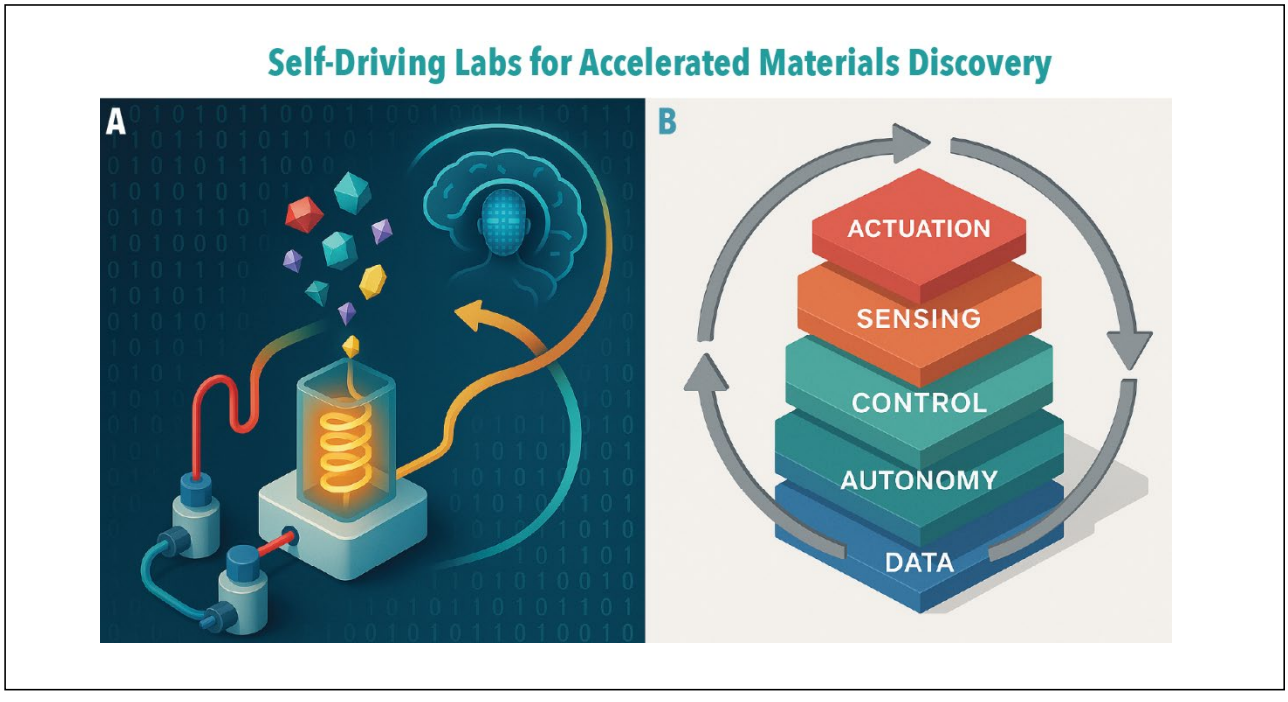

FIGURE 1 (A) An illustration of a self-driving lab for AI-assisted materials discovery. (B) Different layers of a modular SDL, including data, autonomy, control, sensing, and actuation layers.

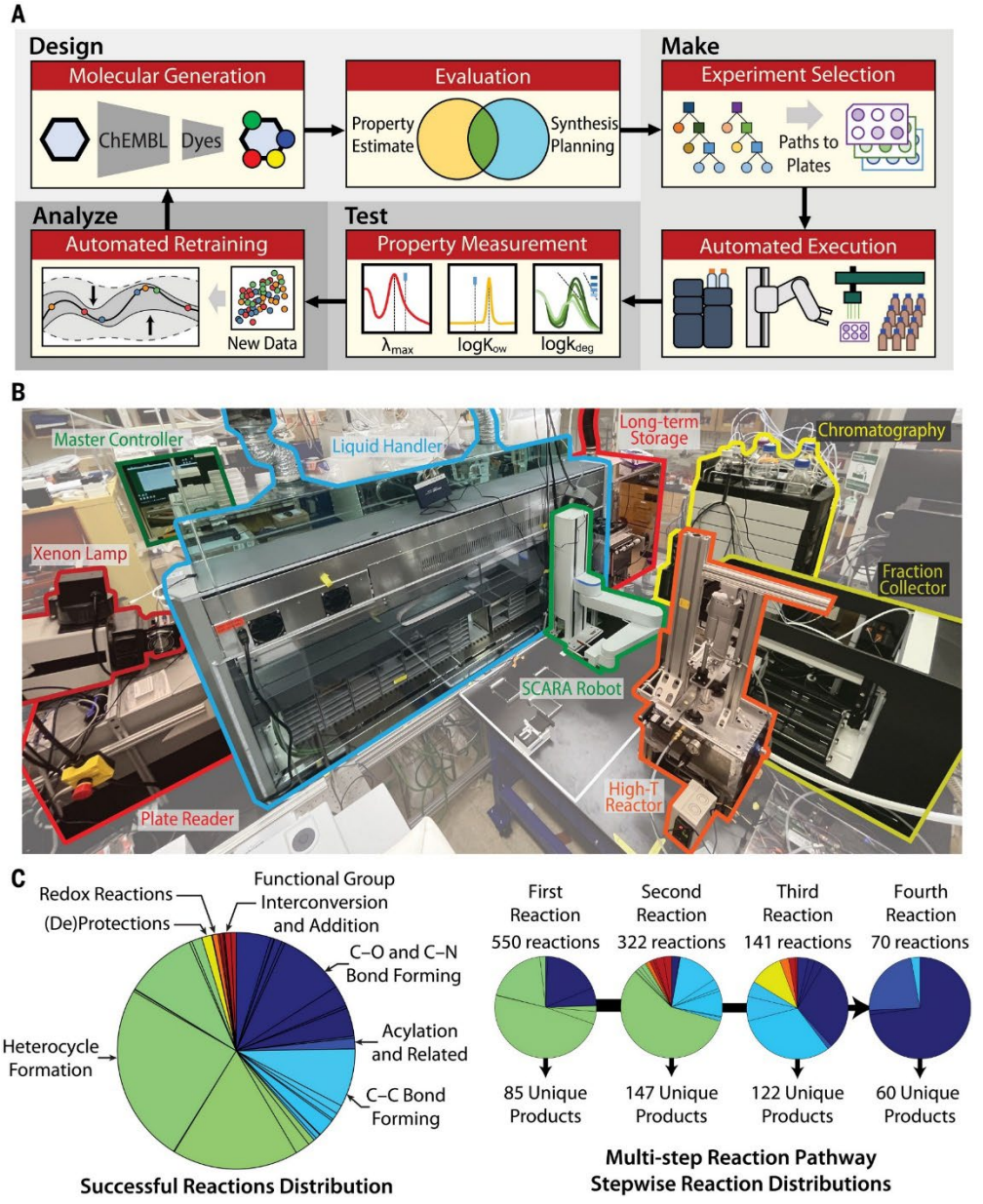

FIGURE 2 An integrated SDL platform and library of reactions it predicted and executed. (A) Schematic of the platform's workflow modules mapped onto the Design–Make–Test–Analyze (DMTA) loop; the loop evaluates three target properties, including maximum absorption wavelength (λmax), octanol-water partition coefficient (log K_{ow}), and photo-oxidative degradation rate (log k_{deg}). (B) Floor plan of the SDL's automated hardware. (C) Sequential distribution of reaction classes autonomously conducted by the SDL shown in panels A and B during the exploratory study. The four inset pie charts trace how the proportion of each reaction class shifts with reaction step; because different pathways terminate after varying numbers of steps, later stages contain fewer total reactions. Reproduced with permission from AAAS, Koscher et al. 2023, Figure 1.

thetic planning, robotic synthesis, and online analytics in a closed-loop format to accelerate the design-make-test-analyze (DMTA) cycle (Koscher et al. 2023). It iteratively proposes dye-like molecules optimized for targeted physicochemical properties, synthesizes them, measures their properties in real time, and retrains its models with the new data. AMMD autonomously discovered and synthesized 294 previously unknown dye-like molecules across three DMTA cycles. The platform showcases how an SDL can explore vast chemical spaces and converge on high-performance molecules with autonomous robotic experimentation.

In practice, SDLs have already demonstrated remarkable results (Table 1). In quantum dot synthesis, SDLs have mapped compositional and process landscapes an order of magnitude faster than manual methods (Bateni et al. 2024; Epps et al. 2020). In polymer discovery, they have uncovered new structure–property relationships that were previously inaccessible to human researchers (Snapp et al. 2024; Wang et al. 2025). These examples underscore the transformative potential of SDLs in bridging the gap between computation and real-world experimentation that is a central goal of the MGI.

SDL Deployment Models: Centralized, Distributed, and Hybrid

Scaling SDLs to fulfill the MGI vision requires thoughtful deployment strategies. Two dominant models are emerging, *Centralized SDL Foundries* and *Distributed Modular Networks* (Canty et al. 2025). Centralized SDL Foundries concentrate advanced capabilities in national labs or consortia. These facilities can host high-end robotics, hazardous materials infrastructure, and specialized characterization tools. They offer economies of scale and can serve as national testbeds for benchmarking, standardization, and training. Researchers can submit digital workflows to be executed remotely, facilitating access to cutting-edge experimentation. In contrast, Distributed SDL Networks enable widespread access by deploying low-cost, modular platforms in individual laboratories. Though more modest in scope, these distributed SDL platforms offer flexibility, local ownership, and rapid iteration. When orchestrated via cloud platforms and harmonized metadata standards, they function as a "virtual foundry," pooling experimental results and accelerating collective progress. A list of available SDL infrastructure

TABLE 1 A summary of recently developed SDLs across different scientific domains

Scientific Domain	Representative SDL(s) and Key Outcome
Colloidal nanocrystals	**AlphaFlow** discovered a new multi-step nanomaterial synthesis chemistry via reinforcement learning guided microfluidic synthesis in 30 days (Volk et al. 2023). **Artificial Chemist** discovered the synthetic route of metal halide perovskite quantum dots for any target bandgap within 90 min (Epps et al. 2020). **SmartDope** discovered the best-in-class doped perovskite quantum dot within one day of autonomous experimentation (Bateni et al. 2024).
Metallic thin films	**ADA** discovered new synthesis conditions that yielded metallic thin films at lower processing temperatures than the state of the art (MacLeod et al. 2022).
Electronic polymer thin films	**Polybot** discovered scale-up fabrication recipes of transparent conductive thin films with average conductivity >4,500 S/cm (Wang et al. 2025).
Homogeneous catalysis	**Fast-Cat** autonomously mapped homogeneous catalytic reactions Pareto fronts in five days (Bennett et al. 2024).
Battery electrolytes and cells	**ODACell** discovered a multi-component hybrid electrolyte with >94% Coulombic efficiency using an AI-guided coin-cell assembly (Yik et al. 2025).
Additive manufacturing	**BEAR** performed >25,000 additive manufacturing/mechanical test cycles to discover an optimal structure reaching 75% energy-absorption efficiency (Snapp et al. 2024).
Small-molecule organic synthesis	**Chemputer** executed digitalized multi-step organic syntheses using batch reactors (Steiner et al. 2019).
Multi-property molecule discovery	**AMMD** discovered 294 unreported dye-like molecules with multi-target objectives (Koscher et al. 2023).
Exploratory synthetic chemistry	**Mobile Robot Chemist** used mobile robots integrated with conventional wet-chemistry workflows for AI-driven reaction discovery (Dai et al. 2024).
Photochemistry	**Robochem** enabled AI-driven optimization, intensification, and scale-up of photocatalytic reactions in flow reactors (Slattery et al. 2024).

across North America is presented in a 2024 MGI report (Subcommittee on the MGI 2024).

A universal SDL model will offer the best of both worlds. Preliminary research can be conducted locally using distributed SDLs, while more complex tasks are escalated to centralized SDL facilities. This layered approach mirrors cloud computing, where local devices handle basic computation and data-intensive tasks are offloaded to data centers. In the SDL context, such a model can maximize both efficiency and accessibility.

Deployment models must also consider interoperability, cybersecurity, and sustainability. Interoperable SDLs require open application programing interfaces (APIs), shared data ontologies, and robust orchestrators. Cybersecurity is critical given the physical risks associated with autonomous experimentation. Sustainability considerations, such as reagent use, waste generation, and energy consumption, must be integrated into the SDL design AND operation. These considerations shape how SDLs are built, governed, and integrated into national infrastructure to align with MGI's long-term goals.

Data, Autonomy, and the MGI Knowledge Loop

At the core of SDL utility is their ability to generate, curate, and interpret data at unprecedented scales and speed. In traditional human-centered experimentation settings, data quality often varies significantly depending on instrumentation, operator expertise, and contextual documentation. SDLs resolve these inconsistencies by encoding every step of the experimental process into machine-readable records. This digitalization includes reagent identities and volumes, as well as equipment settings, environmental conditions, and calibration metadata.

Autonomous agents operating within SDLs are capable of managing and optimizing the computational and experimental data lifecycle. When orchestrated correctly, the SDL can identify correlations and causal links that may be opaque to human interpretation, particularly in high-dimensional design spaces. For example, in exploring the composition–process–property space of multi-cation oxides, an SDL can link trace impurity levels or subtle thermal gradients to variations in material functionality, thereby enabling fine-tuned control on material synthesis, composition, and properties that would otherwise require years of labor-intensive study.

Furthermore, SDLs are natural engines for active learning. Their ability to use real-time feedback to refine predictive models means they can operate efficiently even in data-sparse regimes. Instead of brute-force sampling, SDLs prioritize experiments that maximize information gain. This strategy is particularly valuable in systems with combinatorially large variable spaces, such as doped semiconductors or hybrid organic–inorganic materials, where exhaustive sampling is computationally and experimentally intractable.

A universal SDL model will offer the best of both worlds.

SDLs also improve the feedback loop between simulation and experiment. When integrated with multiscale modeling strategies, SDLs can validate and refine simulations continuously, tightening the predictive cycle (Gongora et al. 2021). By leveraging proxy measurements and uncertainty quantification, SDLs can infer properties not directly observable in the lab (Osterrieder et al. 2023). This integration is core to MGI's mission of accelerating discovery through coupled computation and experiment.

In addition to enabling deeper understanding of materials relationships, SDLs also facilitate rigorous data standardization through embedded provenance protocols. Each SDL-generated dataset can be traced back through its full experimental history, including sensor calibrations, environmental logs, reagent batch numbers, and algorithm version. This capability supports reproducibility and meta-analyses, as well as integration with MGI-curated repositories such as *The Materials Project*, allowing researchers to explore how small differences in conditions or instrumentation affect outcomes. Such high-resolution traceability is foundational for integrating experimental data into machine-readable knowledge graphs that power future hypothesis generation.

One of the most powerful use cases of SDL-generated data is transfer learning, leveraging models trained in one context to make predictions in another. A library of band-gap measurements in one class of semiconductors, for example, may help inform the optimization of a related class with limited prior data. Transfer learning is only effective when datasets are standardized, well-documented, and interoperable. The promise here is not only accelerating new discoveries but also improving generalization and reusability of scientific knowledge. These capabilities close the loop on MGI's core vision: a seamless knowledge cycle from simulation to synthesis to deployment.

Workforce and Ecosystem Evolution

The SDL-driven transformation of experimental science demands a parallel evolution in workforce development and academic structures. SDLs blur disciplinary boundaries, requiring fluency in robotics, automation, programming, analytical chemistry, and data science. To fully realize the SDL-powered MGI vision, educational institutions must modernize training pipelines to prepare a new generation of interdisciplinary researchers.

Within the SDL ecosystem, three complementary roles emerge: *SDL Developers*, responsible for designing and integrating the hardware–software stack; *SDL Technicians*, who maintain systems, calibrate instruments, and ensure operational robustness; and *SDL Users*, domain experts who frame scientific hypotheses, evaluate outputs, and interface with autonomy agents. Developing this tiered skill architecture necessitates new curricula, including interdisciplinary degree programs and hands-on modules with open-source SDL kits (Canty et al. 2025).

Moreover, this evolution presents an opportunity to maximize accessibility and participation in advanced materials research. By lowering the skill barrier required to run complex experiments, SDLs can enable broader participation from all institutions and regions. With appropriate cloud infrastructure and remote interfaces, researchers can design and oversee experiments on a national SDL facility, gaining access to tools and data previously limited to few laboratories.

Developing a robust talent pipeline will also require partnerships with industry and government. Internships and co-op positions at SDL facilities can provide hands-on experience while aligning training with real-world needs. Certification pathways, akin to those in welding or CNC machining, may be introduced for SDL operation, maintenance, and programming. Such credentials would validate workforce readiness and provide upward mobility for technical staff across academia and industry.

Another key component of the SDL workforce ecosystem is the integration of social sciences and ethics. As automation reshapes research dynamics, scholars in science and technology studies, education, and public policy will be essential to monitor impacts, anticipate unintended consequences, and guide appropriate implementation. Embedding these perspectives early into SDL ecosystems will maintain a culture of responsible innovation.

Partnerships and Economic Impact

The economic case for SDL deployment is compelling. In industry, where R&D timelines, time-to-solution, and costs are tightly coupled to competitiveness, the advantages of SDLs are immediate. Autonomous workflows shorten design cycles, improve reproducibility, and reduce experimental waste. For instance, in pharmaceutical development, SDLs have already demonstrated their ability to identify optimal reaction conditions with an order-of-magnitude fewer experiments than the conventional design of experiments approaches. Academia–industry partnerships are pivotal for translating SDL capabilities into commercial impact (Bennett et al. 2024). National labs can serve as pre-competitive testbeds, industry can supply relevant use cases and application constraints; academia can push the frontier of AI, robotics, and experimental automation. Public–private consortia can share infrastructure costs while accelerating the validation and adoption of SDL workflows.

Moreover, SDLs represent a novel paradigm for innovation-driven entrepreneurship by decoupling access to advanced experimental capabilities from direct ownership of capital-intensive infrastructure. This structural shift enables startups and small enterprises to engage in high-impact research and development (R&D) with significantly reduced upfront investment, thereby accelerating design–build–test–learn cycles and facilitating rapid scaling. An analogous model already exists in the pharmaceutical sector through contract research organizations (CROs), which provide specialized R&D capabilities and infrastructure on a service basis to clients lacking in-house resources. While CROs largely emulate the outsourced automation and high-throughput experimentation aspects of the SDL model, SDLs, with integrated AI-assisted decision making, advance this concept further by enabling closed-loop, hypothesis-driven experimentation that adapts in real time to emerging results.

The established CRO ecosystem offers a useful reference point for understanding how a mature SDL ecosystem could function, while also highlighting the potential for SDLs to extend such shared-access models beyond pharmaceuticals to a broader spectrum of scientific and engineering domains. Growing venture capital investment in laboratory automation, particularly in biotechnology and cleantech, reflects this momentum. In this framework, SDLs shift the locus of value creation from physical experimental throughput to *idea* throughput, wherein competitive advantage derives from the development of algorithms, data-driven models, and optimized decision-making strategies rather than sheer experimental capacity.

At the regional level, SDL infrastructure investment can anchor technology clusters, attracting talent, cata-

lyzing spinoffs, and driving economic development. SDL-enabled hubs focused on semiconductors, green chemistry, or battery materials could mirror the role of semiconductor fabs and genomics centers in earlier eras. Policymakers should recognize SDLs as a strategic asset for national and regional innovation competitiveness.

SDLs also create new economic value chains. Companies can build businesses around SDL software stacks and API standards. Vendors of analytical hardware are incentivized to produce SDL-compatible tools with modular designs. Even reagent suppliers may adapt to offer SDL-optimized consumables with QR-coded metadata for seamless integration. As these markets mature, the SDL economy will become a key segment of the broader materials innovation infrastructure.

From a public-sector perspective, SDL investments can also enhance US competitiveness in critical technology domains such as clean energy, semiconductors, and pharmaceuticals. Federal funding for SDL research could be tied to national strategic initiatives, such as CHIPS and Science Act priorities or decarbonization roadmaps, aligning infrastructure development with urgent societal needs. A national SDL backbone can thus become a vital lever for mission-driven research and economic policy.

Trust, Transparency, and Ethical Safeguards

As with any powerful technology, the rise of SDLs brings ethical and philosophical challenges. Building trust requires transparency, reproducibility, and community engagement. The opacity of AI decision making can obscure how experimental strategies are chosen or interpreted. Black-box algorithms can lead to results that are hard to validate or explain. To address these critical matters, the SDL community must prioritize documentation and standardization. Every experiment must be traceable, with rich metadata that allows others to reproduce and interpret results. Benchmarking protocols should be established, allowing performance comparisons across SDL platforms. SDLs must report all data, uncertainty bounds, and operational constraints. Equally important, SDLs must be applied in a transparent and deliberate manner, ensuring that automated decision making aligns with clearly defined scientific objectives and ethical considerations.

Security is also paramount for SDLs. Because SDLs interface with physical matter, software vulnerabilities can have real-world consequences. Protocols for cybersecurity, access control and fail-safe mechanisms must be built into every SDL system. As SDLs become more networked, the risk of tampering increase. Regulatory frameworks may need to evolve to account for these hybrid digital–physical systems. Facile access to SDL infrastructure should also be a priority. Strategies such as open-source platforms, shared facilities, and subsidized cloud access can facilitate access to SDLs. By designing for openness and equity from the outset, the SDL community can ensure that the benefits of autonomy are broadly shared.

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An additional dimension of trust-building involves the human-machine interface. For SDLs to be accepted by the broader scientific community, their decision processes must be interpretable. This need calls for explainable AI techniques that can articulate why an agent selected a particular experiment or rejected a hypothesis. Visual dashboards, natural language logs, and confidence metrics can help bridge the gap between algorithmic reasoning and human intuition.

The establishment of SDL ethics boards may also prove beneficial. These interdisciplinary committees could review autonomous workflows for safety, access, and scientific validity, especially for high-risk applications. Similar to Institutional Review Boards (IRBs) in biomedical research, SDL ethics boards would promote transparency and accountability without impeding innovation.

Public engagement will further enhance legitimacy of SDLs. Communicating how SDLs work, what data they collect, and how they make decisions can demystify the technology. Open lab days, digital twins for citizen science, or interactive dashboards could bring SDLs into classrooms and communities, showcasing their role in accelerating sustainable innovation.

Strategic Recommendations

To fully integrate SDLs into the MGI and national research infrastructure, a coordinated roadmap is essential. In the next 1–3 years, the focus should be on establishing standards and addressing the current SDLs' engineering bottlenecks outlined in Table 2. Table 2 highlights that

TABLE 2 A summary of identified SDL challenges across different scientific domains

Scientific Domain	Challenges	Barriers to Unlock Fully Functional SDLs
High-temperature alloys and ceramics	Reproducible automation and solid-state synthesis at >1000°C; scarce inline phase analytics	Heat-resistant automation, high-throughput in-situ characterization, low-cost and accessible powder-handling tools
Heterogeneous catalysis	High-throughput heterogeneous catalyst synthesis and testing (>100/day)	Modular reactor skids with real-time spectroscopy, autonomous safety interlocks
Microelectronics	Lab-scale end-to-end automation, nanometer tolerances, vacuum tools, multi-step lithography	Accessible fab-class robotics and in-situ multi-modal metrology, hierarchical planners, interoperable process-data standards

SDL maturity is uneven across different disciplines: while fluidic and thin-film chemistries are already automated, domains demanding extreme environments or nanometer precision still face steep technological barriers. For high-temperature alloys and ceramics, the bottleneck is robotic hardware survivability at high temperatures and the lack of in-situ phase probes. Heterogeneous catalysis and microelectronics similarly require purpose-built infrastructure (modular, safety-aware reactor skids and fab-class, multi-modal metrology) plus interoperable data standards to translate SDL principles into fully functional platforms.

Other strategic recommendations include:

- Establishing a national SDL user facility, analogous to supercomputing centers, to provide access and build community expertise.
- Deploying federated SDL networks within 4–7 years to enable collaborative experimentation across institutions (Figure 3) and formalizing interoperability frameworks to allow seamless exchange of workflows and data.
- Scaling workforce development programs, including certifications and interdisciplinary degrees, to meet growing SDL demand.
- Aligning SDL deployment with key MGI priority areas (e.g., semiconductor resilience, clean energy materials, circular economy).
- Fully integrating SDLs into the national R&D ecosystem by year 10.
- Ensuring every major university hosts at least one SDL node for AI-assisted scientific research and workforce training.
- Coordinating shared repositories of workflows and data through national laboratories, and incorporate SDL pipelines into standard product development lifecycles across industry.

These initiatives would help autonomous experimentation evolve from a niche capability into a foundational element of science and engineering.

Another near-term priority is the development of common testing suites for SDL benchmarking. These benchmarks could include standard synthesis targets, characterization routines, and comparison metrics for evaluating performance across different SDL platforms. Such standardized testbeds would enable comparative studies, support best-practices documentation, and cre-

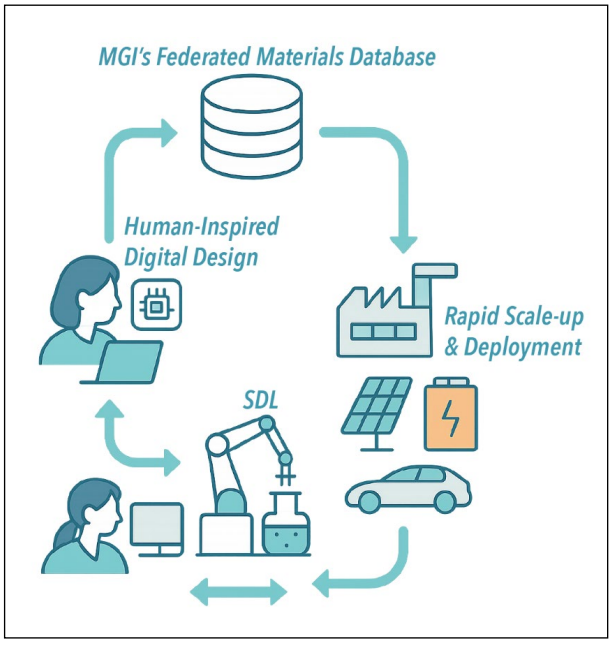

FIGURE 3 An illustration of how distributed SDLs can accelerate materials discovery and deployment with an MGI's federated materials database.

ate a virtuous cycle of performance improvement. As SDL networks grow, federated learning architectures will become essential. Rather than centralizing all data, SDL nodes could train local models and share only aggregated updates, protecting intellectual property while improving global model accuracy. This architecture mirrors developments in healthcare AI and could be adapted to materials science with appropriate data governance protocols.

By the end of the decade, SDLs could also be integrated into autonomous manufacturing ecosystems. For example, in the next decade, an SDL can design a polymer, send its formulation to an additive manufacturing module, evaluates the specific part's mechanical properties, and feed back the data to optimize performance, all with minimal human intervention. This convergence of digital design, experimentation, and production would mark a new era of agile, intelligent manufacturing.

Conclusion

SDLs—a convergence of AI, robotics, and experimental science—are at an inflection point for how we generate scientific knowledge. For the MGI, SDLs offer a tangible path to bridge computation and reality, turning predictive models into validated materials with unprecedented speed. But their true impact lies beyond throughput or efficiency. SDLs can reshape who participates in science, how collaboration happens, and what becomes possible when experimentation itself becomes a programmable, adaptive system. To realize this potential, we must act with vision and coordination. Investment in SDL infrastructure is an investment in the next era of scientific discovery. The MGI began as a bold promise; SDLs are how we fulfill it.

The SDL vision aligns with the scientific ambitions of the MGI and broader societal aspirations: reducing environmental impact, localizing manufacturing, accelerating medicine development, and ensuring rapid and facile access to innovation. It is a vision in which science becomes more dynamic and capable of meeting 21st century challenges.

Investment in SDLs is an investment in the next phase of the MGI. SDLs activate the experimental pillar of the initiative, enable cross-domain data generation, and promote reproducibility and agility. SDLs support both national competitiveness and scientific inclusion. To seize this opportunity, leadership and coordination are essential. Federal agencies must fund and coordinate SDL infrastructure. Universities must rethink curricula and facilities. Industry must invest and co-develop SDLs with academia. And the scientific community must embrace new modes of discovery. With foresight and commitment, the SDL-powered future of the MGI is within reach, and its realization will mark a generational advance in the practice and promise of science.

References

Abolhasani M, Kumacheva E. 2023. The rise of self-driving labs in chemical and materials sciences. Nature Synthesis 2:483–92.

Bateni F, Sadeghi S, Orouji N, Bennett JA, Punati VS, Stark C, Wang J, Rosko MC, Chen O, Castellano FN, and 2 others. 2023. Smart Dope: A self-driving fluidic lab for accelerated development of doped perovskite quantum dots. Advanced Energy Materials 14:2302303.

Bennett JA, Orouji N, Khan M, Sadeghi S, Rodgers J, Abolhasani M. 2024. Autonomous reaction Pareto-front mapping with a self-driving catalysis laboratory. Nature Chemical Engineering 1:240–50.

Boiko DA, MacKnight R, Kline B, Gomes G. 2023. Autonomous chemical research with large language models. Nature 624:570–78.

Canty RB, Bennett JA, Brown KA, Buonassisi T, Kalinin SV, Kitchin JR, Maruyama B, Moore RG, Schrier J, Seifrid M, and 3 others. 2025. Science acceleration and accessibility with self-driving labs. Nature Communications 16:3856.

Curtarolo S, Setyawan W, Wang S, Xue J, Yang K, Taylor RH, Nelson LJ, Hart GLW, Sanvito S, Buongiorno-Nardelli M, and 2 others. 2012. AFLOWLIB.ORG: A distributed materials properties repository from high-throughput ab initio calculations. Computational Materials Science 58:227–35.

Dai T, Vijayakrishnan S, Szczypiński FT, and 8 others. 2024. Autonomous mobile robots for exploratory synthetic chemistry. Nature 635:890–97.

de Pablo JJ, Jackson NE, Webb MA, Chen L-Q, Moore JE, Morgan D, Jacobs R, Pollock T, Schlom DG, Toberer ES, and 14 others. 2019. New frontiers for the Materials Genome Initiative. npj Computational Materials 5:41.

Delgado-Licona F, Addington D, Alsaiari A, Abolhasani M. 2025. Engineering principles for self-driving laboratories. Nature Chemical Engineering 2:277–80.

Epps RW, Bowen MS, Volk AA, Abdel-Latif K, Han S, Reyes KG, Amassian A, Abolhasani M. 2020. Artificial Chemist: An autonomous quantum dot synthesis bot. Advanced Materials 32(30):e2001626. Online at doi.org/10.1002/adma.202001626.

Gongora AE, Snapp KL, Whiting E, Riley P, Reyes KG, Morgan EF, Brown KA. 2021. Using simulation to accelerate

autonomous experimentation: A case study using mechanics. iScience 24:102262.

Jain A, Ong SP, Hautier G, Chen W, Richards WD, Dacek S, Cholia S, Gunter D, Skinner D, Ceder G, and 1 other. 2013. Commentary: The Materials Project: A materials genome approach to accelerating materials innovation. APL Materials 1:011002.

Kirklin S, Saal J, Meredig B, Thompson A, Doak JW, Aykol M, Rühl S, Wolverton C. 2015. The Open Quantum Materials Database (OQMD): Assessing the accuracy of DFT formation energies. npj Computational Materials 1:15010.

Koscher B, Canty RB, McDonald MA, Greenman KP, McGill CJ, Bilodeau CL, Jin W, Wu H, Vermeire FH, Jin B, and 8 others. 2023. Autonomous, multi-property-driven molecular discovery: From predictions to measurements and back. Science 282(6677). Online at www.science.org/doi/10.1126/science.adi1407.

MacLeod BP, Parlane FGL, Morrissey TD, Häse F, Roch LM, Dettelbach KE, Moreira R, Yunker LPE, Rooney MB, Deeth JR, and 10 others. 2020. Self-driving laboratory for accelerated discovery of thin-film materials. Science Advances 6(20):eaaz8867.

MacLeod BP, Parlane FGL, Rupnow CC, Dettelbach KE, Elliott MS, Morrissey TD, Haley TH, Proskurin O, Rooney MB, Taherimakhsousi N,and 7 others. 2022. A self-driving laboratory advances the Pareto front for material properties. Nature Communications 13:995.

MGI [Materials Genome Initiative]. n.d. Materials Genome Initiative. Online at www.mgi.gov.

MGI. 2024a. Accelerated Materials Experimentation Enabled by the Autonomous Innovation Initiative (AMII): A Workshop Report. Online at www.mgi.gov/autonomous-experimentation-materials-rd.

MGI. 2024b. The 2024 MGI challenges. Online at www.mgi.gov/2024-materials-genome-initiative-mgi-challenges.

Osterrieder T, Schmitt F, Lüer L, Wagner J, Heumüller T, Hauch J, Brabec CJ. 2023. Autonomous optimization of an organic solar cell in a 4-dimensional parameter space. Energy & Environmental Science 16:3984–93.

Ruan Y, Lu C, Xu N, He Y, Chen Y, Zhang J, Xuan J, Pan J, Fang Q, Gao H, and 4 others. 2024. An automatic end-to-end chemical synthesis development platform powered by large language models. Nature Communications 15:10160.

Slattery A, Wen Z, Tenblad P, Sanjosé-Orduna J, Pintossi D, den Hartog T, Noël T. 2024. Automated self-optimization, intensification, and scale-up of photocatalysis in flow. Science 383(6681):eadj1817.

Snapp KL, Verdier B, Gongora AE, Silverman S, Adesiji AD, Morgan EF, Lawton TJ, Whiting E, Brown KA. 2024. Superlative mechanical energy absorbing efficiency discovered through self-driving lab-human partnership. Nature Communications 15:4290.

Steiner S, Wolf J, Glatzel S, Andreou A, Granda JM, Keenan G, Hinkley T, Aragon-Camarasa G, Kitson PJ, Angelone D, and 1 other. 2019. Organic synthesis in a modular robotic system driven by a chemical programming language. Science 363(6423):eaav2211.

Szymanski NJ, Rendy B, Fei Y, Kumar RE, He T, Milsted D, McDermott MJ, Gallant M, Cubuk ED, Merchant A, and 6 others. 2023. An autonomous laboratory for the accelerated synthesis of novel materials. Nature 624:86–91.

Volk AA, Epps RW, Yonemoto DT, Masters BS, Castellano FN, Reyes KG, Abolhasani M. 2023. AlphaFlow: autonomous discovery and optimization of multi-step chemistry using a self-driven fluidic lab guided by reinforcement learning. Nature Communications 14:1403. Online at doi.org/10.1038/s41467-023-37139-y.

Wang C, Kim YJ, Vriza A, Batra R, Baskaran A, Shan N, Li N, Darancet P, Ward L, Liu Y, and 7 others. 2025. Autonomous platform for solution processing of electronic polymers. Nature Communications 16:1498.

Watson JD. 1990. The Human Genome Project: Past, present, and future. Science 248(4951):44–49.

Yik JT, Hvarfner C, Sjölund J, Berg EJ, Zhang L. 2025. Accelerating aqueous electrolyte design with automated full-cell battery experimentation and Bayesian optimization. Cell Reports Physical Science 6:102548.

Self-driving labs are the innovation leading to accelerated discovery.

Autonomous Experimentation and Self-Driving Labs for Materials Synthesis Using Deposition Techniques

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Introduction

Autonomous Experimentation (AE), also known as Self-Driving Labs (SDLs), promises to speed materials synthesis research and development (R&D) by orders of magnitude, revolutionizing the research process. AE uses artificial intelligence (AI) and robotics to design, execute, and analyze experiments in rapid, iterative fashion, combining the results from the experiments with modeling and simulation to design the next best experiment to do. The MGI (Materials Genome Initiative) Autonomous Materials Innovation Infrastructure (AMII) report (Boswell-Koller et al. 2024) captures demonstrations and

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advances for materials synthesis that have been made in chemical vapor deposition (CVD), physical vapor deposition (PVD), and electrochemical deposition. By dynamically searching over synthesis parameters, AE can optimize the process quality and speed, resulting in improved and advanced materials at a fraction of the time and labor compared to conventional, human-driven laboratory processes.

SDLs can generate and test scientific hypotheses faster and more effectively than human researchers alone.

More importantly, SDLs can generate and test scientific hypotheses faster and more effectively than human researchers alone. AE experimental campaigns therefore produce deeper scientific understanding of materials phenomena, enabling rational investigations, extrapolation, and exploitation beyond naïve machine learning–only approaches. It is worth noting that the term "Self-Driving Labs" is more common in the chemistry community, whereas "Autonomous Experimentation" is preferred in the materials community. It is also helpful to distinguish AE/SDL from high-throughput or combinatorial methods, which focus on performing many experiments in parallel or rapidly but not autonomously or iteratively by design. Here, we focus on fully autonomous experimentation, where iterative experiments occur in a closed loop without human intervention. Automated—but not autonomous—research is increasingly being pursued as a stepping stone toward full autonomy (Nikolaev et al. 2014). AE can thus be thought of as "human on the loop" rather than "human in the loop."

Here we discuss the future value proposition for AE/SDLs, assess current progress, and discuss future directions and findings from the MGI AMII report (Boswell-Koller et al. 2024). We also consider the implications of AE/SDLs for materials R&D in the future.

Chemical Vapor Deposition

CVD is an important materials synthesis technique for thin film materials, 2-D materials, and nanomaterials (Choy 2019). CVD starts with an input stream of precursor gases that thermally decompose onto a substrate to form the target material. Carbon nanotubes (CNTs) can be synthesized using a metal nanoparticle to catalytically decompose the precursor. Here the CNT is templated by the catalyst, driving the cylindrical structure of the carbon nanotube (Rao et al. 2018).

CVD in general, and CNT synthesis in particular, presents a significant challenge in understanding and optimizing growth. Key control variables include the gas mixtures—typically a hydrocarbon such as ethylene, reducing gases like hydrogen, and oxidants such as water vapor or CO_2 (Bulmer et al. 2023)—as well as experimental parameters like system temperature, temperature ramp rates, and gas flow rates. Interestingly, factors not traditionally considered control variables can also play an important role, such as laboratory humidity, the number of times the furnace tube has been used, and the age of chemical precursors. These factors become especially important when attempting to capture growth phenomena beyond the obvious variables and to explain spurious or intermittent results.

ARES is a CVD AE system developed by the Air Force Research Laboratory that was the first fully autonomous system for materials synthesis (Nikolaev et al. 2016). The system, depicted schematically in Figure 1 (Left), consists of a cold-wall CVD system where growth gases are introduced into a chamber. Small silicon pillars, which are essentially microreactors, are seeded with CNT catalysts. A high-power laser heats a single pillar to the target growth temperature, growing carbon nanotubes. The growth is characterized in real time by analyzing scattered laser light with Raman spectroscopy as the nanotube forms. After the experiment is completed and the results analyzed, an AI planner selects the growth conditions for the next experimental iteration, guided by goals defined by the user (Figure 1 [Right]).

When designing an AE campaign, the first step is to define its objective. For example, one objective might aim to maximize CNT growth rate while minimizing diameter variation (Waelder et al. 2025). Another possible objective is hypothesis testing, as in a 2024 study where we proposed that the CNT catalyst would be most active under synthesis conditions in which the metal catalyst was in equilibrium with its oxide (Waelder et al. 2024). To test this, we systematically varied the growth environment from more oxidizing (e.g., higher water vapor or CO_2 content, lower temperature) to more reducing (e.g., greater hydrocarbon partial pressure, higher temperature), thereby probing catalyst activity for CNT synthesis

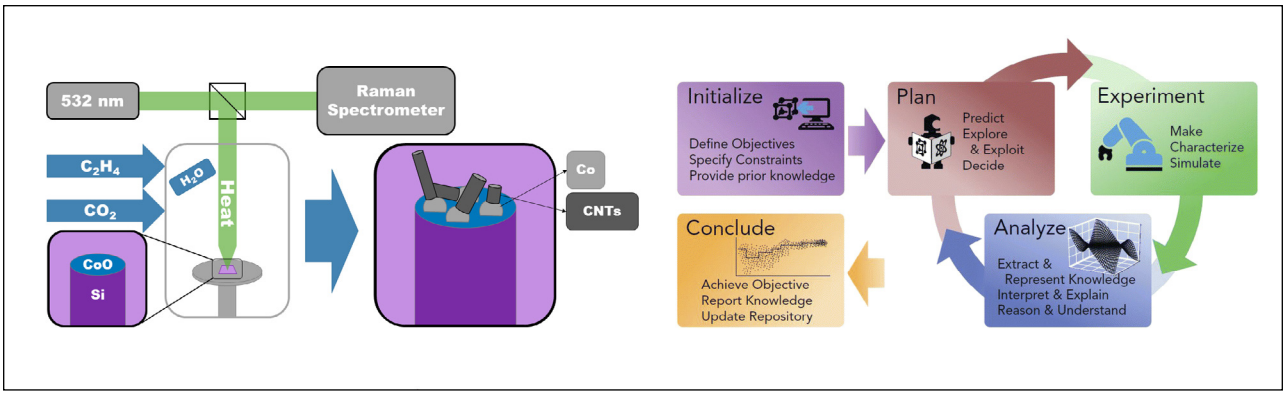

FIGURE 1 (Left) Schematic of ARES carbon nanotube chemical vapor deposition autonomous experimentation system (Waelder et al. 2025). (Right) ARES uses AI decision methods to plan, execute, and analyze CVD experiments in autonomous, iterative closed loop processes (Stach et al. 2021). With permission from respective journals.

(Figure 2) as a function of the reducing potential. In this case, the objective was to confirm or refute the reduction hypothesis rather than to maximize CNT growth rate.

With the reduction hypothesis as the physical phenomenon under investigation, the next step in campaign design is selecting the planner decision method, also known as the acquisition function (Stach et al. 2021). The acquisition function determines the experimental input conditions expected to advance the campaign objective most effectively. Several strategies exist for acquisition functions, including minimizing overall uncertainty, maximizing a particular feature, or combining both.

This highlights an important principle of iterative experimental design: if a campaign identifies a peak, subsequent experiments may test nearby conditions to determine whether even better outcomes exist, an approach known as *exploitation* (Stach et al. 2021). Alternatively, experiments may probe unexplored regions to search for other, potentially superior peaks, an approach known as *exploration*. Acquisition functions typically balance exploration and exploitation within the experimental budget to best meet campaign objectives. Compared with traditional methods such as full factorial or one-variable-at-a-time approaches, iterative optimal experimental design achieves progress much more rapidly (Stach et al. 2021).

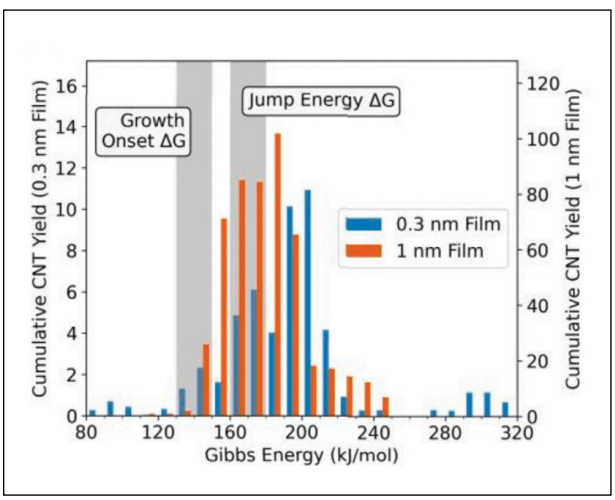

FIGURE 2 Thermodynamics plot showing peak catalyst activity for carbon nanotube synthesis as a function of the free energy of catalyst reduction (Waelder et al. 2024).

We confirmed our hypothesis that the catalyst exhibits its highest activity when the catalyst metal is in equilibrium with its oxide. Using the ARES AE system, we were able to probe the oxidizing and reducing nature of the growth environment across an exceptionally broad range of conditions covering a 500°C temperature window and oxidizing-to-reducing gas partial pressure ratios spanning 8–10 orders of magnitude.

Thus, for AE, a campaign can be framed as a Black-box or naïve optimization of conditions to maximize a target property. However, the more powerful objective is hypothesis testing with SDLs, as the resulting scientific insights can be generalized for broader impact and applied to related material syntheses and reactor scale-up. While there are currently limited examples of fully autonomous CVD systems, we expect a significant increase in their number and capabilities as automation and in situ/in-line characterization advances.

Physical Vapor Deposition

PVD techniques such as magnetron sputtering, molecular beam epitaxy (MBE), and electron-beam evaporation

form the backbone of the electronics industry by enabling crucial thin-film synthesis and device fabrication. PVD tools can produce uniform coatings of a wide range of materials, from nanometer- to micron-scale thicknesses, making them well-suited for materials exploration. Modern advanced PVD systems are often equipped with automated operation capabilities (e.g., sequential wafer or chip transfer, or executing programmed deposition recipes), which serve as key prerequisites for AE workflows. The concept of designing materials through controlled deposition and (multi)layering of ultrathin (sometimes atomically thin) films has long provided the materials science community with a powerful approach to discovering and realizing properties not found in nature.

To accelerate the discovery of new materials and their properties using PVD, high-throughput experimentation provides a particularly powerful platform. In this approach, combinatorial library wafers or chips contain arrays of samples with varying compositions, enabling sequential experiments to be conducted in a straightforward and efficient manner. The ability to synthesize and characterize material arrays sequentially—and even in closed loops—greatly enhances the effectiveness of AE.

In some cases, the exercise of self-driving combinatorial experimentation can be singularly focused on characterization. While fabrication of libraries such as thin-film composition spreads can often be carried out quickly and reliably using PVD techniques (Green et al. 2017), quantitative evaluation of physical properties of interest can be time- and resource-intensive for each individual sample. In such situations, Gaussian process models can effectively guide the measurement sequence across the library. For example, Kusne and colleagues identified the composition of a phase-change memory material with the largest bandgap contrast between amorphous and crystalline phases from a prefabricated ternary thin-film composition spread after measuring only a fraction of the full compositional range (Kusne et al. 2020).

The newly discovered phase-change memory material, $Ge_4Sb_6Te_7$, lies at a structural phase boundary between a host matrix and a secondary phase on the Ge–Sb–Te compositional phase diagram. This composition exhibits unusually large contrast between on and off states and, in recent scaled-up device comparisons, was found to significantly outperform the widely used $Ge_2Sb_2Te_5$ (Khan et al. 2023; Wu et al. 2024). Importantly, the functionality of this material arises from a coherently formed nanocomposite state at the phase boundary. Thus, in this case, autonomous exploration not only led to the discovery of a new material but also revealed a novel strategy for designing high-performance phase-change memory systems.

In another example of AE on a combinatorial library fabricated by a PVD technique, Liang et al. (2024) demonstrated real-time, self-driving, cyclical interaction between experiments and computational predictions for materials exploration. Specifically, they performed rapid mapping of a temperature–composition phase diagram, a fundamental task in the search and discovery of new materials. Thermal processing and experimental determination of compositional phase boundaries in thin films were autonomously integrated with real-time updates of phase diagram predictions through Gibbs free energy minimization.

Using this workflow, the eutectic phase diagram of the Sn–Bi binary thin-film system was accurately determined on the fly from a self-guided campaign that sampled only a small fraction of the entire composition–temperature space, achieving a six-fold reduction in the number of required experiments. This study provided the first demonstration of real-time, autonomous, and iterative integration of experiment and theory carried out entirely without human intervention (Liang et al. 2024).

To establish fully autonomous PVD-based closed-loop cycles that integrate synthesis and characterization at each step, Shimizu and colleagues (2020) demonstrated the successful operation of a robot-controlled multi-chamber vacuum system. By transferring each deposited thin film sample from a sputtering chamber to a materials characterization chamber (for resistance measurements) at each iteration, the robot-based system was able to find optimized materials synthesis conditions within a small number of deposition runs (Shimizu et al. 2020).

While autonomous science systems incorporating sample-handling robots are gaining popularity across various areas of materials science, they can be costly and complex to operate and maintain. In contrast, in situ monitoring of thin-film processes has long been a central practice in the thin-film community. Because modern PVD chambers often accommodate modular in situ characterization tools, any technique that can provide direct feedback on thin-film quality can serve as an effective foundation for closed-loop workflows.

Using this approach, Lippmaa and colleagues (2002) have demonstrated autonomous control of epitaxial unit cell-level growth of oxide thin films implemented in a combinatorial pulsed laser deposition (PLD) system (Figure 3). This PLD system is notable for its ability to fabricate multiple distinct thin-film samples in a single pump-down on one wafer or chip through combinatorial masking, while

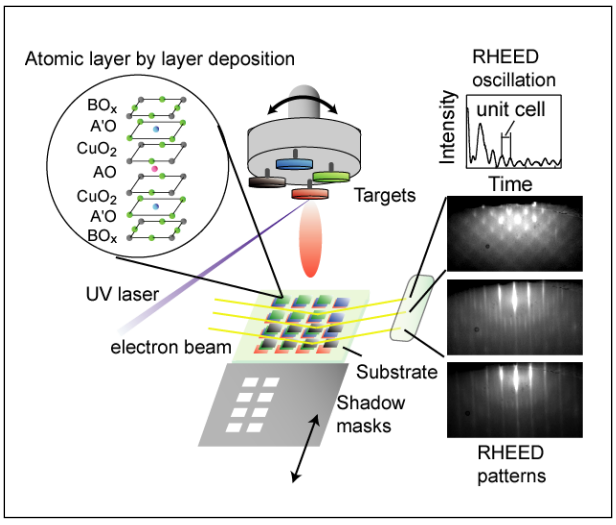

FIGURE 3 Combinatorial pulsed laser deposition system with capability to deposit multiple samples sequentially while electron diffraction for structural monitoring is performed live.

simultaneously employing a reflection high-energy electron diffraction (RHEED) system for *in situ* monitoring of the surface nanostructure at different positions on the library substrate. Building on this, the development of computer vision–based automated quantitative analysis of live RHEED images (Liang et al. 2022) enabled autonomous navigation of multi-dimensional deposition parameter space (temperature, partial pressure, and laser pulse rate), rapidly identifying optimal growth conditions for targeted material phases (Price et al. 2025). Closed-loop PLD has also been demonstrated using Raman spectroscopy as the characterization feedback mechanism (Harris et al. 2024).

In this way, provided that sequential synthesis or deposition and in situ monitoring of relevant material properties are feasible, virtually any PVD system can, in principle, be converted into an autonomous platform. This concept extends beyond PVD, and many additional agile demonstrations of autonomous thin-film—and even bulk—materials synthesis tools are expected in the near future.

Electrochemical Deposition

Electrochemical deposition, or plating, is a widely used technique for producing conformal coatings on surfaces. The first demonstration of the technology was by Luigi Brugnatelli in 1805, when he gold-plated silver medallions (Reid et al. 1975). Copper plating is a common example in introductory chemistry classes, typically performed using a copper sulfate solution and a copper anode. Modern industrial applications include Zn–Ni coatings for automotive components (DeCost et al. 2022) and through-silicon vias for connecting stacked integrated circuit layers (Kim et al. 2022).

At its core, basic level plating is relatively straightforward: a solution containing the target cation is prepared and a sufficiently reducing bias is applied to drive its reduction onto the cathode. Increasing the applied potential (or, more commonly, the applied current) raises the deposition rate, which can influence the morphology of the resulting film. As long as the surface is free of oil, debris, and oxides, electrochemical reduction proceeds without obstruction. To create an alloy, one can simply use a solution containing multiple cations and identify the appropriate redox potential to plate each element. In principle, adjusting the relative concentrations of the cations in solution allows fine-tuning of the deposited composition.

In practice, however, electroplating is much more complex. The choice of metal salt used to supply the cation plays an important role in the deposit, with cyanides generally producing smooth and uniform coatings while modern baths more often use sulfates or chlorides. Similar to physical vapor deposition, processing parameters such as pH, temperature, and agitation are commonly adjusted to control deposition rate and quality. In addition, deposition potential and overall deposition time are frequently used to influence the final coating. For alloys, considering differences in electrochemical redox potential alone does not account for behaviors such as anomalous co-deposition, which can lead to unexpected oversaturation of one (typically less noble) metal in the coating.

Unlike physical vapor deposition, the most challenging part of the plating search space is not the mixing of metals, but rather the identification of the organic and inorganic additives such as brighteners, levelers, surfactants, complexing agents, and pH control agents that facilitate deposition. For instance, during electroplating, the pH often increases as hydronium ions are consumed and hydroxyl ions are produced, leading to the precipitation of metal hydroxides. A buffering agent, such as boric acid, is typically added to maintain the pH and suppress precipitation. Conversely, complexing agents, such as cyanide, bind specifically to the metal cation to form stable complexes in solution, releasing the metal only near the cathode in response to local changes in pH or intermediates. None of these parameters are independent, and changes to one strongly influence the optimal deposition conditions.

There are limited examples of SDLs for electrodeposition reported in the technical literature. Joress and colleagues attempted to mix metal cation salts to facilitate

the autonomous deposition of Ni–Co alloys via a scanning droplet cell system (Joress et al. 2022). In this study, a series of alloys were deposited using mixtures of cobalt sulfate and nickel sulfate exposed to different reduction potentials. Post-deposition analysis revealed that a simple rule of mixtures linearly superimposing the individual metal deposition currents weighted by their relative concentrations was insufficient to predict the composition of the coating. This is consistent with literature reports of weak anomalous co-deposition in the Ni–Co system, although in this case the deviation from solution stoichiometry was only a few percent.

AE will allow the discovery and optimization of materials and processes that are not possible or practical with current approaches.

More recently, Quinn and colleagues (2024) developed a low-cost CNC gantry-based tool to investigate the electrodeposition of poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) films. They aimed to identify correlations between monomer concentration, deposition time, and deposition voltage with the electrochromic color change of the coating and the total charge passed during film reduction. Using this approach, the investigators were able to rapidly converge on a range of optimal deposition times and voltages for color-changing films.

The lack of demonstrated electroplating depositions, coupled with the broad importance of the synthesis method, highlights an opportunity for the AE community. Since most work uses a solution carrying cations and additives, it is readily compatible with Scanning Droplet Cell or pipetting platforms. One challenge is keeping the cations in solution; for example, sudden changes in orifice diameter in a tube adapter can cause a saturated salt solution to precipitate and plug the line. Other considerations include identifying the appropriate figure of merit to guide the optimization. For single-element coatings, simple metrics such as reflectivity, roughness, coating uniformity in color, and linear polarization resistance sweeps can suffice to identify high-quality coatings. However, for multi-element coatings, it is also important to understand both the average composition and its depth dependence, which is challenging to achieve within the loop. In such systems, common electrochemical measurements can also conflate a desired property (e.g., oxygen evolution reaction overpotential) with an undesired property (e.g., dissolution of the coating).

For these reasons, autonomous electrodeposition represents a low-hanging fruit for the community to pursue. There are significant opportunities to use AE to optimize and monitor plating conditions for existing solutions, improving both solution efficiency and coating quality. Looking ahead, substantial gains could be achieved by using such platforms to identify novel plating solution chemistries—including cation concentrations and additives—to produce high-performance coatings. Additionally, AE offers the potential to generate high-quality datasets that can help resolve existing disputes regarding mechanisms and uncover new electrochemical phenomena.

Gaps, Outlook, and Future Directions

The outlook for AE in materials development and synthesis is very bright. Pathfinders in physical and chemical vapor deposition and in electrochemistry research have demonstrated the value of the technology in accelerating research to improve both processes and fundamental understanding. Importantly, AE impacts both science and technological advancement. Moreover, it has the potential to influence domestic and global challenges related to critical minerals, economic competitiveness, human welfare, energy, and the environment.

In the summer of 2024, the MGI Autonomous Materials Innovation Infrastructure Interagency Working Group (AMII-IWG) published a workshop report in support of the MGI 2021 Strategic Plan (Boswell-Koller et al. 2024). The report captured the current state of the AMII based on input from workshop participants across industry, academia, and federal government agencies. The report's findings highlight substantial progress in the United States and summarize existing capabilities. However, significant infrastructure gaps remain, including hardware, software, decision tools, and workforce development, which are necessary to enable AE to be more broadly accessible to researchers. The required infrastructure investment is substantial and indeed comparable to the automotive industry's transition from manual labor to automated assembly-line robots. This involves modernization of R&D, large capital investments in automation, and workforce retraining for automated systems. Digitization of advanced materials R&D also requires major

TABLE 1 The 2024 MGI Challenges

MGI Challenge	Current Issues	Imagined Solutions
Point of care tissue-mimetic materials for biomedical devices and implants	Inadequate materials for implants, potential for leaching, immune response	Personalized soft biomaterial designed and delivered at bedside
Agile manufacturing of affordable multi-functional composites	Limited use of composite materials, high cost, emissions, and weight	Reduced time and cost for composite design and manufacturing
Quantum position, navigation, and timing on a chip	Dependence on aging GPS infrastructure, susceptible to disruption	Devices synchronize flawlessly without reliance on satellites
High performance, low carbon cementitious materials	Cement production generates 8% of global CO_2 emissions	Novel cementitious materials designed using locally sourced feedstocks
Sustainable materials design for semiconductor applications	Need for accelerated design and deployment of new materials	AI-powered autonomous experimentation for rapid material design

investments in software and software engineering. The digital transformation of research and development will continue to evolve, emphasizing data generation, exploitation, and AI-driven reasoning as foundational tools for scientific and technological advancement.

Associated with the AMII were the 2024 MGI Challenges (MGI 2024). The five MGI Challenges, which reflect priorities from multiple federal agencies, are summarized in Table 1. The intent of the Challenges was to "utilize challenges to help unify and promote adoption of the Materials Innovation Infrastructure—through the expansion and integration of capabilities including autonomy, artificial intelligence, and robotics—to realize solutions to challenges of national interest."

Autonomous Experimentation Future of Synthesis

Workforce is a critical issue for AE. First, our STEM workforce is insufficient, and demographic forecasts predict a reduced supply and rapid loss of expertise as the current workforce retires. Second, AE requires a modernized workforce capable of conducting materials R&D while leveraging advances in AI, autonomy, and digital transformation. Addressing this challenge will require retooling university curricula and significant retraining for the current workforce. Often overlooked is the importance of early preparation of K–12 students for future work in AI and autonomy. Developing this future workforce will demand substantial investment in teacher training, curriculum development, and hands-on, experiential, or project-based learning. Finally, public–private partnerships were identified as essential to advancing the AMII.

We expect the near future of AE to focus on building infrastructure and advancing decision methods to accelerate research and reduce the repetitive, mindless tasks faced by bench researchers, allowing humans to concentrate on higher-level research goals and understanding. This represents a shift in the fundamental role of human researchers away from tedium, ironically creating more room for humans (especially students) to exercise greater autonomy in their research. We caution that safety and security considerations must remain central to AE, learning from the autonomy community that delegation of decision authority to a human or to a research robot does not constitute abdication of responsibility for research outcomes.

In the near term, we observe several trends in AE/SDLs. As the technology is still in its early stages, much of the focus will be on expanding laboratory automation, including operando, in situ, and in-line characterization, as well as synthesis, sample transfer, and sample loading. It is encouraging that materials research is a focus of recent advances in AI large language models and foundational models (Ball 2025). We also see progress in AI decision methods that incorporate materials prior knowledge (e.g., phase diagrams) and in-line modeling and simulation into the AE iterative loop. More researchers are integrating explicit hypothesis testing, generation, and regression (Noack and Ushizima 2023). Finally, there are efforts to improve access and reduce barriers to AE. Cloud labs like the Emerald Cloud Lab aim to provide automated and autonomous research fulfillment that is accessible remotely online (Canty et al. 2025). Additional initiatives focus on affordability, including LEGOLAS autonomous chemistry robots from the University of Maryland and the National Institute of Standards and Technology (Saar et al. 2022) and Athena Educational Autonomous Experimentation 3D printers from the Air Force Research Laboratory (Lo et al. 2024), among others.

As AE systems mature, we note a current and natural bias toward replicating human laboratory workflows in AE, rather than taking advantage of de novo AE workflows that can be faster and more efficient, as demonstrated in the PVD community (see above) through the

use of automation and in situ diagnostic tools. Actions or constraints that might be obvious to human researchers are often overlooked when programming an AE robot to conduct research. For example, in an early ARES campaign, we allowed the planner to choose any temperature, and it selected negative absolute temperatures that were clearly unphysical to human researchers. Finally, the phenomenon of serendipitous discovery is often cited as a potential loss with AE. However, AE/SDLs can be programmed to identify unexpected results and flag them for further investigation and attention by human researchers.

In the longer term, we see a revolution in how research is conducted, with ever-increasing speed and progress reducing R&D time from decades to years. We see AE as a force multiplier, enabling one researcher to do the work of a hundred. AE will allow the discovery and optimization of materials and processes that are not possible or practical with current approaches. By enabling exponentially more and better experimentation, AE shifts the balance of risk and reward in deciding what research to pursue. That is, if a researcher can conduct many more experimental iterations, they can attempt high-risk, high-reward AE campaigns that might otherwise not be worth risking progress toward a successful dissertation or research grant.

The impact of AE/SDLs is potentially revolutionary.

However, there are concerns about the changing roles of human researchers as AE expands. What will humans do? Will robots take away jobs? How will human researchers work with AE systems? As with any revolution, these seismic shifts can be concerning and disruptive. We see AE/SDLs as an augmentation to human efforts in the same way that electronic computers freed the human computers of the 1940s to focus on more interesting work. We see human researchers using AE systems to multiply their efforts as farmers use tractors. Because technology advances exponentially (Mokyr 1992), we see this multiplication of effort and speed as necessary to maintain the rate of progress such that AE systems will augment human researchers rather than displace them.

The impact of AE/SDLs is potentially revolutionary. First, there is the prospect of an exponential explosion in materials science advancement, akin to a "Moore's Law" for the speed of research (Seffers 2017). Next, we expect to narrow the "Valley of Death" that prevents many technological advancements from transitioning to use. In addition to accelerating materials R&D from decades to years, we expect materials advances to respond to new needs more rapidly, solving problems in the near term instead of the far term. Finally, we hope to see barriers to AE drop so significantly that citizen scientists can participate in research, unleashing the power of many minds on the vast endeavor of materials R&D. Broadly, we expect AE to impact economic prosperity, national security, and human health and welfare.

References

Ball DW. 2025. The Future of Materials Science: AI, Automation, and Policy Strategies. Mercatus Center, George Mason University. Online at https://www.mercatus.org/research/policy-briefs/future-materials-science-ai-automation-and-policy-strategies.

Boswell-Koller C, Warren J, Maruyama B, Yang C. 2024. Accelerated Materials Experimentation Enabled by the Autonomous Materials Innovation Infrastructure (AMII): A Workshop Report; Subcommittee on the MGI. Online at https://www.mgi.gov/sites/default/files/documents/MGI_Autonomous_Materials_Innovation_Infrastructure_Workshop_Report.pdf.

Bulmer JS, Sloan AWN, Glerum M, Carpena-Núñez J, Waelder R, Humes J, Boies AM, Pasquali M, Rao R, Maruyama B. 2023. Forecasting carbon nanotube diameter in floating catalyst chemical vapor deposition. Carbon 201(5 January):719–33.

Canty RB, Bennett JA, Brown KA, Buonassisi T, Kalinin SV, Kitchin JR, Maruyama B, Moore RG, Schrier J, Seifrid M, Sun S, Vegge T, Abolhasani, M. 2025. Science acceleration and accessibility with self-driving labs. Nature Communications 16(1):3856.

Choy K-L, ed. 2019. Chemical Vapour Deposition (CVD): Advances, Technology and Applications. CRC Press.

DeCost B, Joress H, Sarker S, Mehta A, Hattrick-Simpers J. 2022. Towards automated design of corrosion resistant alloy coatings with an autonomous scanning droplet cell. JOM 74(8):2941–50.

Green ML, Choi CL, Hattrick-Simpers JR, Joshi AM, Takeuchi I, Barron SC, Campo E, Chiang T, Empedocles S, Gregoire JM, and 7 others. 2017. Fulfilling the promise of the Materials Genome Initiative with high-throughput experimental methodologies. Applied Physics Reviews 4(1).

Harris SB, Biswas A, Yun SJ, Roccapriore KM, Rouleau CM, Puretzky AA, Vasudevan RK, Geohegan DB, Xiao K. 2024. Autonomous synthesis of thin film materials with pulsed

laser deposition enabled by in situ spectroscopy and automation. Small Methods 8(9).

Joress H, DeCost B, Hassan N, Braun TM, Gorham JM, Hattrick-Simpers J. 2022. Development of an automated millifluidic platform and data-analysis pipeline for rapid electrochemical corrosion measurements: A pH study on Zn-Ni. Electrochimica Acta 428(October):140866.

Khan AI, Yu H, Zhang H, Goggin JR, Kwon H, Wu X, Perez C, Neilson KM, Asheghi M, Goodson KE, Vora PM, Davydov A, Takeuchi I, Pope E. 2023. Energy efficient neuro-inspired phase–change memory based on Ge4Sb6Te7 as a novel epitaxial nanocomposite. Advanced Materials 35(30):2300107.

Kim S-H, Braun TM, Lee H-J, Moffat TP, Josell D. 2022. Microstructure and texture in copper filled millimeter scale through silicon vias. Journal of The Electrochemical Society 169(3):032508.

Kusne AG, Yu HS, Wu CM, Zhang HR, Hattrick-Simpers J, DeCost B, Sarker S, Oses C, Toher C, Curtarolo S, and 6 others. 2020. On-the-fly closed-loop materials discovery via Bayesian active learning. Nature Communications 11.

Liang H, Stanev V, Kusne AG, Tsukahara Y, Ito K, Takahashi R, Lippmaa M, Takeuchi I. 2022. Application of machine learning to reflection high-energy electron diffraction images for automated structural phase mapping. Physical Review Materials 6.

Liang H, Wang C, Yu H, Kirsch D, Pant R, McDannald A, Kusne AG, Zhao JC, Takeuchi I. 2024. Real-time experiment-theory closed-loop interaction for autonomous materials science. arXiv preprint. arXiv:2410.17430.

Lippmaa M, Koida T, Minami H, Jin Z, Kawasaki M, Koinuma H. 2002. Design of compact pulsed laser deposition chambers for the growth of combinatorial oxide thin film libraries. Applied Surface Science 189(3–4):205-9.

Lo S, Baird SG, Schrier J, Blaiszik B, Carson N, Foster I, Aguilar-Granda A, Kalinin SV, Maruyama B, Politi M, Tran H. 2024. Review of low-cost self-driving laboratories in chemistry and materials science: The "frugal twin" concept. Digital Discovery 3(5):842–68.

MGI [Materials Genome Initiative]. 2024. The 2024 Materials Genome Initiative (MGI) challenges. Online at https://www.mgi.gov/2024-materials-genome-initiative-mgi-challenges.

Mokyr J. 1992. The Lever of Riches: Technological Creativity and Economic Progress. Oxford University Press.

Nikolaev P, Hooper D, Perea-Lopez N, Terrones M, Maruyama B. 2014. Discovery of wall-selective carbon nanotube growth conditions via automated experimentation. ACS Nano 8(10):10214–22.

Nikolaev P, Hooper D, Webber F, Rao R, Decker K, Krein M, Poleski J, Barto R, Maruyama B. 2016. Autonomy in materials research: A case study in carbon nanotube growth. npj Computational Materials 2:16031.

Noack M, Ushizima D., eds. 2023. Methods and Applications of Autonomous Experimentation. CRC Press.

Price C, Takeuchi I, Rondinelli J, Chen W, Hinkle C. 2025. AI-accelerated electronic materials discovery and development. Computer 58(2):98–104.

Quinn H, Robben GA, Zheng Z, Gardner AL, Werner JG, Brown KA. 2024. PANDA: A self-driving lab for studying electrodeposited polymer films. Materials Horizons 11(21):5331–40.

Rao R, Pint CL, Islam AE, Weatherup RS, Hofmann S, Meshot ER, Wu FQ, Zhou CW, Dee N, Amama PB, and 32 others. 2018. Carbon nanotubes and related nanomaterials: Critical advances and challenges for synthesis toward mainstream commercial applications. ACS Nano 12(12):11756–84.

Reid FH, Goldie W, Brooman EW. 1975. Gold plating technology. Journal of The Electrochemical Society 122(6).

Saar L, Liang H, Wang A, McDannald A, Rodriguez E, Takeuchi I, Kusne AG. 2022. The LEGOLAS Kit: A low-cost robot science kit for education with symbolic regression for hypothesis discovery and validation. MRS Bulletin 47:881–85.

Seffers GI. 2017. Scientists pick AI for lab partner. Signal. Online at https://www.afcea.org/signal-media/scientists-pick-ai-lab-partner.

Shimizu R, Kobayashi S, Watanabe Y, Ando Y, Hitosugi T. 2020. Autonomous materials synthesis by machine learning and robotics. APL Materials 8:111110.

Stach E, DeCost B, Kusne AG, Hattrick-Simpers J, Brown KA, Reyes KG, Schrier J, Billinge S, Buonassisi T, Foster I, and 11 others. 2021. Autonomous experimentation systems for materials development: A community perspective. Matter 4(9):2702–26.

Waelder R, Park C, Sloan A, Carpena-Núñez J, Yoho J, Gorsse S, Rao R, Maruyama B. 2024. Improved understanding of carbon nanotube growth via autonomous jump regression targeting of catalyst activity. Carbon 228:119356.

Waelder R, Kim W, Pitt MA, Myung JI, Maruyama B. 2025. Multi-objective Bayesian optimization of carbon nanotube yield and diameter control at synthesis. APL Machine Learning 3:026114.

Wu X, Khan AI, Lee H, Hsu C-F, Zhang H, Yu H, Roy N, Davydov AV, Takeuchi I, Bao X. 2024. Novel nanocomposite-superlattices for low energy and high stability nanoscale phase-change memory. Nature Communications 15:13.

From human intuition to machine intelligence:

the next frontier in microscopy.

Self-Driving Microscopy for AI/ML-Enabled Physics Discovery and Materials Optimization

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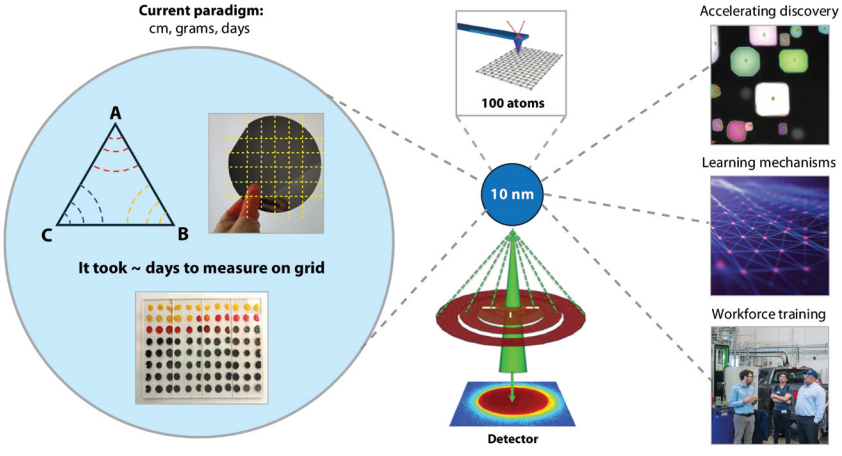

Closing the materials discovery loop is now achievable by integrating artificial intelligence with microscopy to create autonomous systems that can rapidly characterize vast material libraries, learn new physical laws, and fabricate structures atom by atom.

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Introduction: Our Material Future

Materials are the bedrock of economy and foundation for all real-world technologies. The viability of space travel, grid energy storage, solar to fuels conversion, methane removal, and photovoltaic energy solutions hinge on the discovery and optimization of novel materials and rapid scaling toward manufacturing. The last 20 years have seen an exponential growth in the theoretical predictive capability for crystalline materials and small molecules. However, it is only in the last five years that we have seen the rapid expansion of high-throughput synthesis enabled by laboratory robotics and microfluidics, as well as a resurgence of combinatorial synthesis (Abolhasani and Kumacheva 2023; Epps and Abolhasani 2021; Jiang et al. 2022; Rajan 2008; Soldatov et al. 2021; Szymanski et al. 2023). Combinatorial synthesis, microfluidics, and ultimately dip-pen megalibraries have demonstrated the ability to "write" multicomponent nanomaterials at high throughput scale, generating millions of material examples in the 3D, 4D, and 5D composition spaces (Chen et al. 2016, 2019; Jibril et al. 2022).

The lesson of the past two decades is that scaling computation or synthesis individually, even by many orders of magnitude, is insufficient for expediting materials discovery. Rather, the key is to accelerate the feedback loop between theory and hypothesis making, experiment planning, synthesis, and characterization with subsequent update of theoretical models. With the recent advances in high throughput computational screening and synthesis (Colón and Snurr 2014; Daglar and Keskin 2020; Greenaway et al. 2018; Manly et al. 2001), the remaining bottleneck for accelerated materials discovery now is closing the characterization loop and, in particular, extending characterization from static to dynamic to learn materials evolution during the processing. This is a highly complex challenge. While theoretical workflows are often homogeneous and experimental efforts typically focus on a single material family or preparation method, characterization spans multiple techniques, often providing information on complementary aspects of materials behavior and requiring integration into single model.

A key requirement for accelerated materials discovery is shifting characterization cycles to time scales on the order of seconds and length scales on the order of microns and smaller to match the throughput of existing fast synthesis methods. This consideration propels microscopy techniques to the forefront. Electron microscopy and associated spectroscopies offer a high-veracity method for probing the structure and chemical properties on the single nanoparticle level (Christopher et al. 2020; Colliex et al. 2016; Egerton 2011; Kociak et al. 2014), but generally suffer from slow sample preparation (El Kirat et al. 2005; Ghomrasni et al. 2020; Thompson et al. 2016). Similarly, scanning probe microscopy excels in probing functionalities including piezoelectricity (Martin 1972), photovoltage (Kuk et al. 1991; Weaver and Wickramasinghe 1991), and electrochemical properties on the nanometer scale (Bentley et al. 2019; Gewirth and Niece 1997; Takahashi et al. 2017), and are ideally suited for exploring combinatorial spread libraries[1] and droplet libraries.[2]

Microscopy experiments can vary greatly in quality and reproducibility, even among researchers in the same group, let alone across groups or over time.

Materials discovery via microscopy gives rise to a unique challenge. These instruments can operate much faster than human decision making and often create bespoke data sets. At the same time, exploration of positionally encoded combinatorial systems via grid search methods is still intractable. The confluence of these two factors makes a case for the machine learning (ML)-enabled autonomous microscopy. Here, we provide an overview of the emergent trends in automated microscopy, highlighting both challenges and opportunities for these methods to aid materials discovery and design.

Why Automation in Microscopy

Classical microscopy has traditionally relied on rectangular and fixed-time scanning patterns, a practice shaped by both technological limitations and human biases. These approaches are easily implemented and visualized, leading to a standard sequence of operations: tuning the microscope, imaging, and spectroscopic measurements. The human operator performs multiple and repetitive

[1] Combinatorial spread library is a sample prepared such that there is a concentration gradient encoded via spatial location.

[2] The library of different materials compositions prepared by drop casting.

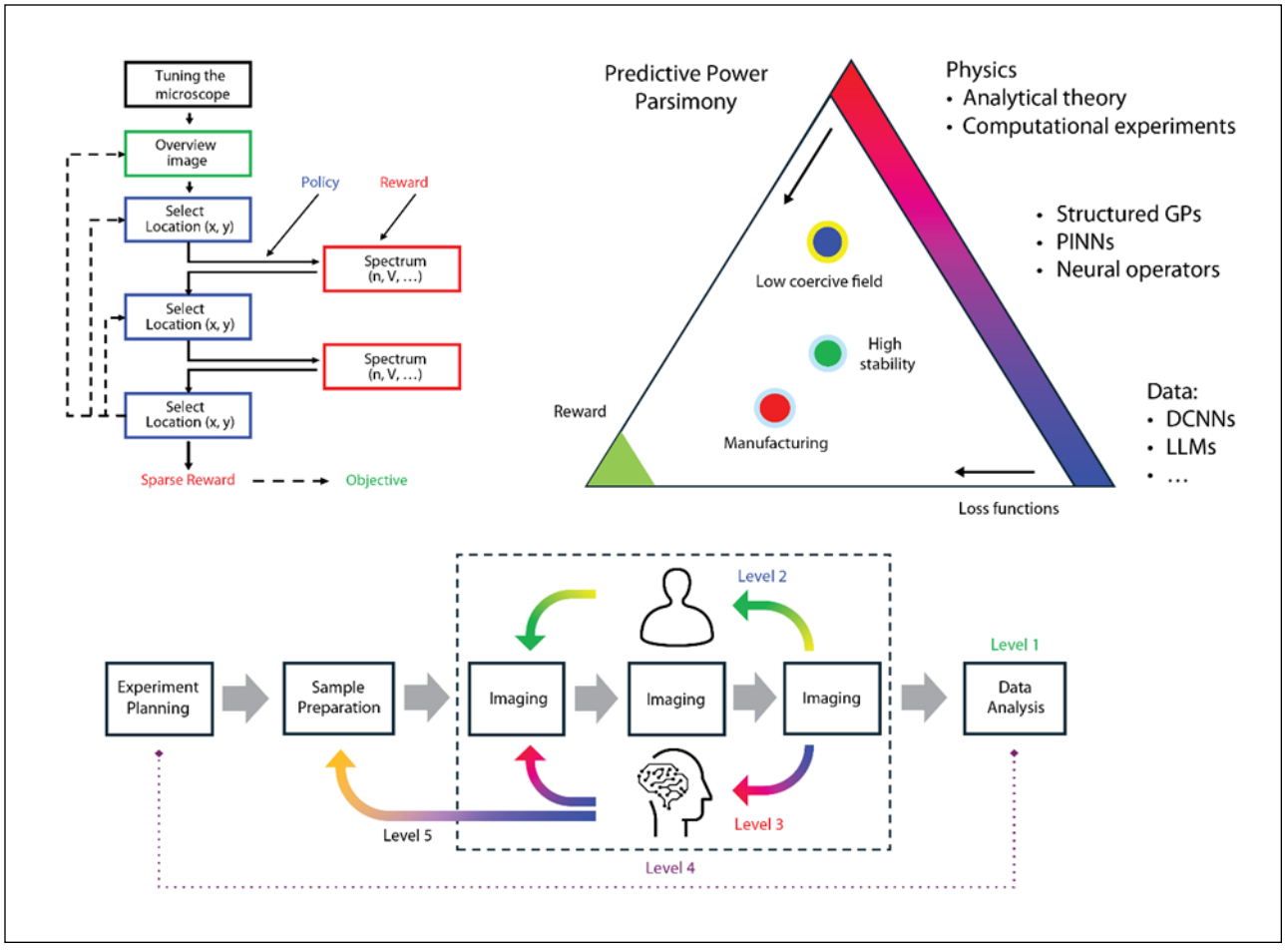

FIGURE 1 (Top Left) Operation of microscope can be represented as a linear set of operations that can be either defined based on known policies, or policies can be learned based on external reward functions. (Top Right) Relationship among data, physics, and reward. Traditionally only the simplest reward functions are used, as compared to very complex real-world objectives. (Bottom) Levels of decision making in microscopy workflows.

simple operations, such as tuning the microscope, selecting objects for investigation, and conducting spectroscopy (Figure 1 [Top Left]). However, the sequence of these seemingly straightforward operations reflects a complex decision-making process informed by the operator's expertise and guided by experimental goals, with results continuously monitored and goals refined during the experiment. As a result, microscopy experiments can vary greatly in quality and reproducibility, even among researchers in the same group, let alone across groups or over time.

Here, we discuss AI-enabled microscopy as a tool for materials and physics discovery, focusing on the levels of autonomous and human in the loop decision making. Exploring the materials at the limits of microscope data acquisition rates requires translating the operator's objectives into a structured framework that ML methods can define and execute. This is particularly important because experimental goals like physics discovery or materials optimization vary between scientists and are often not explicitly defined.

Rewards, Objectives, and Hyperlanguages

Translating the complex decision-making process of human operators into automated workflows requires building the corresponding ML framework. This in turn requires defining several core concepts including *reward*, *objectives*, and *hyperlanguage*.

A *reward* is an immediate, measurable outcome of an experiment—typically quantifiable and directly tied to the optimization goals. Rewards can be simple, instrument-specific metrics such as achieving higher resolution or maximizing signal intensity, or more complex domain

specific metrics such as minimization of the peak corresponding to the undesired impurity, limited certain types of deleterious defects, or establishing preferred grain orientation.

Objectives, on the other hand, are long-term scientific goals. These can include fundamental goals such as understanding material behavior or discovering a new physical law or applied goal as making better solar energy material or stable battery. Objectives typically require multiple experiments and iterations to approach, and the relationship between experimental reward and objectives is often uncertain. The key part of experimental planning is building rewards that align with objectives. This process is probabilistic in nature, often involving specific hypotheses and heavily depending on human heuristics informed by prior observations, physics, and domain-specific intuition.

Finally, *hyperlanguage* serves as a unifying framework that defines the possible operations that can be executed on the microscope, connecting the ML abstractions to the executable real-world operations. In the language of reinforcement learning, actions are expressed in hyperlanguage.

It is important to note that the rewards in ML are necessarily domain related. Quoting Peter Norvig (Russell and Norvig 2020), "Somewhat remarkably, almost all AI research until very recently has assumed that the performance measure can be exactly and correctly specified in the form of utility or reward function." Traditional rewards in ML or physics are very simple, including loss functions or parsimony or predictive power of models. These contrast with far more complex real-world objectives and reward functions (Figure 1 [Top Right]). Correspondingly, experiment planning by a domain expert always implicitly or explicitly includes the definition of the probabilistic reward(s) expected to align with the project objective. While humans often perform this intuitively, building automated instruments and self-driving labs requires the rewards to be formulated explicitly.

Levels of ML in Microscopy

Both electron and scanning probe microscopes can operate at rates well above human reaction times and generate data volumes and dimensionality far beyond human analytical capabilities. ML and AI offer the opportunity to enable discovery at these time scales and with such complex objects. The application of ML in microscopy for materials discovery requires classification of the decision-making levels within the experimental workflow (Figure 1 [Bottom]).

- *Level 1* represents a scenario where data are analyzed post-experiment, but the experimental progression remains fixed (as already determined by the human operator) and cannot be adjusted based on after-the-fact analysis.

- *Level 2* introduces real-time data analysis, allowing insights to be gained during the experiment; however, decisions are still made and implemented manually by human operators.

- *Level 3* involves ML agents that can execute microscope commands during the experiment, driven by predefined reward functions available in real time and potentially with a human in the loop.

- *Level 4* extends this autonomy, enabling the microscope to conduct experiments independently based on reward functions, while also integrating interactions with theory-in-the-loop systems to refine its actions.

- *Level 5* goes further, incorporating upstream experimental planning, where the microscope not only executes experiments but also controls sample preparation methods, creating a fully autonomous end-to-end experimental workflow. In this scheme, Level 5 decision making establishes the connection between a single tool and broader up- and downstream decision making, allowing integration into autonomous instrument networks.

Level 1: Post-acquisition Analysis

Until the late 20th century, electron microscopy was largely constrained by data analysis challenges, with data typically recorded on film or as relatively small image or spectroscopic datasets. The rapid emergence of personal computing and, more recently, cloud computing over the past 25 years has revolutionized data storage and enabled the use of highly information-rich detectors. This technological leap has made it possible to generate datasets with images containing up to 10^9 pixels, along with hyperspectral data of comparable complexity.

This explosion of data necessitated the development of advanced analysis methods, ranging from physics-based reconstructions to ML-driven dimensionality reduction and segmentation techniques. Physics-based reconstructions condense raw, high-volume data into a smaller set of material-specific, microscope-independent descrip-

tors. Dimensionality reduction methods reduce data volume while presenting it in low-dimensional formats more suitable for human interpretation, spanning simple techniques like principal component analysis to more complex nonlinear approaches based on variational autoencoders. Segmentation methods, meanwhile, use prior knowledge embedded in pretrained networks to identify and isolate features of interest within the dataset, enabling targeted and efficient analysis. Many of these methods are reviewed by Kalinin et al. (2022) and Smeaton et al. (2024). However, a key limitation of post-acquisition analysis is that the experimental data have already been collected, meaning the course of the experiment cannot be altered after the fact.

Level 2: Real-time Data Analytics

In traditional microscopy, all critical decisions—such as selecting regions for imaging, determining scan sizes and pixel densities, choosing areas for spectroscopic measurements, and defining measurement parameters—were made manually by human operators. These decisions relied on prior observations and the operator's expertise. However, this process is highly subjective, varying significantly with the operator's experience. Moreover, many phenomena of interest, such as topological defects or domain walls, are difficult to detect, or even interpret, by eye in raw images. For large, noisy, fast, or high-dimensional datasets, human perception is fundamentally limited, making manual decision making increasingly impractical.

This challenge has driven interest in real-time ML-based imaging and spectral analysis workflows that operate during data acquisition, transforming streaming high-dimensional data into forms more suitable for human interpretation. In this framework, humans still decide on the next operation, but the data are processed in real time to enhance interpretability. Despite the availability of advanced ML methods for post-acquisition analysis, implementing real-time ML remains a non-trivial problem. For supervised methods, a major challenge lies in addressing distribution shift, where small changes in microscope imaging parameters can cause substantial variations in ML outputs. This issue is common in computer vision, as shown by the immense effort required for autonomous driving systems. Furthermore, scientific exploration inherently involves encountering objects or phenomena not represented in training datasets. This is especially true for mesoscopic and scanning probe microscopy (SPM) imaging, where objects of interest are often less well defined compared to atomically resolved imaging under ideal conditions.

Applications of real-time analytics include representing high-dimensional or complex datasets in a form that supports human perception and identification. This includes visualization of defects in high-noise images and mapping physical order parameter fields such as strain, polarization, and octahedral tilts. An example of a few-shot learning–based model (Akers et al. 2021; Ter-Petrosyan et al. 2024), which leverages pre-trained encoders and requires only a limited number of examples to distinguish features of interest, is shown in Figure 2. While such models may offer less descriptive power, they can be adapted to novel scenarios and updated in real time as new contextual information or tasks arise. Alternatively, lightweight forecasting models, such as those based on simple recurrent neural networks or more sophisticated transformers, may be used in conjunction with real-time imaging or spectroscopy data to maintain a continuous prediction of the state of a system or chemical reaction (Lewis et al. 2022). These models are particularly useful for informing real-time decision making, as described below, since they encode knowledge of the response times of both the imaging system and the material system (Hujsak et al. 2016, 2018).

Even unsupervised methods, such as dimensionality reduction, present challenges. They often require careful tuning of numerous hyperparameters and can yield multiple or non-unique representations of the data. To overcome these limitations, reward-based analysis workflows offer a promising alternative. By leveraging defined reward functions, these workflows can construct robust and explainable pipelines, enabling automated, reproducible, and interpretable analysis of streaming microscopy data (Barakati et al. 2024). Integrating real-time ML with microscopy thus bridges the gap between complex data acquisition and human decision making, paving the way for more effective and insightful experimentation.

Level 3: Real Time Decision Making

The effective timescale for human decision making is typically on the order of 0.3–1 second for rapid, instinctive decisions and considerably longer for decisions requiring deeper thought. These timescales are substantially slower than the intrinsic data acquisition rates of electron microscopes and many scanning probe techniques, which can operate on millisecond or faster timescales. Moreover, sustained human decision making is constrained by fatigue and other limitations, whereas instruments can

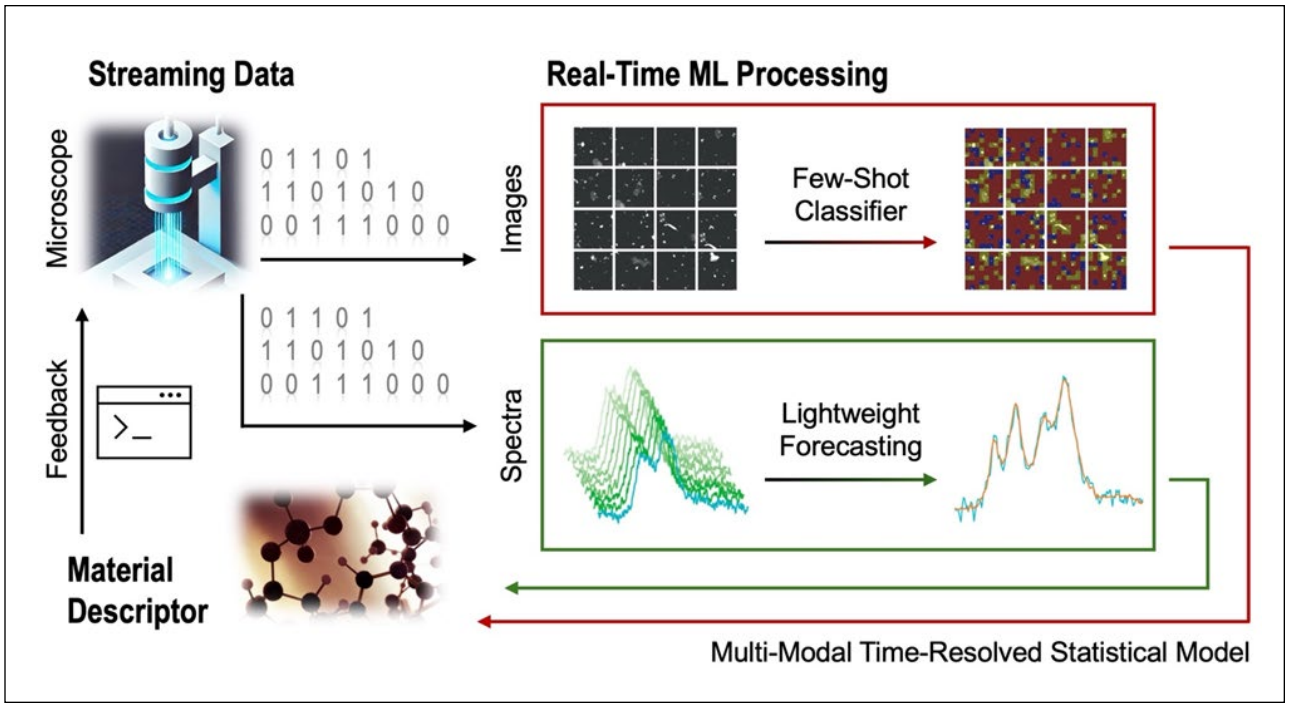

FIGURE 2 By implementing real-time ML, microscopy and spectroscopy data can be immediately interpreted and used for experimental optimization. This figure illustrates two examples: (Top) rapid segmentation of image features using few-shot learning and (Bottom) predictive forecasting of spectral changes with lightweight models. Insights generated by such methods enable dynamic adjustments of experimental parameters. Adapted from Akers et al. (2021) and Lewis et al. (2022), respectively, under CC-BY 4.0 licenses.

operate autonomously for days. These factors suggest that transitioning from human-based to AI/ML-driven decision making could increase the efficiency of microscope use by a factor of 10 to 1,000, provided the quality of AI decisions matches or exceeds that of human operators.

Realizing this potential, however, requires addressing two key challenges. The first is the development of robust Application Programming Interfaces that provide ML agents with direct access to the same control commands available to human operators, expressed through a defined hyperlanguage. This represents a significant engineering task. While the concept of AI-centric microscopes has gained traction globally, progress has been hindered by the cost and complexity of moving away from traditional human-operated systems at the customer level. At the same time, instrument vendors have been slow to adopt AI-native designs due to limited financial incentives outside niche applications. Consequently, early efforts by the materials community relied on fragmented, custom-built solutions to enable AI integration. These included modular access to low-level data streams, real-time visualization, and embedding AI agents into control workflows (Olszta et al. 2022). Current instruments are still designed around human-centric architectures, limiting their response time, precision, and reproducibility (Fiedler et al. 2023). To fully harness the potential of autonomous experimentation, a new generation of hardware–software co-design is required, incorporating modular operating systems, high-speed data streams, and real-time AI integration.

A second, and less obvious, challenge involves building decision-making workflows using these defined hyperlanguage commands. This process represents a highly multistep decision-making framework. One approach is to predefine state–action policies, where a fixed policy determines actions at each stage before the experiment begins. Examples include spectroscopic measurements on defined objects of interest, such as domain walls or grain boundaries (Liu et al. 2023), or specific atom types or defects (Roccapriore et al. 2022a). Another approach is to adopt myopic workflows, where the reward function is defined and optimized at each step. An example is the use of deep kernel learning to explore structure–property relationships, where decisions are made based on a consistent reward function (Liu et al. 2022; Roccapriore et al. 2022c). The applications of these approaches include

broad exploration of structure–property relationships, either for known objects of interest or for the discovery of microstructural elements that maximize functionality of interest. For the latter, the key requirement is that the functionality must be estimable from the spectral data.

This capability opens the door to a fully automated materials discovery process, where the microscope is not just a passive observer but an active participant in designing and creating new materials.

In practice, human decision making in microscopy is far more complex, with reward functions evolving dynamically during experiments. For instance, initial operations may focus on instrument optimization, followed by exploration of statistically significant regions or curiosity-driven investigations of anomalies visible in structural images. Later stages often transition to hypothesis-driven exploration, such as focusing on topological defects based on their potential to exhibit unique properties. Building ML workflows capable of adapting to shifting reward functions requires either setting the reward sequence in advance, designing human-in-the-loop systems (Kalinin et al. 2024) where the operator adjusts the reward functions in real time, or developing multistage decision-making workflows capable of autonomous adaptation.

Level 4: Knowledge Extraction from Data

One of the primary goals of experimentation is the accrual of new knowledge, which can range from gathering statistical information on microstructures and atomic configurations to uncovering phenomenological laws governing material behavior and even advancing our understanding of fundamental physics. The better the physical models we develop, the greater the predictive power of theory in driving real-world material innovations. In this context, a more objective (though still difficult to quantify) measure of an experiment's value is its ability to generate new knowledge. Achieving this requires integrating theory into the experimental loop, enabling a synergistic interplay between data and predictive models.

Astronomers have long used observations of celestial motion to deduce fundamental physical laws, such as Kepler's and Newton's laws, transforming our understanding of the universe. Similarly, modern microscopy provides an unprecedented opportunity to extract physical laws directly from observations of dynamic processes, such as particle growth, microstructure formation, and particle motion. With significant investments in in situ and operando microscopy techniques ranging from environmental electron microscopy to liquid cell transmission electron microscopy and scanning probe microscopy, scientists can now access real-time nanoscale processes under realistic conditions (Smeaton et al. 2024). These advancements have already demonstrated the feasibility of extracting physical parameters, such as diffusion and reaction coefficients, directly from observed data (Ievlev et al. 2015) or learning interaction parameters of spin models from atomically resolved imaging (Valleti 2021), proving that physics discovery from experimental observations is achievable.

The future lies in moving beyond purely data-driven approaches by integrating experimental data with external sources, such as material parameters, compositional insights, and density functional theory models. This integration—shifting from isolated observations to context-informed discovery—will allow the derivation of new physical laws while bridging the gap between nanoscale dynamics and predictive, theory-driven understanding. Such theory may inform emerging materials "frontier" models, an experimental analogue to the Materials Project,[3] as evidenced by the successful adaptation of current foundation models to microscopy (Abebe et al. 2025). Incorporating theory-in-the-loop not only enhances the ability to design experiments with more targeted objectives but also ensures that the knowledge generated contributes directly to advancing materials science and fundamental physics.

Level 5: Upstream Integration with Materials Synthesis and Processing

Traditionally, materials discovery has been followed by characterization, where new materials are systematically analyzed to uncover their properties. However, using microscopes for rapid characterization raises an intriguing possibility: can microscopes directly control synthesis tools? This question becomes particularly relevant in the

[3] https://next-gen.materialsproject.org.

context of combinatorial libraries, which allow exploration across multi-dimensional composition spaces (2D, 3D, and 4D) by synthesizing films or samples with systematic variations in composition.

Advanced microscopes could take this further by not only characterizing samples but also directly controlling synthesis tools, provided sample preparation is fast enough. By integrating sample synthesis and preparation into an autonomous feedback loop, microscopes can iteratively guide the selection of compositions or processing conditions to optimize desired properties. Through combined automated control and real-time data analysis, it is possible to gain new knowledge of kinetic responses and phase transitions, such as radiation-induced oxygen vacancy formation in thin films (Lewis et al. 2022). Currently, human cognition limits the ability to register changes and process relevant feedback, but emerging autonomous systems will not face this constraint. This capability opens the door to a fully automated materials discovery process, where the microscope is not just a passive observer but an active participant in designing and creating new materials.

Microscopy for Materials Discovery: The Future

To illustrate the concept above, we present three emerging applications of ML-enabled Scanning Transmission Electron Microscopy (STEM) and Scanning Probe Microscopy (SPM) for materials discovery.

Materials Discovery in Combinatorial Libraries

SPM is built around the concept of a cantilever sensor, which combines exceptionally high force sensitivity with the capability to probe currents flowing through the tip–surface junction. This force sensitivity enables the detection of electrostatic, magnetic, or electromechanical forces, making SPM a versatile tool for investigating phenomena in nanometer-scale volumes at reasonably fast timescales. However, a significant limitation of many SPM modes is that the measured signals often represent a convolution of surface topography and material properties, reducing the amount of directly useful information. Despite this, even weakly informative signals can serve as proxies for tasks such as exploring combinatorial spread libraries, where the materials' topography reflects composition-dependent growth behaviors.

Some SPM modalities, such as piezoelectric measurements, photovoltage measurements, and to a lesser extent conductivity measurements, are less sensitive to topographic variations, providing more direct access to material functionalities. Furthermore, the integration of SPM with optical methods, such as NanoIR, unlocks an even broader range of capabilities. This makes SPM a powerful tool for rapidly probing the evolution of material functionalities within the compositional space of combinatorial libraries. These libraries conventionally encode binary and ternary phase diagrams, while more complex compositional spaces can be explored using droplet or nanoparticle libraries. However, given the finite throughput of SPM, exploring these high-dimensional spaces requires ML-enabled search strategies rather than simple grid-based methods.

The emergence of autonomous science represents a watershed moment with the potential to transform the materials and chemical sciences.

A limitation of traditional spread libraries is that they typically allow variation of compositional spaces but not processing conditions, apart from thermal gradient samples. Looking ahead, a more advanced scenario involves integrating SPM downstream of synthesis robots capable of varying both compositional and processing spaces in very high dimensions. This integration would enable the systematic exploration of material functionalities across a far more complex experimental landscape, making SPM a cornerstone of autonomous and high-throughput materials discovery workflows.

An even broader range of opportunities is offered by electron microscopy, which provides nanoscale analogs of conventional macroscopic characterization methods. For instance, structural imaging in STEM yields direct information on atomic structures, while electron beam diffraction offers insights roughly equivalent to X-ray scattering. Energy Dispersive X-ray Spectroscopy (EDS) provides local chemical composition, and Electron Energy Loss Spectroscopy (EELS) delivers both chemical information and data on local low-energy excitations, such as plasmons and vibrational excitations, similar to infrared spectroscopy. Although the signal formation mechanisms of these methods are considerably more complex than their macroscopic photon- and X-ray-based counterparts, rapid advancements in instrumentation and data analyt-

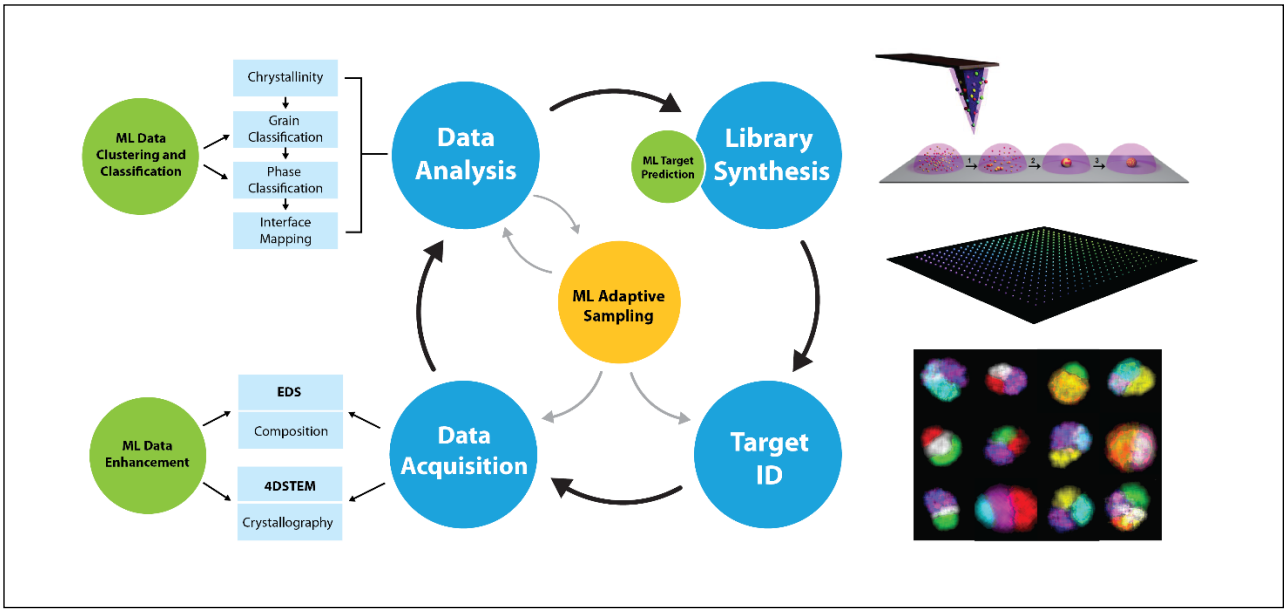

FIGURE 3 Workflow and associated rapid characterization approach for megalibraries (Chen et al. 2016). The center schematic depicts the ML-enabled workflow, comprising identification of target, followed by adaptive sampling for data acquisition and data analytics. The right-side panel shows schematic representation of probe-based synthesis (Top) of megalibraries (Middle) and montage of EDS map of multicomponent and multiphase nanoparticles (Bottom). The left side panel illustrates the role of specific EM methods (Bottom Left) and materials/related parameters necessary for identifying key structural attributes of the nanoparticles.

ics frameworks promise significant improvements in their interpretation in terms of relevant material properties in the coming years. Even now, multi-modal ML models can effectively fuse and distill actionable materials descriptors from such data, informing synthesis and processing (Ter-Petrosyan et al. 2024).

Building upon these advancements, STEM is rapidly becoming a powerful tool for exploring materials, particularly at the nanoscale. A critical requirement for leveraging its full potential is the integration of sample preparation with imaging and analysis workflows. While electron microscopy measurements themselves are relatively fast, sample preparation remains a bottleneck, significantly limiting overall throughput. One solution to this challenge involves the use of "megalibraries" (Kluender et al. 2019; Wahl et al. 2023), where dip-pen lithography creates multidimensional particle libraries directly on an electron-transparent silicon (Si)-rich silicon nitride (SiNx) membrane as a sample holder. These libraries enable the systematic exploration of compositional and structural spaces, with each particle studied individually as well as collectively. Beyond this, other strategies for exploring compositional and processing spaces could be developed, paving the way for electron microscopy to play a central role in high-throughput materials discovery.

In recent years, significant advancements in AI-enabled microscopy have emerged, demonstrating practical implementations of the ML-driven search strategies needed for exploring combinatorial libraries. These innovations include binary classification systems that efficiently distinguish high-quality nanoparticles with exceptional precision, rapid image segmentation pipelines that dramatically reduce acquisition time while maintaining high accuracy, and automated preprocessing frameworks that enhance model performance while reducing computational demands. Collectively, these approaches represent crucial steps toward closing the materials discovery loop by enabling the high-throughput characterization of megalibraries, where millions of distinct nanoparticles with varying compositions can be systematically explored (Figure 3). By integrating these AI-driven techniques with microscopy workflows, researchers can now navigate complex compositional spaces far more efficiently than traditional grid-based methods, accelerating the identification of promising materials for further analysis and development.

Atomic Fabrication

The last note left by Richard Feynman on his blackboard was, "What I cannot create, I do not understand." Building solid-state quantum computers, creating nanoro-

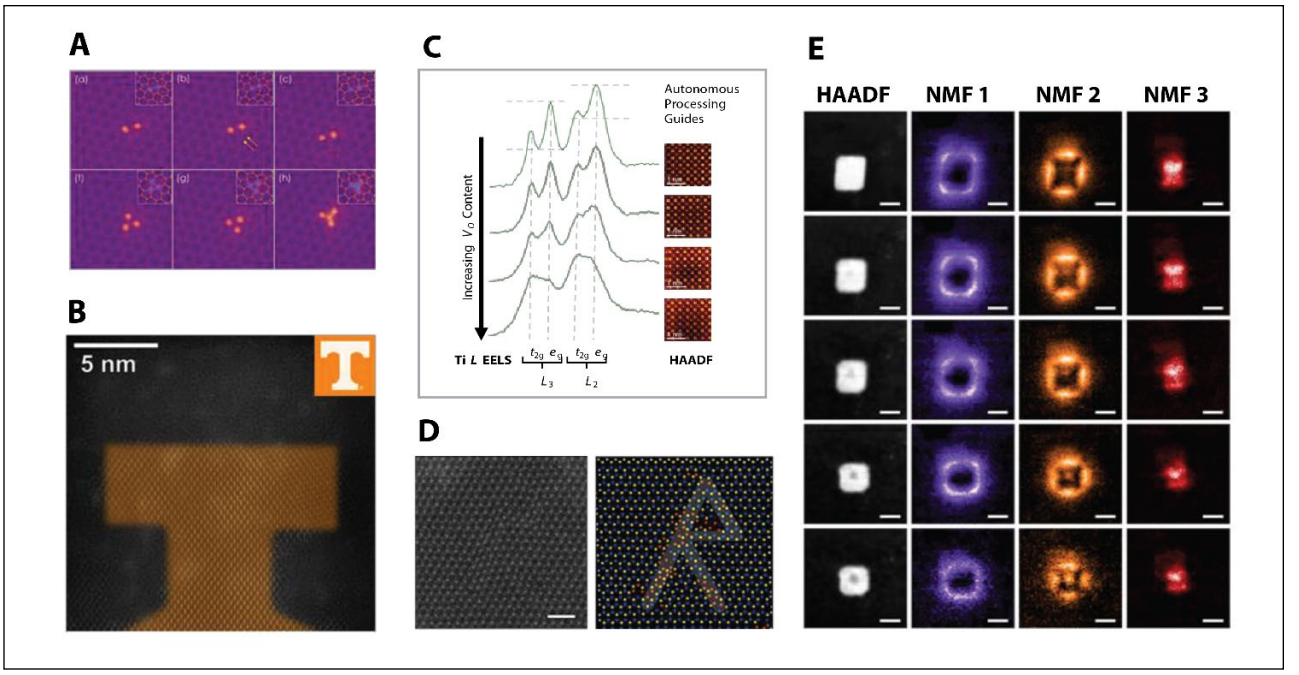

FIGURE 4 Examples of direct atomic fabrication by electron beam. (A) Assembly of multiatomic artificial molecules of Si in graphene (Dyck et al. 2018). (B) Letter "T" formed by crystallizing amorphous Si by electron beam (courtesy of G. Duscher). (C) Autonomous manipulation of oxygen vacancies using the electron beam. (D) Letter "R" formed by removing S atoms from MoS_2. (E) Evolution of plasmonic responses during direct electron beam manipulation of a nanoparticle (Roccapriore et al. 2022b).

bots, and designing new classes of biological molecules and catalysts all require the capability to manipulate and assemble matter atom by atom, probe the resulting structures, and connect them to the macroscopic world. The current paradigm of top-down fabrication, based on lithographic methods, is reaching the limit of ~2 nm device structures—an order of magnitude above atomic spacing—is limited to a single materials class, and relies on a globe-spanning supply and manufacturing chain. Until recently, the two low-cost, low-footprint paradigms for bottom-up atomic fabrication were chemical synthesis and scanning tunneling microscopy (STM)-based direct atomic manipulation. Synthesis is massively parallel, but developing synthetic pathways to complex molecular machines—and especially their assembly—is exceptionally time-consuming, with only the simplest architectures realized experimentally. In comparison, STM-based atomic manipulation has developed slowly and has been demonstrated only for special classes of materials.

Electron beam damage has been known in electron microscopy since the first experiments by Ernst Ruska before World War II. It was one of the primary factors (along with resolution) driving the development of electron microscopy over decades, first toward high-voltage instruments in the 1980s and then, from the late 1990s, toward aberration-corrected (AC) instruments. The broad introduction of AC microscopes over the last decade has allowed investigators to localize beam damage to a single atomic column or chemical bond (Markevich et al. 2016), opening a new paradigm for direct atomic-level manipulation of matter (Figure 4). Over the same period, this approach has enabled direct atomic motion (Dyck et al. 2017; Susi et al. 2017), the construction of homo- and multiatomic artificial molecules in 2D materials (Dyck et al. 2018), and atomic-plane sculpting of 2D and 3D materials (Jesse et al. 2015).

By combining imaging (e.g., HAADF[4]-STEM) and spectroscopic signals (e.g., EELS, EDS) in a multi-modal approach, it is possible to obtain highly localized information about point defects. The complexity of these interactions—for example, electron beam radiation coupling to oxygen vacancy formation (Lewis et al. 2022)—necessitates new ML models. Such models should process multimodal data and predict appropriate beam parameters to achieve a desired defect configuration. By incorporating these ML predictions into an automated feedback loop, real-time control is achieved, overcoming human reaction

[4] High-angle annular dark-field.

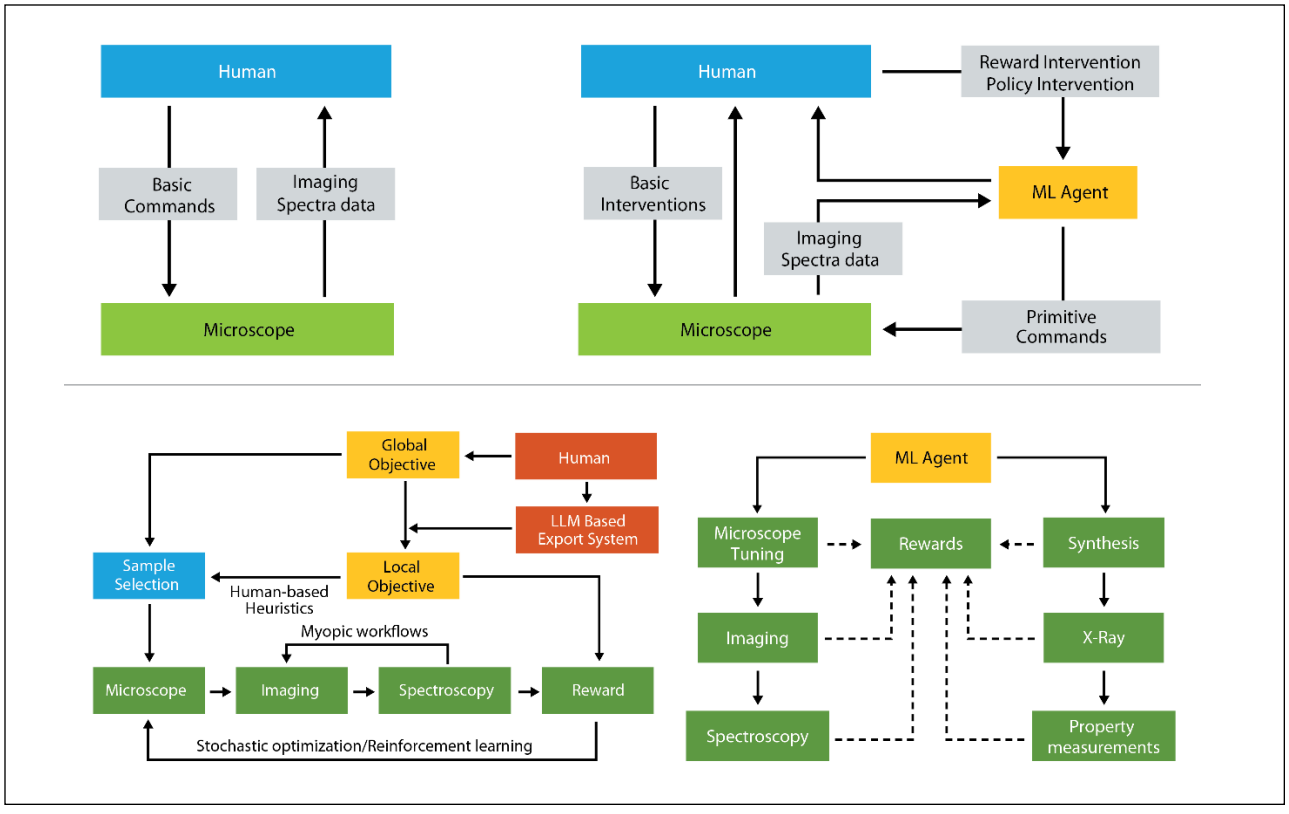

FIGURE 5 Transition from current human operated microscopy to myopic human-in-the-loop workflows to autonomous microscopy and multi-instrument autonomous facilities.

time limitations. The microscope thus transitions into an autonomous atomic-scale factory.

Integrating Multiple Tools

Paralleling other domains, there is an increasing need to develop ML models capable of multi-modal reasoning to improve discriminating ability and aid in hypothesis generation (Figure 5). It is often tacitly assumed that more modalities (e.g., imaging, spectroscopic, diffraction) are better. While correct in principle, this neglects the real cost of acquiring additional data in terms of time, dose, or instrument usage that may damage the material during analysis. Multi-modal data often exhibit a high degree of sparsity or redundancy that is not fully considered when assessing each modality independently. Thus, it is critical to understand each data stream's characteristics, how sample features are represented, how the data are collected, and related factors. To date, there have been few, if any, systematic studies of these characteristics in relation to specific material properties, such as crystallinity and alloying element distribution (Ter-Petrosyan et al. 2024). As a result, models may inadvertently bias toward one modality and unintentionally disregard key features of others. These models provide an opportunity to learn how to prioritize experiments to extract the most information at the least cost, effectively shortcutting the discovery process.

Summary

The emergence of autonomous science represents a watershed moment with the potential to transform the materials and chemical sciences. In electron microscopy, initial engineering has given way to practical automation systems, but more work is needed to make autonomous microscopy a reality. The next generation of hardware must be designed with autonomy in mind. We should carefully consider our data budget and design architectures capable of reasoning in sparse and unexplored settings. It is also increasingly important to account for the cost and idiosyncrasies of handling multi-modal data, which can provide a more comprehensive picture of materials. Nonetheless, early successes have demonstrated the potential of these methods to transform how materials are made, measured, and modeled.

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References

Abebe W, Strube J, Guo L, Tallent NR, Bel O, Spurgeon S, Doty C, Jannesari A. 2025. SAM-I-Am: Semantic boosting for zero-shot atomic-scale electron micrograph segmentation. Computational Materials Science 246:113400.

Abolhasani M, Kumacheva E. 2023. The rise of self-driving labs in chemical and materials sciences. Nature Synthesis 2(6):483–92.

Akers S, Kautz E, Trevino-Gavito A, Olszta M, Matthews BE, Wang L, Du Y, Spurgeon SR. 2021. Rapid and flexible segmentation of electron microscopy data using few-shot machine learning. npj Computational Materials 7(1):187.

Barakati K, Pratiush U, Houston AC, Duscher G, Kalinin SV. 2024. Unsupervised reward-driven image segmentation in automated scanning transmission electron microscopy experiments. arXiv preprint arXiv:2409.12462.

Bentley CL, Edmondson J, Meloni GN, Perry D, Shkirskiy V, Unwin PR. 2019. Nanoscale electrochemical mapping. Analytical Chemistry 91(1):84–108.

Chen P-C, Liu X, Hedrick JL, Xie Z, Wang S, Lin Q-Y, Hersam MC, Dravid VP, Mirkin CA. 2016. Polyelemental nanoparticle libraries. Science 352(6293):1565–69.

Chen P-C, Liu M, Du JS, Meckes B, Wang S, Lin H, Dravid VP, Wolverton C, Mirkin CA. 2019. Interface and heterostructure design in polyelemental nanoparticles. Science 363(6430):959–64.

Christopher J, Taleb M, Maity A, Hentschel M, Giessen H, Talebi N. 2020. Electron-driven photon sources for correlative electron-photon spectroscopy with electron microscopes. Nanophotonics 9(15):4381–406.

Colliex C, Kociak M, Stéphan O. 2016. Electron Energy Loss Spectroscopy imaging of surface plasmons at the nanometer scale. Ultramicroscopy 162:A1–A24.

Colón YJ, Snurr RQ. 2014. High-throughput computational screening of metal–organic frameworks. Chemical Society Reviews 43(16):5735–49.

Daglar H, Keskin S. 2020. Recent advances, opportunities, and challenges in high-throughput computational screening of MOFs for gas separations. Coordination Chemistry Reviews 422:213470.

Dyck O, Kim S, Kalinin SV, Jesse S. 2017. Placing single atoms in graphene with a scanning transmission electron microscope. Applied Physics Letters 111(11).

Dyck O, Kim S, Jimenez-Izal E, Alexandrova AN, Kalinin SV, Jesse S. 2018. Building structures atom by atom via electron beam manipulation. Small 14(38):1801771.

Egerton RF. 2011. Electron Energy-Loss Spectroscopy in the Electron Microscope, 3rd ed. Springer Science & Business Media.

El Kirat K, Burton I, Dupres V, Dufrêne Y. 2005. Sample preparation procedures for biological atomic force microscopy. Journal of Microscopy 218(3):199–207.

Epps RW, Abolhasani M. 2021. Modern nanoscience: Convergence of AI, robotics, and colloidal synthesis. Applied Physics Reviews 8(4).

Fiedler KR, Olszta MJ, Yano KH, Doty C, Hopkins D, Akers S, Spurgeon SR. 2023. Evaluating stage motion for automated electron microscopy. Microscopy and Microanalysis 29(6):1931–39.

Gewirth AA, Niece BK. 1997. Electrochemical applications of in situ scanning probe microscopy. Chemical Reviews 97(4):1129–62.

Ghomrasni NB, Chivas-Joly C, Devoille L, Hochepied J-F, Feltin N. 2020. Challenges in sample preparation for measuring nanoparticles size by scanning electron microscopy from suspensions, powder form and complex media. Powder Technology 359:226–37.

Greenaway R, Santolini V, Bennison M, Alston B, Pugh C, Little M, Miklitz M, Eden-Rump E, Clowes R, Shakil A, and 5 others. 2018. High-throughput discovery of organic cages

and catenanes using computational screening fused with robotic synthesis. Nature Communications 9(1):2849.

Hujsak K, Myers BD, Roth E, Li Y, Dravid VP. 2016. Suppressing electron exposure artifacts: An electron scanning paradigm with Bayesian machine learning. Microscopy and Microanalysis 22(4):778–88.

Hujsak KA, Roth EW, Kellogg W, Li Y, Dravid VP. 2018. High speed/low dose analytical electron microscopy with dynamic sampling. Micron 108:31–40.

Ievlev AV, Jesse S, Cochell TJ, Unocic RR, Protopopescu VA, Kalinin SV. 2015. Quantitative description of crystal nucleation and growth from in situ liquid scanning transmission electron microscopy. ACS Nano 9(12):11784–91.

Jesse S, He Q, Lupini AR, Leonard DN, Oxley MP, Ovchinnikov O, Unocic RR, Tselev A, Fuentes-Cabrera M, Sumpter BG, Pennycook SJ, Kalinin SV, Borisevich AY. 2015. Atomic-level sculpting of crystalline oxides: Toward bulk nanofabrication with single atomic plane precision. Small 11(44):5895–900.

Jiang Y, Salley D, Sharma A, Keenan G, Mullin M, Cronin L. 2022. An artificial intelligence enabled chemical synthesis robot for exploration and optimization of nanomaterials. Science Advances 8(40):eabo2626.

Jibril L, Cheng M, Wahl CB, Dravid VP, Mirkin CA. 2022. Polymer-mediated particle coarsening within hollow silica shell nanoreactors. Chemistry of Materials 34(11):5094–102.

Kalinin SV, Ophus C, Voyles PM, Erni R, Kepaptsoglou D, Grillo V, Lupini AR, Oxley MP, Schwenker E, Chan MK, and 6 others. 2022. Machine learning in scanning transmission electron microscopy. Nature Reviews Methods Primers 2(1):11.

Kalinin SV, Ziatdinov M, Ahmadi M, Ghosh A, Roccapriore K, Liu Y, Vasudevan RK. 2024. Designing workflows for materials characterization. Applied Physics Reviews 11(1).

Kluender EJ, Hedrick JL, Brown KA, Rao R, Meckes B, Du JS, Moreau LM, Maruyama B, Mirkin CA. 2019. Catalyst discovery through megalibraries of nanomaterials. Proceedings of the National Academy of Sciences 116(1):40–5.

Kociak M, Stéphan O, Gloter A, Zagonel LF, Tizei LH, Tencé M, March K, Blazit JD, Mahfoud Z, Losquin A. 2014. Seeing and measuring in colours: Electron microscopy and spectroscopies applied to nano-optics. Comptes Rendus Physique 15(2–3):158–75.

Kuk Y, Becker R, Silverman P, Kochanski G. 1991. Photovoltage on silicon surfaces measured by scanning tunneling microscopy. Journal of Vacuum Science & Technology B 9(2):545–50.

Lewis NR, Jin Y, Tang X, Shah V, Doty C, Matthews BE, Akers S, Spurgeon SR. 2022. Forecasting of in situ electron energy loss spectroscopy. npj Computational Materials 8(1):252.

Liu Y, Kelley KP, Vasudevan RK, Funakubo H, Ziatdinov MA, Kalinin SV. 2022. Experimental discovery of structure-property relationships in ferroelectric materials via active learning. Nature Machine Intelligence 4(4):341–50.

Liu Y, Yang J, Lawrie BJ, Kelley KP, Ziatdinov M, Kalinin SV, Ahmadi M. 2023. Disentangling electronic transport and hysteresis at individual grain boundaries in hybrid perovskites via automated scanning probe microscopy. ACS Nano 17(10):9647–57.

Manly CJ, Louise-May S, Hammer JD. 2001. The impact of informatics and computational chemistry on synthesis and screening. Drug Discovery Today 6(21):1101–10.

Markevich A, Kurasch S, Lehtinen O, Reimer O, Feng X, Mullen K, Turchanin A, Khlobystov AN, Kaiser U, Besley E. 2016. Electron beam controlled covalent attachment of small organic molecules to graphene. Nanoscale 8(5):2711–19.

Martin RM. 1972. Piezoelectricity. Physical Review B 5(4):1607.

Olszta M, Hopkins D, Fiedler KR, Oostrom M, Akers S, Spurgeon SR. 2022. An automated scanning transmission electron microscope guided by sparse data analytics. Microscopy and Microanalysis 28(5):1611–21.

Rajan K. 2008. Combinatorial materials sciences: Experimental strategies for accelerated knowledge discovery. Annual Review of Material Research 38(1):299–322.

Roccapriore KM, Boebinger MG, Dyck O, Ghosh A, Unocic RR, Kalinin SV, Ziatdinov M. 2022a. Probing electron beam induced transformations on a single-defect level via automated scanning transmission electron microscopy. ACS Nano 16(10):17116–127.

Roccapriore KM, Cho SH, Lupini AR, Milliron DJ, Kalinin SV. 2022b. Sculpting the plasmonic responses of nanoparticles by directed electron beam irradiation. Small 18(1):2105099.

Roccapriore KM, Kalinin SV, Ziatdinov M. 2022c. Physics discovery in nanoplasmonic systems via autonomous experiments in scanning transmission electron microscopy. Advanced Science (Weinheim) 9(36):e2203422.

Russell SJ, Norvig P. 2020. Artificial Intelligence: A Modern Approach. 4th edition. Pearson.

Smeaton MA, Abellan P, Spurgeon SR, Unocic RR, Jungjohann KL. 2024. Tutorial on in situ and operando (scanning) transmission electron microscopy for analysis of nanoscale structure–property relationships. ACS Nano 18(52):35091–103.

Soldatov MA, Butova VV, Pashkov D, Butakova MA, Medvedev PV, Chernov AV, Soldatov AV. 2021. Self-driving laboratories for development of new functional materials and optimizing known reactions. Nanomaterials 11(3):619.

Susi T, Meyer JC, Kotakoski J. 2017. Manipulating low-dimensional materials down to the level of single atoms with electron irradiation. Ultramicroscopy 180:163–72.

Szymanski NJ, Rendy B, Fei Y, Kumar RE, He T, Milsted D, McDermott MJ, Gallant M, Cubuk ED, Merchant A. 2023. An autonomous laboratory for the accelerated synthesis of novel materials. Nature 624(7990):86–91.

Takahashi Y, Kumatani A, Shiku H, Matsue T. 2017. Scanning probe microscopy for nanoscale electrochemical imaging. Analytical Chemistry 89(1):342–57.

Ter-Petrosyan A, Holden M, Bilbrey JA, Akers S, Doty C, Yano KH, Wang L, Paudel R, Lang E, Hattar K, and 5 others. 2024. Revealing the evolution of order in materials microstructures using multi-modal computer vision. arXiv preprint arXiv:2411.09896.

Thompson RF, Walker M, Siebert CA, Muench SP, Ranson NA. 2016. An introduction to sample preparation and imaging by cryo-electron microscopy for structural biology. Methods 100:3–15.

Valleti SMP, Zou Q, Xue R, Vlcek L, Ziatdinov M, Vasudevan R, Fu M, Yan J, Mandrus D, Gai Z, Kalinin SV. 2021. Bayesian learning of adatom interactions from atomically resolved imaging data. ACS Nano 15(6):9649–57.

Wahl CB, Mirkin CA, Dravid VP. 2023. Towards autonomous electron microscopy for high-throughput materials discovery. Microscopy and Microanalysis 29(Suppl 1):1913–14.

Weaver J, Wickramasinghe H. 1991. Semiconductor characterization by scanning force microscope surface photovoltage microscopy. Journal of Vacuum Science & Technology B 9(3):1562–65.

Where AI meets chemistry: accelerating materials innovation.

Frontiers in Polymer Materials, Sustainability, and AI/ML-Based Self-Driving Laboratories (SDLs)

Rigoberto Advincula

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The ability to conduct empirical experiments or process optimization guided by the scientific method (hypothesis-driven) is the driving force behind advances in science and engineering. Experiments that test theories and simulations serve as a reality check, enabling the discovery of new phenomena or efficiencies that lead to widely adopted industrial technologies. As Max Planck is famously quoted as saying,

> "Experiment is the only means of knowledge at our disposal. Everything else is poetry, imagination."

A future has just arrived—an intelligent operating system for conducting experiments, embodied by an automated laboratory-operated robot and controlled by computers that autonomously set or reset experimental parameters—essentially, a 24/7 assistant that never sleeps. This assistant continuously analyzes vast amounts of data, identifies gaps in the experiment or process, sends instructions for recalculation or new simulation, and resets the experimental setup for the next phase. This represents the future of self-driving laboratories (SDLs), driven by artificial intelligence and machine learning (AI/ML) in the fields of chemistry and materials science (Abolhasani and Kumacheva 2023; Tom et al. 2024). They are poised to facilitate new scientific discover-

ies, optimize process engineering, and rapidly accelerate research and development (R&D) for manufacturing.

In the context of materials, specifically polymer materials, this assistant could identify and discover new polymers with optimized properties for various applications. It could also design new synthesis routes, predict thermo-mechanical properties and degradation, and develop strategies for sustainability and recyclability. It may even predict project costs and environmental impacts, going beyond the current capabilities of life cycle analysis and technoeconomic analysis methods. Moreover, it can recalculate these in real time as new information or experimental pathways emerge.

Will this be possible for today's polymer science and engineering? Can we solve the plastic conundrum? This article explores the potential of AI/ML to drive innovation in polymer materials and examines the role of SDLs in addressing challenges in polymer science and engineering.

Polymer Materials in Society

Polymer materials play a crucial role in many aspects of society and daily life. Plastics are ubiquitous, and we accept them as an integral part of everyday living. By definition, polymer materials consist of large molecules, or macromolecules, and therefore naturally have high molecular weight (MW). They are composed of monomers, repeating structural units connected in linear, branched, or architected configurations. Their distribution, or polydispersity, is a key feature that determines their processability. From semi-crystallinity to optical and dielectric properties, polymers offer advantages that enable them to replace steel, glass, and ceramics in various applications, particularly when the proper weight-to-strength ratio is achieved.

However, future research and innovation focus on understanding field effects in macromolecular synthesis, novel depolymerization or dynamic bonding rearrangements, and new structure–composition–property relationships in polymers. An emphasis on materials physics, architected microstructures, and advanced processing techniques, such as additive manufacturing (AM), requires new creative tools that can be enhanced with AI/ML tools (Advincula et al. 2025; Chen et al. 2025). Similar trends will emerge in more ML-driven analytical and characterization of advanced polymer materials.

It is intriguing to consider whether many Nobel Prizes related to polymer chemistry and physics—such as those awarded to Staudinger, Ziegler and Natta, Flory, Merrifield, De Gennes, Heeger, MacDiarmid, Grubbs, Lehn, Stoddart, and others (Nobel Prize Organisation n.d.; Seymour et al. 1989)—might have been awarded earlier had AI/ML and SDLs been available to them. At the same time, the knowledge from their contributions serves as a foundation for future work using these new tools. Breakthroughs in polymers have led to advances in catalysis and manufacturing, lighter-weight vehicles with plastic parts, electrically conducting polymers and devices, liquid crystal displays, the total synthesis of biopolymer-based drugs, improvements in biomedical devices, and high-performance composites.

Polymer materials play a crucial role in many aspects of society and daily life.

Polymer Synthesis Tied to Properties

It is helpful to categorize polymer synthesis and mechanisms into broad classes: step-growth and chain-growth reaction mechanisms (Lodge and Hiemenz 2020; Saldívar-Guerra and Vivaldo-Lima 2013). The use of a catalyst refers to agents, such as organometallic compounds or enzymes, that broadly accelerate and mediate the reaction process. The most common commodity plastics, such as polyethylene, polypropylene, polystyrene, polybutadiene, and ABS, are made through chain-addition reaction mechanisms. Popular polymers, such as polyesters, nylons, and polycarbonates, are produced through step-growth polymerization mechanisms; however, some can also be synthesized using ring-opening addition methods. They are distinguished by their MW, polydispersity, living or nonliving mechanisms, and the use of media (solutions or dispersions) and bulk polymerization methods.

Polymers are not limited to linear structures, though; they can also be synthesized as grafts, blocks, hyperbranched structures, or even controlled microstructures. Copolymers are formed from two or more monomer compositions that can be connected in statistical, alternating, or block arrangements, and their structures can be predicted using the Mayo–Lewis equation. Overall, nanophase, mesophase, and microphase behaviors contribute to the observed macroscopic properties.

Lastly, polymers can also be categorized as thermosets or elastomers, based on their degree of crosslinking and distinct thermo-mechanical properties (brittle but tough, or rubbery). Popular thermosets include epoxy, vinyl esters, phenolic resins (also known as phenol-formaldehyde), and polyurethane. Representative elastomers include natural rubber, silicone, thermoplastic polyurethane, and other synthetic rubbers.

Polymers, Plastics, and Recycling

Most polymer products are formulated with additives to optimize their properties for processing and specific applications. For polymers, the term "plastic" is more commonly used, and resins, epoxies, paints, adhesives, and films are also identified as standard formulations with a majority polymer composition. Formulation is a crucial process in the polymer conversion industry. The versatile properties, cost-effectiveness, and applicability of polymers across sectors—including packaging, medical supplies, coatings, military, automotive, aerospace, semiconductors, and building construction—underscore their importance and the performance of the final products.

The development of smart and innovative functional polymers will open new opportunities in coatings, smart packaging, electronics, sensors, medical devices, and drug delivery systems.

The term "recycling" is now primarily associated with plastic-related activities (Collias and Layman 2021). Yet, less than 10% of plastics are ever recycled, with the rest returning to the environment or being incinerated, often in their original state and potentially in a non-degradable form. Is it possible to convert our major classes of plastics into sustainable and even upcycled polymer materials?

Typically, plastics are sourced from petroleum-based feedstocks. However, natural polymers and biopolymers constitute the majority of biomass (cellulose or non-cellulose) from plants, trees, and agriculture (Das et al. 2023). There are many types of biodegradable polymer materials, including polylactide, polyhydroxyalkanoates, and other lactic acid copolymers, as well as natural or synthetic polybutadienes, which can be classified as part of the biobased feedstock category. The term "bioplastics," or sometimes biodegradable polymers, is often associated with these classes.

These polymers also constitute living matter, including polysaccharides, polynucleotides, and polypeptides. Their self-assembly, or intelligent assembly, facilitated by enzymes and DNA, enables them to function correctly within living systems. Polymers are also referred to as soft matter (van Saarloos et al. 2024), a subset of condensed matter that focuses on the physics and phenomena of such systems, including biological ones. Thus, they are not only essential for life but also serve as critical materials for many industries.

The development of smart and innovative functional polymers will open new opportunities in coatings, smart packaging, electronics, sensors, medical devices, and drug delivery systems. Smart polymers can be stimuli-responsive to various triggers, including pH, light, temperature, chemicals, and electric fields, leading to applications such as smart textiles and wearables, autonomous self-healing materials, and novel drug-releasing polymer excipients or implants. Additive manufacturing, better known as 3D printing, has advanced beyond rapid prototyping into limited production. Combining AM with stimuli-responsive polymers gives rise to a new concept known as "4D printing." By enabling economic production and greater design freedom, these polymers can become part of specialty polymer or product lines in any primary polymer manufacturing industry.

The New AI/ML-Driven Research and Optimization Tools in SDLs

Is there a role for AI/ML and SDLs in the future of polymer materials? More interestingly, will the polymer scientist or engineer continue to be essential in driving polymer innovation and sustainability? Is the "scientist-in-the-loop" still critical in the laboratory of the future? The automated research laboratory will combine mechatronics, simulation, robotics, and data analysis to accelerate research and discovery. The combination of AI/ML with SDLs can automate the design, architecture, formulation, execution, and analysis of experiments, leading to more efficient polymer materials research and development (Beaucage et al. 2024) (Figure 1). For now, the answer should be "yes": we still need the human-in-the-loop to utilize this tool.

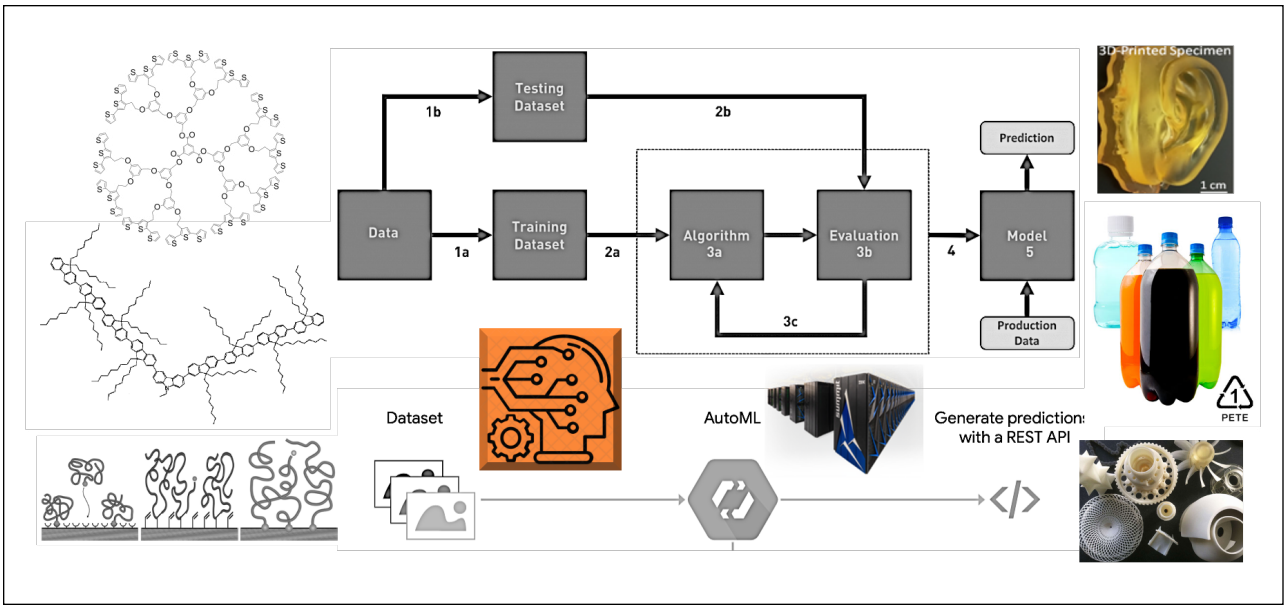

FIGURE 1 The steps leading from macromolecule discovery workflows to AI/ML-optimized polymers and products.

Simulation and Theory Lead the Way

To start, simulation and theoretical predictions can be more directly linked with an automated laboratory (Gartner and Jayaraman 2019). Quantum chemical calculations, ranging from atomistic to coarse-grained methods, including molecular dynamics (MD), are crucial for predicting bond connectivities and reaction pathways. The use of density functional theory (DFT) is key to achieving optimal reactivity. Simulating pseudo-chiral and conformational properties is essential for understanding multiphase behavior beyond MD.

For practical correlation of the effects of MW or polydispersity, it is necessary to refine assumptions based on self-consistent field theories. In linking mesoscopic to macroscopic properties, finite element analysis and multi-physics simulations stand out as predictive tools for the desired processing methods and functional properties. Creating these digital twins ensures that algorithm development and experimental work are fundamentally grounded in reality. These simulation tools are essential for guiding the execution of real-time experiments and dynamically adjusting reaction parameters to optimize, for example, synthesis conditions.

The generation of hypotheses begins with molecular bonding and macromolecular-driven paradigms, based on bond reactivity, reactivity ratios (for copolymers), and conformational and configurational considerations, including Kuhn and segment lengths (Rubinstein and Colby 2003). In this way, predictive modeling can be employed, where ML models analyze polymer structures and properties to predict new microstructures and their corresponding characteristics. For blends, formulations, chi-interactions, and solubility parameters are essential. A data-driven design will utilize new generative AI algorithms to uncover novel relationships between polymer characteristics and performance. Lastly, the goal could be the optimization of existing synthesis routes, reaction conditions, and catalysis to reduce the number of variables and enable a more straightforward scale-up of manufacturing processes. Specific examples of hypothesis-driven research leading the way in simulation and algorithm development include copolymerization (Kuenneth et al. 2021), catalytic olefin polymerization (Vittoria et al. 2022), and the design of polymer blend electrolytes (Wheatle et al. 2020). A key future direction is the application of agentic AI (AI capable of goal-driven actions and independent decision making) and multi-agent AI with graph reasoning for generating new research directions and paths to discovery (Ghafarollahi and Buehler 2024).

Codes and LLMs Enable Faster Data Analytics

Recently, efforts have been made to provide codes and molecular labeling of polymer materials that incorporate

the polymer's structure and, potentially, its function or properties. These methods for labeling polymer materials or coding will enable tracing based on structure, composition, sequencing, and function, which can significantly aid in accelerating simulation and data curation. The Simplified Molecular Input Line Entry System (SMILES) is an example. SMILES provides a specification in the form of line notation with short ASCII strings, representing entries in polymer databases that can be used as indexing identifiers (Lin et al. 2019). This refinement essentially serves as a more effective reference language. It can even be implemented in large language models (LLMs) with the development of more efficient Retrieval Augmented Generation (RAG) systems. For polymers, this involves indexing, retrieval, and generation. The LLM can use this "augmentation" to generate more precise and cited responses, rather than relying solely on general training data. First, the polymer data is processed and converted into a searchable format using numerical vectors, and then stored in a vector database. To retrieve information, a user submits a query, and the system searches the vector database to find the most relevant results. The retrieved data is then incorporated into the prompt sent to the LLM (Yu et al. 2024).

An open AI platform such as ChatGPT could be particularly useful for polymer scientists and engineers. Such a platform could lead to more efficient data analytics for potential synthesis routes, characterization, and forensic analysis of failures. It could also allow for faster design and modification of new, functional, and biodegradable polymeric materials for advanced applications.

Engineering the Science of Polymers from Statistics to Digital Twins

In chemical engineering, ML is a subset that, when applied, enables feedback-loop methods for optimizing process or reaction yields. It allows computers to learn from data and refine predictions without explicit reprogramming. Process modeling based on grounded thermodynamic and kinetic principles includes mass transport and diffusion conditions. Often overlooked in continuous flow processing, such as in solution or melt, is treating these fluids as complex systems that can be modeled using statistical mechanics. In process optimization, parameters such as pressure, temperature, volume, flow rate, and dosing compositions must be controlled to achieve higher yields. By applying statistical or matrix process optimization methods, careful algorithm development can reduce the number of experiments and focus on more critical parameters beyond those addressed by principal component analysis. For example, a 60% reduction in the number of experiments while achieving a 90% reaction yield can be a game-changer for streamlining process development.

Typically, experimental work relies heavily on expert intuition and even trial-and-error methods. This approach can be wasteful, however, and may be a poor economic driver for product launches. A data-driven approach to R&D experimentation, from start to finish, is required, grounded in predictive modeling and macromolecular information. Bayesian optimization platforms, combined with chemical descriptor databases, can bring reaction models closer to alignment with real-world chemistry and process engineering.

Statistics Is Key to the Design of Experiments

Statistical methods are fundamental to ML approaches (Bzdok et al. 2018). They provide tools to analyze data, build models, and evaluate their performance in experiments. Several key statistical concepts, including regression analysis, probability distributions, hypothesis testing, and clustering, can be more effectively applied in the design of experiments for polymer research. These methods facilitate the understanding of data, the identification of patterns, and the making of predictions.

Beyond statistical methods, several ML-directed algorithms include regression analysis, decision trees, random forests, Bayesian optimization, and neural networks. By understanding the different types of ML algorithms (supervised or unsupervised learning) and their respective strengths, polymer scientists and engineers can make more informed decisions about which algorithm is best suited for a particular task and apply it in scientific experiments or process optimization. Unfortunately, statistics is not as widely emphasized in STEM education as a foundation for sound decision making in designing and planning experiments.

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Digital Twins and Neural Networks

An optimized system, built on carefully simulated digital twins, could, in the future, adapt or reconfigure the simu-

lation by learning from real-time experimental feedback. This would iteratively refine reaction conditions to minimize material waste (or the number of experiments) and enhance polymer properties in real time. It could also accelerate discovery cycles by incorporating more generative AI or deep learning (DL) methods.

DL relies on neural networks, mathematical models inspired by the brain's psychological functions. These artificial neural networks consist of layers of interconnected neurons that process and learn from data. The input layer receives raw data, which is then processed through hidden layers where patterns are identified before reaching the output layer and subsequently generates predictions or classifications. Convolutional neural networks are primarily used in image processing, detecting spatial hierarchies of patterns, and performing best with GPU support. Recurrent neural networks are well suited for handling sequential data, making them ideal for time-series analysis and language modeling. Deep neural networks with multiple hidden layers are used for highly complex, nonlinear problems. Given the complexity of polymer synthesis, characterization, and property prediction, DL will become increasingly integrated into polymer informatics, characterization, and experimental workflows to enhance efficiency and accuracy.

Building an Autonomous-ML Research Using an SDL with Flow Chemistry

For an SDL, other tasks such as the use of alternative reagents, storage, improved quality control, and data analytics can make experiments more seamless and faster. This operational system for an ML-driven experimental setup is best implemented with an automated, continuous-flow chemistry or reactor setup at the bench scale (Knox et al. 2025; Pittaway et al. 2025; Sumpter et al. 2023) (Figure 2). This is where most polymer chemists can work on different algorithms, test mechanistic hypotheses, demonstrate controlled kinetics, and enable plug flow (for solutions) and packed-bed (for heterogeneous catalyst supports) columns, all conducted under chemical engineering operation parameters.

Building an SDL Requires a Team and Automation Technology

Building a bench-scale setup requires skills in chemistry, chemical engineering, mechatronics, robotics, applied computing or programming, and device interfacing. By controlling flow rate (mass transport), reaction space engineering, leveraging microfluidics or microreactors, and regulating pressure, volume, and temperature per unit operation in time and space series, it is possible to leverage AI/ML-optimized protocols. By building moni-

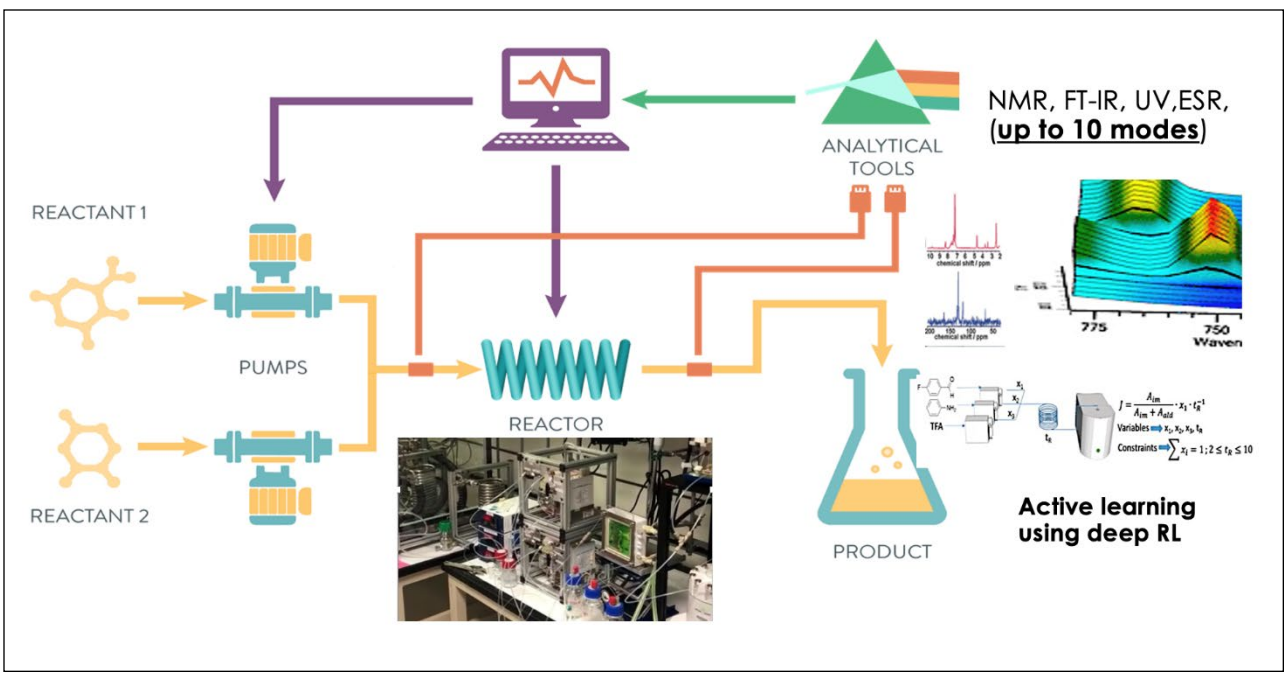

FIGURE 2 A bench-scale AI/AI-driven reaction setup as part of an SDL facility. Such facilities can produce a significant amount of data for polymer science.

toring stations or employing analytical and characterization methods under flow and in situ (e.g., online NMR, IR, Raman, UV-vis, ESR), data can be collected from multiple viewpoints in real time. The key to control is an edge server or computer that can both manage and process data gathered from monitoring stations and sensors. A feedback loop mechanism can integrate decision making and set or reset points. This edge server, when connected to high-performance computing platforms and potentially exascale supercomputers, enables the recreation of digital twins in real time. Cloud data storage is crucial in such circumstances for collecting and archiving the large amounts of data expected from this bench-scale chemistry operation.

This approach is not only a vision for polymer chemistry but is also becoming increasingly advanced in the pharmaceutical and drug discovery industries. If fully implemented, it represents an auto-ML-driven discovery and research operation platform that will accelerate polymer science and engineering. By coupling robotics, programmable mechatronics, and additive manufacturing, this system offers a valuable platform for both academic and industrial research communities. We have been leading efforts in AI/ML-driven SDL development for polymers at Oak Ridge National Laboratory (ORNL 2025) and are part of the lead project with the INTERSECT initiative. Many other national laboratories and academic institutions are also pursuing similar efforts in materials research (Ferreira Da Silva et al. 2024).

Challenges remain in integrating SDLs into materials and polymer research laboratories. These include

- lack of standards and integration of instruments with different application programming interfaces (APIs) and their ability to communicate with a standard operating system and edge server;
- real-time measurements and instrumentation that are closer to the chemistry of chemical intermediates or transition states for kinetic and thermodynamic control;
- hypothesis development to help researchers appreciate simulation methods and the hierarchy that relates them to real or multiphase environments, beyond vacuum or homogeneous conditions; and
- costs of scaling SDLs for manufacturing compared with laboratory bench-scale setups.

The last of these may be the most immediate to overcome if SDLs are to be more widely utilized for materials and polymer research. Recently, some articles have emphasized user-automation infrastructures (Pelkie et al. 2025) and the democratization of SDLs through decentralization (Bayley et al. 2024). Another recent paper focused on the use of low-cost 3D printing for laboratory automation, integrated with ML and AI algorithms to enable flexible and affordable SDLs (Doloi et al. 2025).

Replicating an Expert Polymer Scientist Is Still No Easy Task

An AI-driven SDL will be required for seamless integration of AI, automation, and laboratory workflows in polymer science and engineering, extending beyond current human capabilities and addressing the immense combinatorial complexity in polymers. The use of both ML and DL will unlock new possibilities by predicting material properties, designing novel polymers, and optimizing synthesis conditions with high efficiency. It will also accelerate formulation development with additives and optimize processes for cost-effective manufacturing. Specifically, Reinforcement Learning (RL), a distinct type of ML in which models learn by interacting with an environment and receiving rewards for taking optimal actions, will be essential. RL algorithms can be complex and are designed to discover optimal strategies, making them particularly suited for decision making. They can be powerful tools for optimizing polymerization processes and autonomous experimental control, bringing SDLs closer to duplicating human heuristics and scientific expertise.

It is time to rethink training and education for future polymer scientists and engineers. Many researchers, while intrigued by AI's potential, are overwhelmed by its complexity due to a lack of training and experience.

One immediate step is implementing more agentic AI in SDLs. This can enhance the pace of scientific discovery by automating repetitive, time-consuming tasks. It is not necessary to automate the entire research or discovery process; instead, embedding more agentic and proactive AI can lead to faster decision making and automation of tasks. Examples include scripting peak analysis of spectra in real time, real-time optimization using specific algorithms, and independent command-control protocols on instrumentation (Flores-Leonar et al. 2020). By embedding agentic AI protocols, researchers will have more opportunities to focus on creative ideation and experimental planning, potentially reducing the costs associated with automation. Agentic AI can also be applied in experiment design, data analysis, and even report generation (Gridach et al. 2025).

The goal, however, is not to replace humans in the lab but to assist them in accomplishing tasks and connect them with expertise. Will SDLs displace jobs for polymer scientists and engineers? Perhaps, but learning to utilize AI/ML tools and maintaining a high level of skill and experience will remain indispensable. Ultimately, the "expert-in-the-loop" and human judgment will be difficult to replicate.

Going Back to the Plastics Economy

In our current linear plastic economy, we are burdened with the dual task of cleanup and transitioning to a more circular economy (DOE 2023). A key objective for more ML-driven R&D and the use of SDLs is to capitalize on opportunities for sustainable polymer synthesis, enabling the production of chemical intermediates and monomers through optimized bio-refineries and harnessing the potential of enzyme catalysis in polymer synthesis. The use of renewable resources, such as biomass, agro-waste, or even CO_2 as part of the upstream raw materials has gained traction (Sun and Wang 2024). One possibility is to utilize AI/ML in designing pathways for polymer construction and deconstruction, with an emphasis on chemical upcycling (Figure 3). Mixed plastics can be converted to key oligomeric intermediates and incorporate

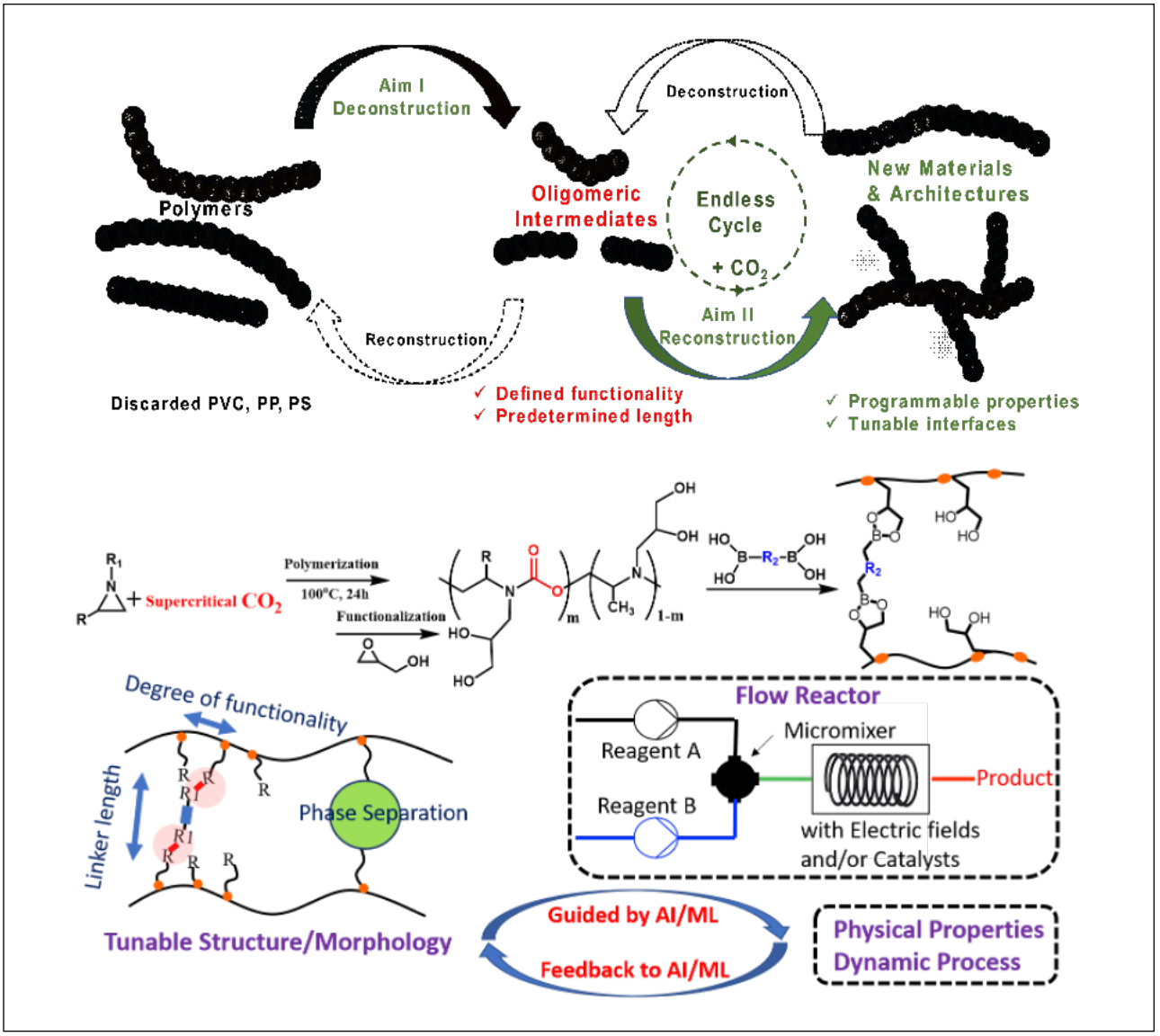

FIGURE 3 A path to chemical upcycling of plastics through construction–deconstruction synthesis and using CO_2 as a key intermediate with vitrimeric properties. This can be done with an AI/ML-driven SDL set-up guided by simulation and digital twins.

CO_2 as a key monomer, resulting in a polymer that may also be vitrimeric in nature and reformed with dynamic bonds. Controlling phase separation and bond reformation can yield new recyclable attributes and improved thermo-mechanical properties.

AI will fundamentally transform how polymer research is conducted, shifting from empirical iteration to data-driven hypothesis generation and informed decision making.

It remains essential, however, to develop new chemistry and processing methods that are designed from the outset (polymer genome) to achieve higher performance and upcycling potential. If pursued with the tools of AI/ML and SDL, this approach offers the possibility to mitigate some of the irreversible damage to the environment and food chain (e.g., microplastics). Reducing packaging waste and single-use plastics may be achieved by redesigning the life cycle of polymer materials. Looking ahead, it will be essential to strive for multiple uses of polymeric materials—from design and production to consumption, repair, reuse, and recycling. Encouragingly, numerous programs and projects are already underway in institutions and national laboratories across the United States, Europe, and Asia, with clear goals for both the upstream and downstream aspects of the plastics economy.

Final Observations

In conclusion, AI/ML-driven SDLs can significantly accelerate the discovery of new polymer materials and enhance process and formulation optimization. The convergence of AI and polymer science will unlock new possibilities, from predictive modeling to autonomous research workflows. As AI-driven methodologies mature, the next frontier will not only involve discovering novel macromolecules but also designing the algorithms that enable their discovery—generative AI. Moving forward, RL is expected to play a larger role in self-optimizing polymerization processes and unraveling complex composition–processing–property relationships. Rather than simply accelerating workflows, AI will fundamentally transform how polymer research is conducted, shifting from empirical iteration to data-driven hypothesis generation and informed decision making.

SDLs will be essential tools in this transformation. With advances in robotic synthesis, in situ characterization, and self-learning models, these labs will accelerate research in real time, dynamically adjusting synthesis conditions to optimize properties with minimal human intervention. This shift will redefine the role of polymer scientists, moving from experiment control to precision-driven material design and intervention. By reducing experimental time, SDLs can enable the simultaneous and continuous execution of multiple experiments, facilitating the solution of complex problems. Optimizing experimental parameters with digital twins and AI/ML algorithms can help identify the optimal conditions for achieving desired material properties. And LLMs with RAGs can accelerate the identification of valuable training data and experimental protocols, enabling the exploration of vast chemical and macromolecular spaces to determine the most efficient synthesis routes and processing or recycling strategies. The time has come to deploy more AI/ML tools, agentic AI, and SDLs in polymer science and engineering.

References

Abolhasani M, Kumacheva E. 2023. The rise of self-driving labs in chemical and materials sciences. Nature Synthesis 2:483–92.

Advincula R, Yuan Y, Wang H, Wang Q, Chen J. 2025. Bridging additive manufacturing and electronics printing in the age of AI. Nanomaterials 15(11):843.

Bayley O, Savino E, Slattery A, Noel T. 2024. Autonomous chemistry: Navigating self-driving labs in chemical and material sciences. Matter 7:2382–98.

Beaucage P, Sutherland D, Martin T. 2024. Automation and machine learning for accelerated polymer characterization and development: Past, potential, and a path forward. Macromolecules 57(18):8661–70.

Bzdok D, Altman N, Krzywinski M. 2018. Statistics versus machine learning. Nature Methods 15:233–34.

Chen J, Yuan Y, Ziabari AK, Xu X, Zhang H, Christakopoulos P, Bonnesen PV, Ivanov IN, Ganesh P, Wang C, Jaimes KP. 2024. AI for manufacturing and healthcare: A chemistry and engineering perspective. arXiv arXiv:2405.01520.

Collias D, James M, Layman J. 2021. Circular Economy of Polymers: Topics in Recycling Technologies. Washington, DC: American Chemical Society; ACS Publications.

Das A, Ringu T, Ghosh S, Pramanik N 2023. A comprehensive review on recent advances in preparation, physicochemical characterization, and bioengineering applications of biopolymers. Polymer Bulletin 80(7):7247–312.

DOE [Department of Energy]. 2023. Strategy for Plastics Innovation. Online at https://www.energy.gov/sites/default/files/2023-01/DOE-strat-for-plastics-innova_1-19-23.pdf.

Doloi S, Das M, Li Y, Cho ZH, Xiao X, Hanna JV, Osvaldo M, Tat LN. 2025. Democratizing self-driving labs: Advances in low-cost 3D printing for laboratory automation. Digital Discovery 4(7):1685–721.

Ferreira Da Silva R, Moore R, Mintz B, Advincula R, Al Najjar L, and 27 others. 2024. Shaping the Future of Self-Driving Autonomous Laboratories Workshop. Technical Report, ORNL/TM-2024/3714. Online at https://www.osti.gov/servlets/purl/2481197.

Flores-Leonar MM, Mejía-Mendoza LM, Aguilar-Granda A, Sanchez-Lengeling B, Tribukait H, Amador-Bedolla C, Aspuru-Guzik A. 2020. Materials acceleration platforms: On the way to autonomous experimentation. Current Opinion in Green and Sustainable Chemistry 25:100370.

Gartner T, Jayaraman A. 2019. Modeling and simulations of polymers: a roadmap. Macromolecules 52(3):755–86.

Ghafarollahi A, Buehler M. 2025. SciAgents: Automating scientific discovery through bioinspired multi-agent intelligent graph reasoning. Advanced Materials 37(22):2413523.

Gridach M, Nanavati J, El Abidine K, Mendes L, Mack C. 2025. Agentic AI for scientific discovery: A survey of progress, challenges, and future directions. arXiv. arXiv:2503.08979.

Knox ST, Wu KE, Islam N, O'Connell R, Pittaway PM, Chingono KE, Oyekan J, Panoutsos G, Chamberlain TW, Bourne RA, Warren NJ. 2025. Self-driving laboratory platform for many-objective self-optimisation of polymer nanoparticle synthesis with cloud-integrated machine learning and orthogonal online analytics. Polymer Chemistry 16(12):1355–64.

Kuenneth C, Schertzer W, Ramprasad R. 2021. Copolymer informatics with multitask deep neural networks. Macromolecules 54(13):5957–61.

Lin T, Coley C, Mochigase H, Beech H, Wang, W, Wand Z, Woods E, Craig S, Johnson J, Kalow J, Jensen K, Olsen B. 2019. BigSMILES: A structurally-based line notation for describing macromolecules. ACS Central Science 5(9):1523–31.

Lodge T, Hiemenz P. 2020. Polymer Chemistry (3rd ed.). CRC Press.

Nobel Prize Organisation. n.d. All Nobel Prizes. Online at https://www.nobelprize.org/prizes/lists/all-nobel-prizes.

ORNL (Oak Ridge National Laboratory). 2025. Creating the laboratory of the future. Online at https://www.ornl.gov/file/labs-future/display.

Pelkie B, Baird S, Aissi E, Aspuru-Takata K, Cao Y, and 22 others. 2025. Democratizing self-driving labs through user-developed automation infrastructure. Working Paper, Version 1. ChemRxiv 1–18.

Pittaway PM, Knox ST, Cayre OJ, Kapur N, Golden L, Drillieres S, Warren NJ. 2025. Self-driving laboratory for emulsion polymerization. Chemical Engineering Journal 507:160700.

Rubinstein M, Colby R. 2003. Polymer Physics. Oxford University Press. Online at https://doi.org/10.1093/oso/9780198520597.001.0001.

Saldívar-Guerra E, Vivaldo-Lima E. 2013. Handbook of Polymer Synthesis, Characterization, and Processing. John Wiley & Sons.

Seymour R, Mark H, Pauling L, Fisher C, Stahl A, Sperling L, Marvel C, Carraher C. 1989. Pioneers in Polymer Science. Springer Science & Business Media.

Sumpter B, Hong K, Vasudevan R, Ivanov I, Advincula R. 2023. Autonomous continuous flow reactor synthesis for scalable atom-precision. Carbon Trends 10:100234.

Sun C, Wang Y. 2024. Catalytic upcycling plastics with CO_2: A novel strategy for carbon waste valorization. Chem Catalysis 4(3):100934.

Tom G, Schmid SP, Baird SG, Cao Y, Darvish K, Hao H, Lo S, Pablo-García S, Rajaonson EM, Skreta M, Yoshikawa N. 2024. Self-driving laboratories for chemistry and materials science. Chemical Reviews 124(16):9633–732.

van Saarloos W, Vitelli V, Zeravcic Z. 2024. Soft Matter: Concepts, Phenomena, and Applications. Online at https://softmatterbook.online.

Vittoria A, Urciuoli G, Costanzo S, Tammaro D, Cannavacciuolo FD, Pasquino R, Cipullo R, Auriemma F, Grizzuti N, Maffettone PL, Busico V. 2022. Extending the high-throughput experimentation (HTE) approach to catalytic olefin polymerizations: From catalysts to materials. Macromolecules 55(12):5017–26.

Wheatle B, Fuentes E, Lynd N, Ganesan V. 2020. Design of polymer blend electrolytes through a machine learning approach. Macromolecules 53(21):9449–59.

Yu S, Ran N, Liu J. 2024. Large-language models: The game-changers for materials science research. Artificial Intelligence Chemistry 2(2):100076.

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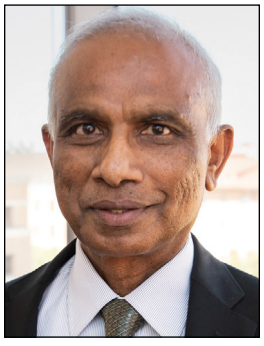

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Energy storage with batteries has become an integral part of our daily life, ranging from portable electronics, such as cellphones and laptops, to electric vehicles (EVs). They have the potential to transform grid storage of electricity as well. Batteries also play a critical role in national defense, ranging from soldier power to communication devices to vehicles. The global lithium-ion battery market was projected to be valued at around $60 billion USD in 2024 and to reach ~$182 billion in 2030 (The Research Insights 2025).

For a battery technology to be widely adopted, several critical parameters need to be considered: cost ($ kW^{-1} h^{-1}), energy density (W h kg^{-1} or W h L^{-1}), power density (W kg^{-1} or W L^{-1}), charge–discharge cycle life, safety, and environmental (toxicity) impact. These parameters are linked to severe materials challenges (Figure 1). The dominant factors that need to be considered depend on the application. For instance, for portable electronics, user time between charges (energy density) is dominant because these batteries are small and cost is not an impediment. For EVs, driving range (energy density), cost, safety, cycle life, and fast charge (power density) are all critical factors, generally decreasing in priority as battery size increases. And for grid-scale storage, the

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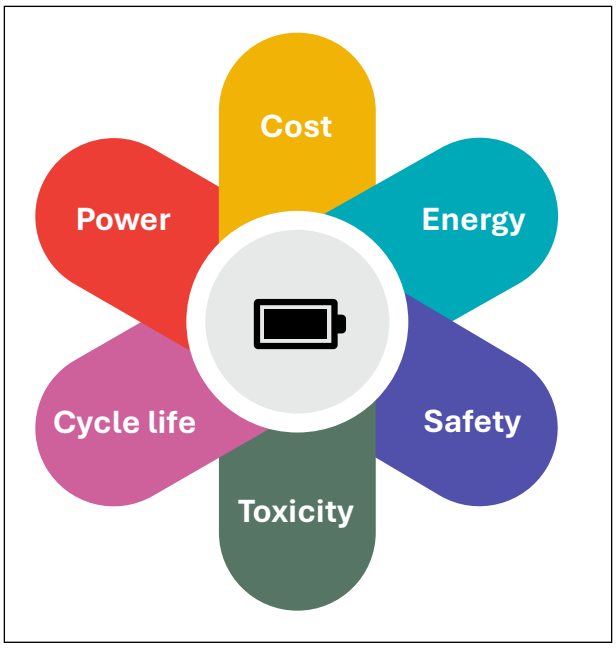

FIGURE 1 Key performance parameters that need to be considered for battery technology.

dominant considerations are cost, reliability (cycle life), and safety, given the large size of the batteries.

The Cost and Supply-Chain Challenge

The battery market is dominated by lithium-ion batteries due to their high energy density and long shelf-life. However, they employ expensive metals like cobalt, nickel, and lithium that are naturally scarce. As the battery industry rapidly expands for transportation and grid storage applications, cost—while ensuring adequate safety—will remain the dominant concern. Raw materials availability, their processing, and cell manufacturing all contribute to cost. Other performance factors such as cycle life (durability) and safety also impact the cost. A battery with a long cycle life requires fewer replacements, lowering overall costs; similarly, strong safety performance simplifies operation and management, further reducing costs.

Battery raw materials abundance and origin also impact the supply chain, national security, and national economy for the United States. For example, cobalt—which still dominates portable electronics batteries—is a critical metal that is mined largely in the Democratic Republic of Congo in Central Africa where child labor presents ethical issues. Lithium mining in South America poses environmental hazards and social concerns. Factors such as these can pose supply-chain challenges to the United States.

Therefore, it is imperative for the scientific community and industry to explore and develop affordable, supply-chain-friendly battery chemistries and materials with adequate safety—particularly for EVs and grid storage—in order to relieve the United States and society in general from its dependence on critical materials like cobalt, nickel, and lithium. Artificial intelligence (AI) can play a role in this regard if appropriately integrated with physical intuition and scientific curiosity. Accordingly, this article first gives an overview of how we arrived at where we are now with battery technologies, reviewing the scientific and engineering innovations that have occurred over the past half century. Then, it focuses on how the power of AI could help accelerate the discovery of new materials and battery chemistries, highlighting the recent developments and accomplishments with AI.

Energy storage with batteries has become an integral part of our daily life, ranging from portable electronics, such as cellphones and laptops, to electric vehicles.

How Did We Get to Where We Are Now?

Lithium-ion batteries operate on intercalation chemistry, in which lithium ions are reversibly inserted into and extracted from the anode (negative electrode) and cathode (positive electrode). The anode and cathode are separated by an electronically insulating but ionically conducting electrolyte, which transports lithium ions (the working ion) between the electrodes to maintain charge neutrality, while electrons flow through the external circuit to perform useful work. Both the anode and cathode should ideally be good electronic and lithium-ion conductors to transport electrons and working ions and support acceptable charge–discharge rates and power density. The anode should have high negative electrochemical reduction potential while the cathode should have high positive electrochemical reduction potential to maximize the operating cell voltage. In addition, both the anode and cathode should facilitate a large degree of reversible

lithium intercalation/deintercalation to maximize the amount of charge stored (cell capacity).

The product of cell voltage and capacity determines energy density. The reversibility of the two electrodes over many charge–discharge cycles along with their interfacial stability in contact with the electrolyte determines the cell cycle life and durability. Issues like metallic dendrite formation, internal short circuits, cell swelling, and gas evolution as the cell cycles, along with electrolyte flammability, can degrade cell safety. Toxicity associated with the materials, processing, and manufacturing determines the environmental (including human health) impact. These factors and the costs associated with them highlight the significant challenges inherent in materials design, development, and implementation.

Although intercalation chemistry of ions or guest molecules into solid hosts was known for close to two centuries, Stanley Whittingham was the first to demonstrate a rechargeable lithium battery in 1976, employing lithium metal as an anode and titanium disulfide (TiS_2) with a layered crystal structure as a cathode (Whittingham 1976). Direct metal-metal (Ti-Ti) interaction and the two-dimensional layered structure supported good lithium-ion conductivity. Following the demonstration with TiS_2, several layered sulfides and selenides were investigated as cathodes, and rechargeable lithium batteries with metallic lithium anode and a sulfide cathode began being marketed in the 1980s. Unfortunately, dendrite growth with lithium metal and internal short-circuit led to fire hazards, resulting in an abandoning of the technology.

John Goodenough, drawing on over two decades of experience studying the electronic and magnetic properties of transition-metal oxides at Lincoln Laboratory, Massachusetts, began focusing on oxides as cathodes after joining the University of Oxford in 1976. Kiochi Mizushima, who came on leave from Tokyo University as a visiting scientist to work with Goodenough, identified layered lithium cobalt oxide ($LiCoO_2$) as a cathode in 1980 (Mizushima et al. 1980). As with TiS_2, the direct metal-metal (Co-Co) interaction and the two-dimensional layered structure facilitate good electronic and lithium-ion conductivity. Akira Yoshino at Asahi Kasei Corporation in Japan worked on carbonaceous materials as anodes. He demonstrated the first rechargeable lithium-ion cell, employing $LiCoO_2$ cathode and a carbon-based anode (petroleum coke) in 1985 (Yoshino et al. 1987). Following this, Sony Corporation commercialized lithium-ion technology in 1991 with LiCoO2 cathode and a coke anode. Later, in 1997, the industry transitioned to graphite anode as it displays a flatter discharge voltage (Figure 2). For their work, Whittingham, Goodenough, and Yoshino were awarded the Nobel Prize in Chemistry in 2019.

Commercialized lithium-ion technology offered two critical advantages. First, replacing a sulfide cathode like TiS_2 with an oxide cathode like $LiCoO_2$ enabled a

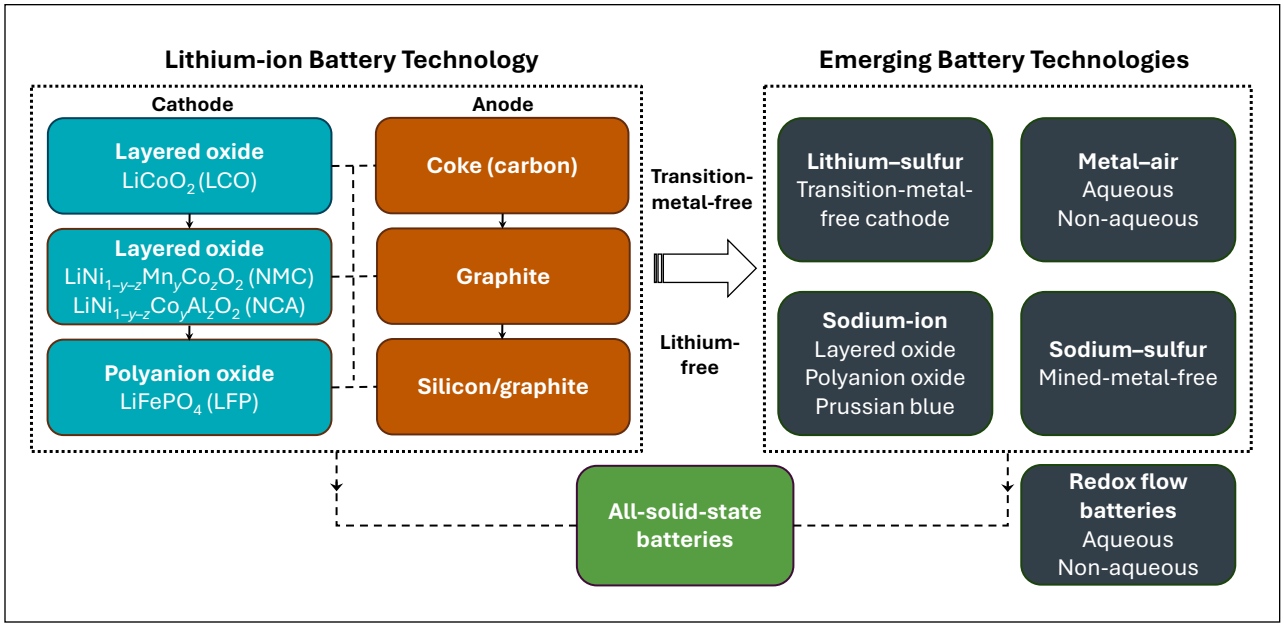

FIGURE 2 An overview of cathode and anode development for lithium-ion batteries over four decades and transition to emerging next-generation battery technologies.

higher cell voltage of ~4 V versus <2.5 V with a sulfide cathode. Second, because the cathode already contained lithium in it, it eliminated the need to use lithium metal as an anode and allowed lithium-free anodes like graphite. Present-day lithium-ion technology is based on this "rocking chair" concept in which the lithium ions shuttle between the two electrodes during the charge–discharge process without involving metallic lithium.

The Cathode Challenge

About 75% of the cost of a lithium-ion battery comes from its materials, with roughly half of that attributed to the cathode, which relies on costly metals like cobalt and nickel (Li et al. 2020). The cathode also imposes key limits on energy density due to surface instability with liquid organic electrolytes, restricting the operating voltage to below 4.3 V, and a relatively low charge-storage capacity (<220 A h kg^{-1}) compared with ~370 A h kg^{-1} for graphite anodes. In addition, oxide cathodes can release oxygen gas during overcharge, posing fire hazards and safety concerns.

Following the discovery of layered $LiCoO_2$, lithium manganese oxide ($LiMn_2O_4$) with a spinel structure was identified in 1983 by Michael Thackeray, who, while on leave from the Council for Scientific and Industrial Research in South Africa, worked with Goodenough as a visiting scientist at Oxford (Thackeray et al. 1983). The three-dimensional spinel framework, characterized by direct Mn–Mn interactions and 3D lithium-ion diffusion pathways, enabled faster charge–discharge rates and greater structural stability compared to the two-dimensional layered $LiCoO_2$. $LiMn_2O_4$ also exhibited reduced oxygen release, improved safety, and a significant cost advantage since Mn is abundant and inexpensive relative to cobalt. However, dissolution of Mn^{2+} in the presence of trace protons in liquid electrolytes, followed by its migration to the anode, catalyzes electrolyte reduction on the graphite surface, increases cell impedance, and shortens cycle life. Consequently, despite its favorable cost and safety profile, $LiMn_2O_4$ could not be widely adopted due to the persistent issue of manganese dissolution.

Since the commercialization of $LiCoO_2$ in 1991, the prevailing trend over the past 35 years has been to progressively substitute cobalt with nickel and manganese to produce layered lithium nickel manganese cobalt oxide cathodes ($LiCo_{1-2x}Mn_xNi_xO_2$). This strategy is motivated by two factors: (1) both manganese and nickel are less expensive than cobalt, and (2) Ni^{3+} can be oxidized nearly to Ni^{4+}, enabling higher charge-storage capacity compared with $LiCoO_2$ (Chebiam et al. 2001). Consequently, cathode compositions evolved from $LiCoO_2$ to $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ (NMC 111), $LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$ (NMC 622), and $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC 811), as well as $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (NCA) (Figure 2). Today, NMC 811 is widely regarded as the industry standard, while R&D efforts continue to push nickel content toward ~90% compositions that are beginning to see adoption. This compositional shift increases charge-storage capacity from ~150 A h kg^{-1} for $LiCoO_2$ to ~230 A h kg^{-1} for $LiNiO_2$, translating into higher energy densities. More recently, the Manthiram group demonstrated cobalt-free layered oxide cathodes, such as $LiNi_{0.9}Mn_{0.05}Al_{0.05}O_2$(NMA), which are now being manufactured by TexPower in Houston (Li et al. 2020).

The Departure from Oxide Cathodes to Find a Pathway to Utilize Iron

Iron is the least expensive transition metal and the fourth most abundant element in Earth's crust. Its extraction and processing are low-cost and it is used in a variety of applications like steel. Despite its ubiquity, no way had been found to employ iron oxides as cathodes for lithium-ion batteries until recently. When Arumugam Manthiram arrived at Oxford in 1985 to work with Goodenough as a visiting scientist, cobalt- and manganese-based oxides ($LiCoO_2$ and $LiMn_2O_4$) were known cathodes, but iron oxides were not. Drawing on his background in polyanion oxide chemistry from earlier work on lanthanide molybdates in India (Manthiram and Gopalakrishnan 1984), Manthiram first explored lithium insertion/extraction in the polyanion oxide iron molybdate ($Fe_2(MoO_4)_3$) and subsequently in iron tungstate ($Fe_2(WO_4)_3$) (Manthiram and Goodenough 1987). Both compounds exhibited a cell voltage of ~3 V with flat voltage profiles—significantly higher than that of Fe_2O_3 (<2.5 V)—despite all being governed by the Fe^{2+}/Fe^{3+} redox couple. In 1986, Manthiram and Goodenough moved to The University of Texas at Austin (UT Austin), where Manthiram turned to iron sulfate ($Fe_2(SO_4)_3$). Remarkably, it displayed an even higher cell voltage of ~3.6 V compared to $Fe_2(MoO_4)_3$ and $Fe_2(WO_4)_3$, again with the same structure and the same Fe^{2+}/Fe^{3+} redox couple (Manthiram and Goodenough, 1989).

The marked increase in cell voltage—by more than 1 V—when moving from a simple oxide such as Fe_2O_3 to polyanion oxides led Manthiram and Goodenough to recognize the inductive effect of counter cations (Mo^{6+},

W^{6+}, or S^{6+}) on lowering the redox energy of $Fe^{2+/3+}$ in polyanion oxides compared to that in an oxide (Fe_2O_3) and thereby raising the cell voltage. The more covalent Mo-O and W-O bonds compared to the Fe-O bonds weaken the Fe-O covalency through inductive effect and lower the $Fe^{2+/3+}$ redox energy. The even more covalent S-O bond compared to the Mo-O and W-O bonds weakens the Fe-O covalence further, thereby lowering the $Fe^{2+/3+}$ redox energy even much more (Manthiram 2020) and raising the cell voltage even further. Intrigued by these findings, a PhD student Geeta Ahuja then pursued with Manthiram and Goodenough transition-metal phosphates, which comprised part of her dissertation in 1991 (Ahuja 1991). Based on the above foundation, Goodenough with his students identified lithium iron phosphate ($LiFePO_4$) with the olivine structure and a flat 3.5 V profile as a cathode in 1997 (Padhi et al. 1997) (Figure 2)—a decade later after Manthiram laid the groundwork with polyanion oxide pathway to employ iron in cathodes (Manthiram and Goodenough 1987, 1989).

Collectively, the work of Manthiram and Goodenough in the late 1980s led to:

- establishing a pathway to employ iron—the least expensive metal with suitable properties—in lithium-ion batteries;
- opening the broad field of polyanion cathodes, including $LiFePO_4$ (LFP), $Li_3V_2(PO_4)_3$ (LVP), $Na_3V_2(PO_4)_3$ (NVP), $Na_3V_2(PO4)_2F_3$ (NVPF), and others for both lithium-ion and sodium-ion batteries (Masquelier and Croguennec 2013);
- uncovering the inductive effect of counter-cations, which enabled higher cell voltages with more stable, lower-valent redox couples such as $Fe^{2+/3+}$; and
- improving thermal stability, safety, and cycle life through the tightly bound oxygen in covalently bonded polyanion groups and the use of stable lower-valent redox couples.

By 2024, about 40% of the lithium-ion battery market—worth $24 billion USD—was based on LFP cathodes. The abundance, low cost, and supply-chain advantages of iron, combined with the enhanced safety of polyanion oxide cathodes, are now driving industry adoption of LFP even further. Its market share is projected to rise well above 40%, particularly with the rapid growth of energy storage applications.

However, despite the notable cost, supply-chain, and safety advantages of polyanion oxide cathodes, LFP has drawbacks. It is less dense than oxide cathodes such as NMC and is intrinsically a poor electronic and ionic conductor, which limits charge transport. An analogous polyanion oxide, $LiMn_{1-x}Fe_xPO_4$ (LMFP) has recently attracted considerable interest. LMFP operates at a higher voltage, thereby offering higher energy density.

The unique opportunity for three visiting researchers from Japan, South Africa, and India to work with Goodenough in the 1980 without overlapping led to the development of three distinct families of cathodes: layered oxides, spinel oxides, and polyanion oxides. Of these, layered oxides and polyanion oxides are now widely used in commercial lithium-ion batteries. Looking ahead, the cost and supply-chain benefits of iron and manganese, coupled with improved safety and longer cycle life, are expected to further expand the market share of LFP and LMFP cathodes in both Western countries and emerging markets such as India. Moreover, blending a cobalt-lean or cobalt-free layered NMC oxide with LMFP or LFP can reduce costs while minimizing energy density penalties, and at the same time improve safety and cycle life compared to using NMC alone (Lee et al. 2024).

Moving Forward

Cost, sustainability, and supply chain challenges are driving interest in alternative materials and battery chemistries. Examples include lithium-ion batteries based on more abundant metals, sodium-ion batteries (using sodium instead of lithium as the working ion), and lithium-sulfur or sodium-sulfur batteries, in which sulfur serves as the cathode without additional metals (Figure 2). However, most of these technologies remain at the R&D or prototype stage.

With lithium-ion batteries, there is significant interest in replacing graphite with silicon anodes, as silicon is abundant and offers an order-of-magnitude higher charge-storage capacity. Unfortunately, large volume changes during cycling and aggressive surface reactivity with the liquid electrolyte severely shorten cycle life. As a compromise, commercial cells currently use silicon-graphite composite anodes containing <10% silicon (Figure 2). Renewed efforts are also underway to employ lithium metal anodes. For instance, the US Department of Energy–funded Battery500 Consortium is targeting an energy density of 500 W h kg^{-1} with lithium-metal

anodes, compared to ~300 W h kg^{-1} in today's state-of-the-art lithium-ion cells.

In sodium-ion batteries, layered oxides can be synthesized largely with manganese and iron, minimizing expensive nickel and further lowering costs. Other promising cathodes include polyanion oxides such as NVP and NVPF, and Prussian blue analogs such as $Na_2FeFe(CN)_6$ and $Na_2FeMn(CN)_6$. While Prussian blue analogs are low cost, they suffer from toxic gas release and safety concerns, and both these and polyanion cathodes deliver lower energy density than layered oxides. Sodium-ion batteries also require hard carbon anodes (short-range order) instead of graphite (long-range order), lowering the cell voltage and complicating performance consistency. Overall, sodium-ion batteries typically exhibit lower energy density than lithium-ion batteries, and the current goal is to bring sodium-ion technology to parity with LFP-based lithium-ion cells.

Sulfur provides notable benefits, including an order-of-magnitude higher capacity than oxide or polyanion cathodes, broad abundance, favorable supply-chain availability, and low cost as a petrochemical byproduct. Sodium–sulfur batteries, in particular, can be considered "mined-metal-free" since sodium is widely available in seawater. However, sulfur's poor ionic and electronic conductivity necessitates large amounts of conductive carbon and liquid electrolyte, reducing the practical energy density. Moreover, during discharge, soluble higher-order polysulfides form and shuttle between the sulfur cathode and lithium- or sodium-metal anode, causing severe capacity fading. Thus, despite sulfur's compelling cost and supply-chain advantages, fundamental scientific challenges must be overcome for commercialization.

Electrolytes play a pivotal role in all of these battery chemistries. With the high negative electrochemical reduction potentials, anodes (graphite, silicon, lithium metal, hard carbon, sodium metal) and highly oxidizing cathodes (e.g., NMC) react with liquid electrolytes, forming solid-electrolyte interphase (SEI) and cathode-electrolyte interphase (CEI) layers. These interphases consume active lithium or sodium and impede ionic transport. Complex solvent and additive blends that are often found through trial-and-error are used to mitigate these effects. Challenges are especially severe with metal anodes due to repeated plating/stripping and new surface formation, as well as with silicon anodes because of volume expansion and nanoscale particle size. Flammable solvents further raise fire-safety risks.

While the solid electrodes or electrolytes with fixed atomic positions in the crystal lattice are more straightforward to model and characterize, liquid electrolytes with multiple solvents and salts present far greater complexity. Solvation structures and the associated solvation/desolvation dynamics strongly influence SEI, CEI, and overall performance. Here, AI tools can accelerate the discovery of high-performance electrolyte formulations with balanced compatibility across electrodes.

Cost, sustainability, and supply chain challenges are driving interest in alternative materials and battery chemistries.

To address liquid-electrolyte limitations, all-solid-state batteries are being aggressively pursued with lithium- and sodium-metal anodes and both oxide and sulfur cathodes (Figure 2). Solid-state designs promise higher energy density by leveraging high-capacity metal anodes and eliminating the weight of liquid electrolytes, while also improving safety by removing flammable solvents. Yet, ion transport across solid–solid interfaces remains sluggish, and manufacturing large, defect-free separators with today's ceramic oxide or sulfide electrolytes is difficult. Solid electrolytes can also form undesirable SEI or CEI layers, depending on material pairings.

For large-scale grid storage employing batteries, cost and reliability become critical. In this context, redox flow batteries are being developed with aqueous and nonaqueous liquid electrodes (Figure 2). A key challenge with this technology is species crossover through conventional porous polymer separators. One strategy to mitigate crossover is to use solid-state electrolyte separators, which conduct ions through lattice sites without pores (Manthiram et al. 2017). This approach enables hybrid chemistries, for example coupling aqueous and nonaqueous, or acidic and basic electrodes within a single system.

Empowering Accelerated Development with AI

A vast amount of experimental and computational data accumulated over more than four decades with various battery chemistries and materials are available in the published literature, public databases, and in industry. As we march into the "fourth paradigm" (data-driven approach) of materials research driven by data, advances in AI are

rapidly reshaping with respect to how researchers discover and optimize battery materials (Lombardo et al. 2022; Wang et al. 2024). The premise is whether one can use the wealth of data available with AI and machine learning (ML) to accelerate the developments with the desired battery performance metrics.

AI/ML Basics

AI broadly refers to computer systems that perform tasks usually requiring human intelligence; ML is a core subset of AI that uses algorithms or statistical models to learn patterns from data, enabling predictive modeling without explicit rule-based programming. ML algorithms mainly consist of unsupervised learning, supervised learning, and reinforcement learning.

Supervised learning trains models on labeled data (i.e., the target or outcome variable is known) to predict outputs for new, unseen inputs. This method is widely used in applications like image recognition, speech recognition, spam detection, and predictive analytics. These models learn to map inputs to desired outputs by minimizing error on known examples. In battery research, supervised learning is applied to predict key materials properties based on structural, chemical, or thermodynamic descriptors. Common tasks include regression (e.g., predicting continuous values like ionic conductivity, voltage, or capacity) and classification (e.g., determining whether a material is stable within a voltage window or whether a certain formulation leads to dendrite formation).

In contrast, unsupervised learning is used when the data lacks explicit labels. This method aims to detect underlying patterns, groupings, or structures within data without prior annotation. In the context of battery research, unsupervised learning can be applied to cluster materials based on structural or compositional similarity, reveal trends in electrolyte solvation structures, or reduce the dimensionality of complex simulation data.

Self-supervised learning is a specialized form of unsupervised learning in which models generate pseudo-labels from unlabeled data, enabling them to capture meaningful patterns and feature representations without extensive manual annotation. This approach has become central in natural language processing (NLP) and computer vision, where models are pre-trained on large datasets by exploiting inherent data structures and then fine-tuned for specific applications. In materials engineering and battery research, self-supervised learning can be applied to molecular graphs, atomic environments, or spectral data to extract rich descriptors that are later fine-tuned for tasks such as property prediction or structure classification.

Meanwhile, there is also semi-supervised learning, which combines supervised learning and unsupervised learning by using both labeled and unlabeled data to train the models. This method leverages a small set of labeled data along with a large amount of unlabeled data to improve learning efficiency. It is particularly useful in situations where obtaining a sufficient amount of labeled data can be expensive or time-consuming, but large amounts of unlabeled data are relatively easy to acquire.

Reinforcement learning (RL) is an ML technique that is used to guide decision-making processes. It involves an autonomous agent that interacts with an environment and learns optimal strategies through trial and error in the absence of any guidance from a human user. In battery research, RL can be used to optimize formulations, cycling protocols, or synthesis conditions with minimal experiments. When coupled with automated experimentation in closed-loop systems, they enable self-driving labs that rapidly converge on optimal materials candidates, significantly reducing development time and experimental costs.

As the traditional ML techniques reach their limitations in handling large volumes of high-dimensional, unstructured data, deep learning (DL) has emerged as a powerful alternative to tackle the challenges by utilizing multilayered neural networks. Different forms of DL have been used in many of the AI applications in our lives today, such as ChatGPT and self-driving cars. In materials engineering, DL enables the direct use of raw or minimally processed data, such as atomic configurations, spectral data, and crystallographic data to model target properties. These models can learn hierarchical and spatial features automatically, making them especially powerful for tasks like capturing complex structure-property relationships, representing compositional effects, or even generating new candidate materials in a multi-dimensional chemical space.

Moreover, concepts like active learning, which emphasizes efficiency by enabling AI systems to identify the most informative data points for labeling or experimentation, and transfer learning, which allows models trained on one type of material system to be adapted to another, are also promising ML techniques that can be employed in battery materials research.

AI-Assisted Data Acquisition

At the heart of all the ML approaches lies data: AI and ML flourish only when presented with abundant, diverse, high-quality datasets to learn from (Figure 3) and the per-

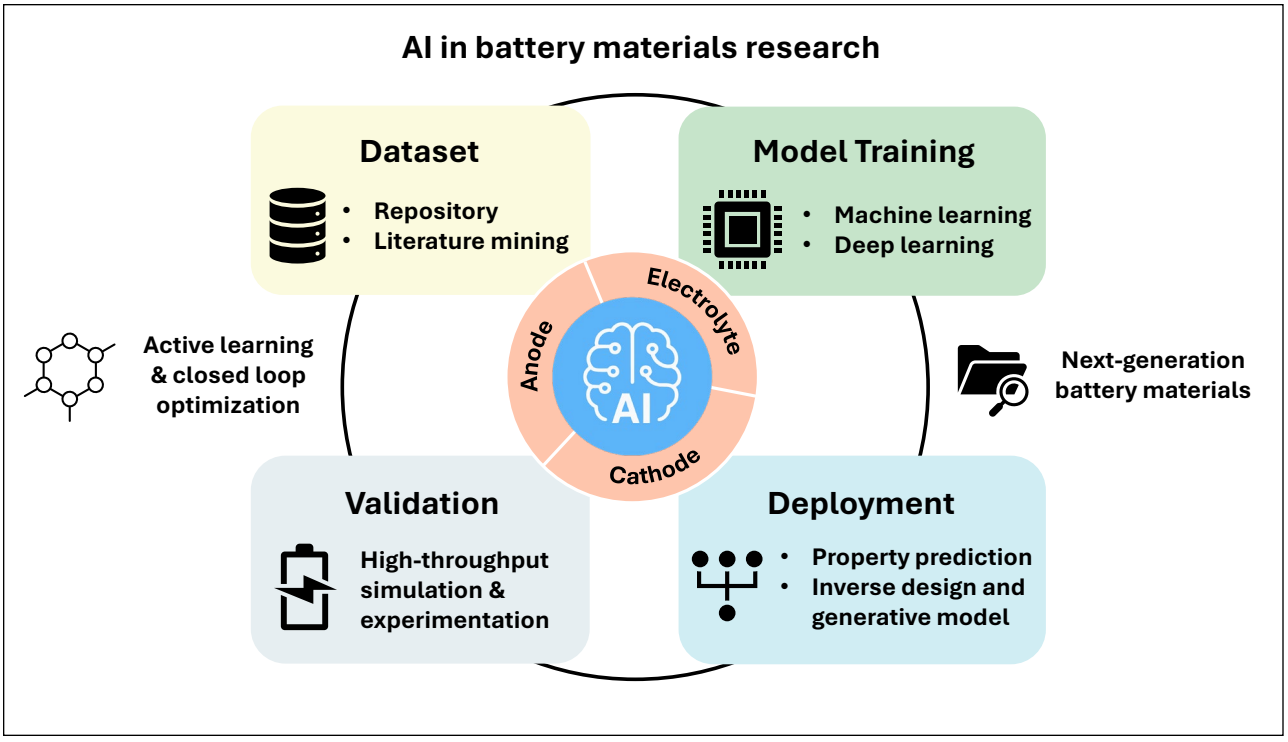

FIGURE 3 Typical workflow for AI-assisted battery materials research.

formance of AI models is tightly coupled to the diversity, relevance, and quality of the data they are trained on. AI learns by example, so the effectiveness of a model depends on how well the training data represents the chemical and structural landscape of interest. Therefore, before training AI models for battery-related research, they need to be provided with rich and accessible datasets that accurately reflect the complex behavior of battery materials. This includes experimental data from electrochemical tests, physical characterization, and spectroscopy, computational data from first-principles calculations, and molecular dynamics simulations.

A straightforward approach to data acquisition is mining published literature and patents, which contain decades of experimental and computational results. While searchable databases provide direct access, they may lack the specific data types or scale needed for battery researchers to train ML models. In such cases, AI can help through automated literature mining (Kononova et al. 2021). Modern NLP tools, including large language models (LLMs), can extract structured data from unstructured text, allowing researchers to collect property measurements, synthesis parameters, and performance metrics from thousands of scientific documents (Miret and Krishnan 2025).

Beyond mining existing resources, another way to acquire battery-relevant data is by generating large-scale datasets through high-throughput computational or experimental methods augmented by AI. On the computational side, ML-based interatomic potentials and surrogate models can deliver accuracy comparable to costly density functional theory (DFT) calculations, but at a fraction of the time. These models have been applied to predict electronic structures, density, viscosity, ionic conductivity, and other physicochemical properties (Gong et al. 2025). The resulting simulated datasets can then serve as inputs for downstream ML pipelines or as validation sets in materials screening workflows. For example, NVIDIA's collaboration with SES AI employed GPU-accelerated ML to solve structures and compute electronic properties for more than 100 million candidate electrolyte molecules—including highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) levels as well as electrostatic potentials—effectively mapping the "molecular universe" of battery chemistry with unprecedented efficiency (Xu et al. 2025).

Additionally, high-throughput experimentation can generate experimental data orders of magnitude faster than manual approaches. The integration of robotics and AI into laboratory automation has given rise to self-driv-

ing laboratories that autonomously plan, execute, and analyze experiments. For instance, researchers have developed robotic systems that move between stations, mixing and testing compounds under AI guidance. One of the earliest demonstrations came from the University of Liverpool, where a "mobile robotic chemist" autonomously explored a photocatalyst formulation space, conducting 688 experiments in just eight days (Burger et al. 2020). Battery researchers have likewise been early adopters. At Carnegie Mellon University (CMU), scientists developed the battery-focused test stand "Otto," which screened 140 electrolyte formulations in 40 hours (Dave et al. 2020). Such automated systems are often integrated with active learning or Bayesian optimization to create closed-loop frameworks that continuously refine experimental strategies based on feedback, accelerating the discovery of promising new materials.

Predicting and Optimizing Battery Materials

With carefully designed algorithms and proper training on high-quality datasets, AI methods can be applied to specific battery materials and properties (Lombardo et al. 2022) (Figure 4). In cathode discovery, models are used to predict intrinsic properties, such as crystal structure, density, and conductivity, as well as performance metrics, such as capacity, cycle life, redox energy, thermal stability, and rate capability. AI tools can screen vast compositional spaces, identify promising dopant elements, and estimate electrochemical performance based on structure and chemical composition. A recent example is DRXNet, a DL model developed by Gerbrand Ceder's group (Zhong et al. 2024). DRXNet predicts accessible capacities and voltage profiles for new Li–Mn–O–F compositions as well as for high-entropy disordered rock salt (DRX) systems containing diverse metal species. By serving as a universal surrogate, it enables rapid screening of thousands of hypothetical DRX cathodes, thereby accelerating the discovery of new electrode materials.

AI is also increasingly applied to electrolyte design. For liquid electrolytes, ML models can predict critical properties such as ionic conductivity, interfacial stability, and electrochemical stability windows (oxidative/reductive limits) (Kumar et al. 2025). ML and surrogate models have also been used to study solvation structures and intermolecular interactions (Gao et al. 2023). Solid-state electrolytes, another major focus area, similarly benefit

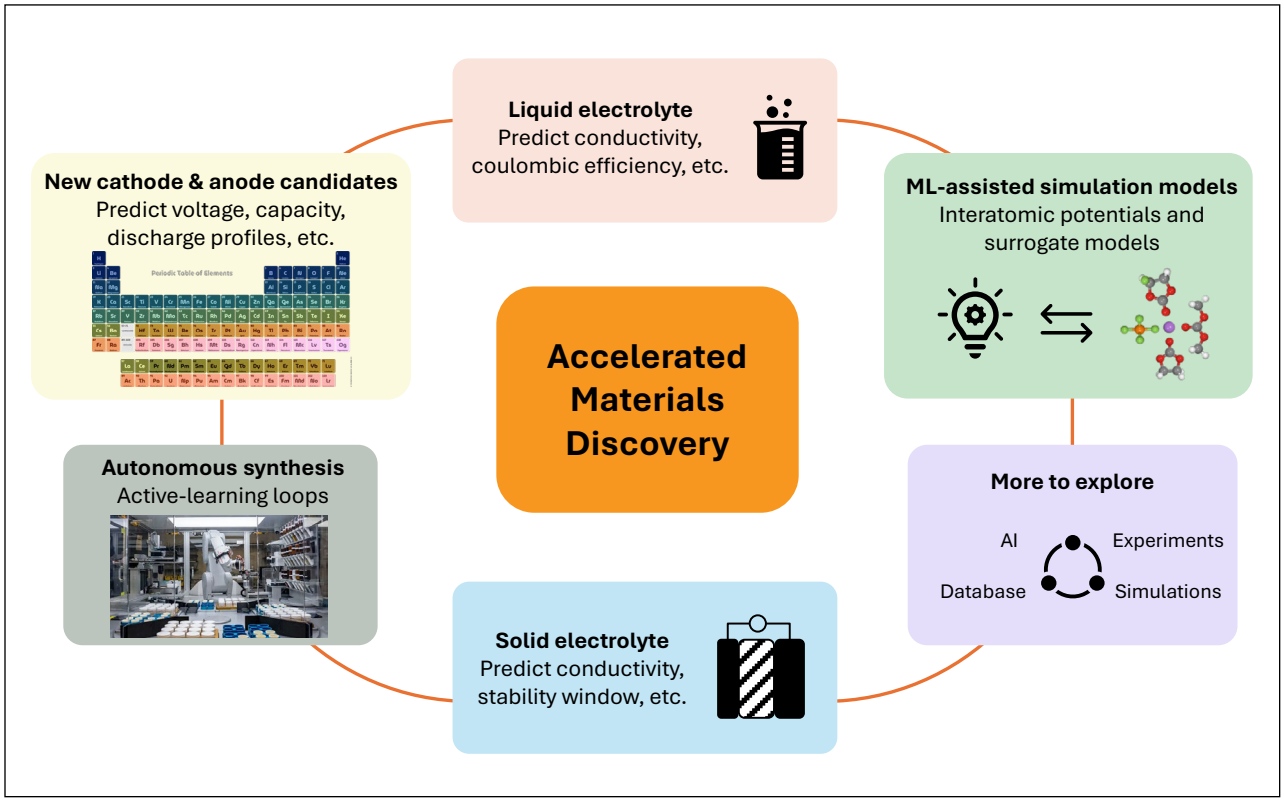

FIGURE 4 Applications of AI methods in different battery components or research processes for accelerated battery materials discovery. Credit: Fabio Crameri/S-ink for the periodic table and Berkeley Lab for the A-lab photo.

from ML predictions of ionic conductivity, structural stability, and electrochemical compatibility. Recent advances in DL have enabled models that operate directly on unstructured inputs such as molecular graphs or atomistic geometries. These methods are particularly powerful for capturing subtle structure–property relationships across high-dimensional chemical spaces, reducing reliance on expert intuition and improving predictive performance (Zhang et al. 2024). In parallel, state-of-the-art generative ML approaches are being developed to propose entirely new electrolyte molecules or mixtures, for both liquid and solid-state systems. By learning patterns from existing electrolyte databases and sampling new molecular graphs with desired properties, these models can effectively "invent" novel chemistries (Wang 2025; Yang et al. 2025). In essence, AI is transforming battery R&D into a data-driven optimization problem: given design targets, it can navigate multidimensional chemical space to suggest top candidates and experimental plans.

AI-Driven Battery Research Efforts

Several high-profile projects exemplify the AI-driven paradigm, particularly in demonstrating the power of closed-loop operations where AI systems iteratively generate hypotheses, guide experiments, and refine their models with newly acquired data. These autonomous cycles of prediction, testing, and learning are transforming materials discovery from a manual, intuition-driven pursuit into a scalable, data-centric process. A few illustrative examples are highlighted below.

CMU's Clio

A team from CMU demonstrated an autonomous workflow combining active learning with high-throughput experimentation to optimize liquid electrolytes for lithium batteries (Dave et al. 2022). The platform iteratively tested candidate mixtures in coin cells, using Bayesian optimization to prioritize formulations that improved ionic conductivity and electrochemical stability. Over a series of closed-loop cycles, the system converged on novel electrolyte compositions that outperformed benchmark formulations, showcasing the power of AI-guided experimentation to accelerate materials optimization.

Google DeepMind's GNoME (graph networks for materials exploration)

In 2023, DeepMind used deep graph neural networks to explore inorganic crystal space, predicting 2.2 million new crystalline compounds, of which about 380,000 were calculated to be thermodynamically stable (Merchant et al. 2023). Notably for battery research, GNoME identified 528 potential lithium-ion conductors, any of which could serve as novel solid electrolytes or cathode components. The model was trained on existing materials databases (e.g., the Materials Project) and employed active learning loops—predicting candidates and then verifying them with DFT—to achieve this unprecedented scale. DeepMind has released its 380,000 most stable predictions publicly. While some concerns remain regarding the true novelty of these materials (Cheetham and Seshadri 2024), collaborators at Lawrence Berkeley National Laboratory have already begun using these predictions to guide autonomous synthesis efforts, as discussed in the next example.

Autonomous Laboratories (Robotic Chemists, A-Lab)

Beyond predictive modeling, the emergence of fully automated laboratories marks a significant advance in closed-loop experimentation for battery materials. A-Lab, developed at Berkeley Lab, exemplifies this paradigm by integrating robotic synthesis, automated characterization, and AI-driven decision making into a self-driving platform for materials discovery (Szymanski et al. 2023). The system operates by autonomously selecting candidate materials, synthesizing and characterizing them, and using ML to analyze the resulting data and propose the next set of experiments—all with minimal human intervention. In their demonstration, the A-Lab team synthesized and characterized more than 41 previously unreported inorganic compounds, showcasing the potential of autonomous labs to dramatically accelerate discovery and ease experimental bottlenecks in battery materials innovation. Looking ahead, these platforms could be extended beyond synthesizability to investigate factors such as microstructure and materials performance.

Microsoft Azure and Pacific Northwest National Laboratory Collaboration

In early 2024, Microsoft and the Pacific Northwest National Laboratory showcased how AI and cloud-scale computing can compress years of discovery into months (Chen et al. 2024; Xu et al. 2024). Using Azure Quantum Elements, AI models narrowed a pool of ~32 million inorganic formulas to about 500,000 predicted to be thermodynamically stable. From this set, ~18 candidates were selected (in roughly 80 computing hours) for synthesis and testing in a battery context. One of these proved to be a solid-state electrolyte that synergistically combined

lithium and sodium ions. This material reduced lithium content requirements by ~70% while maintaining ionic conductivity, challenging prior assumptions about the stability of mixed-ion systems.

Future Outlook: Challenges and Opportunities

The AI revolution in battery research is still in its early stages, and progress on multiple fronts is needed to realize its full potential. First, experimental infrastructure must expand. Automated laboratories with broader capabilities, including high-throughput synthesis, characterization, and electrochemical testing, are essential for generating reliable data at scale.

In the coming years, AI could become as indispensable to battery research as electrochemistry itself.

Second, data quality and accessibility must be improved. Beyond existing public databases such as Materials Project, AFLOW, and OQMD, training powerful ML models will require large, high-quality, open-source datasets of battery materials spanning diverse chemistries and conditions. Equally important are standardized protocols for reporting experimental and computational results, including metadata such as synthesis or fabrication details, test conditions, and computational parameters. Such standardization would enhance data interoperability and reusability in line with the FAIR (Findable, Accessible, Interoperable, and Reusable) principles, which are critical for data-driven approaches. At present, much of the published literature lacks accurate metadata and consistent evaluation methods. Addressing these gaps will require coordinated community efforts such as the proposed "Battery Data Genome" initiative (Ward et al. 2022) along with incentives for companies and labs to share data.

Third, new AI tools and platforms may need to be tailored specifically for battery research. Advances in accuracy and the development of multiscale models will be critical to link atomic-scale predictions with real-world device performance, bridging gaps between atomistic ML models, continuum battery models, and circuit-level simulations. Equally important is usability: accessible ML frameworks, cloud-based platforms, and educational resources can lower barriers to adoption and enable broader use of AI among battery scientists.

In the coming years, AI could become as indispensable to battery research as electrochemistry itself. By combining human ingenuity with machine intelligence, the field can more rapidly identify breakthrough materials, whether high-capacity cathodes, safer electrolytes and electrodes, or durable solid-state systems. Ultimately, an ecosystem of standardized data, interpretable models, and autonomous labs could transform battery R&D from an artisanal trial-and-error practice into a data- and AI-driven engineering discipline. Seamless collaboration and communication between experienced experimentalists and computational experts will be essential, ensuring the human expertise needed to guide and accelerate discoveries in energy storage.

Summary

Half a century of concerted basic science and engineering research has led to today's lithium-ion battery technology. About 50% of materials cost is from the cathode, and basic science research in the 1980s offered pathways to lower the cost and ease supply chain—from cobalt oxide to manganese oxide to iron polyanion oxide cathodes. As the battery market expands to large-scale applications such as EVs and grid storage, cost and supply-chain challenges are poised to become increasingly critical.

Efforts must focus on eliminating scarce critical metals such as cobalt and nickel, while advancing battery chemistries based on earth-abundant elements like iron, manganese, sulfur, and sodium, as well as organic materials. Replacing liquid electrolytes with solid-state alternatives offers the potential to improve safety and increase energy density. With the vast troves of experimental data available in the literature and industry, AI can help accelerate the discovery of cost-effective, supply-chain-resilient chemistries and materials. Appropriately combining machine intelligence with human ingenuity could enable rapid, transformative advances in energy storage.

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References

Ahuja G. 1991. An Investigation of Some Lithium Insertion Compounds. PhD Dissertation, Chapter 5, pp. 92–114, The University of Texas at Austin.

Baker N. 2024. Unlocking a new era for scientific discovery with AI: How Microsoft's AI screened over 32 million candidates to find a better battery. January 9. Online at https://azure.microsoft.com/en-us/blog/quantum/2024/01/09/unlocking-a-new-era-for-scientific-discovery-with-ai-how-microsofts-ai-screened-over-32-million-candidates-to-find-a-better-battery.

Burger B, Maffettone PM, Gusev VV, Aitchison CM, Bai Y, Wang X, Li X, Alston BM, Li B, Clowes R, and 4 others. 2020. A mobile robotic chemist. Nature 583:237–41.

Chebiam RV, Kannan AM, Prado F, Manthiram A. 2001. Comparison of the chemical stability of the high energy density cathodes of lithium-ion batteries. Electrochemistry Communications 3(11):624–27.

Cheetham AK, Seshadri R. 2024. Artificial intelligence driving materials discovery? Perspective on the article: Scaling deep learning for materials discovery. Chemistry of Materials 36(8):3490–95.

Chen C, Nguyen DT, Lee SJ, Baker NA, Karakoti AS, Lauw L, Owen C, Mueller KT, Bilodeau BA, Murugesan V, Toyer M. 2024. Accelerating computational materials discovery with machine learning and cloud high-performance computing: From large-scale screening to experimental validation. Journal of the American Chemical Society 146(29):20009–18.

Dave A, Mitchell J, Kandasamy K, Wang H, Burke S, Paria B, Póczos B, Whitacre J, Viswanathan V. 2020. Autonomous discovery of battery electrolytes with robotic experimentation and machine learning. Cell Reports Physical Science 1(12):100264.

Dave A, Mitchell J, Burke S, Lin H, Whitacre J, Viswanathan V. 2022. Autonomous optimization of non-aqueous Li-ion battery electrolytes via robotic experimentation and machine learning coupling. Nature Communications 13:5454.

Gao Y, Yao N, Chen X, Yu L, Zhang R, Zhang Q. 2023. Data-driven insight into the reductive stability of ion–solvent complexes in lithium battery electrolytes. Journal of the American Chemical Society 145(43):23764–70.

Gong S, Zhang Y, Mu Z, Pu Z, Wang H, Han X, Yu Z, Chen M, Zheng T, Wang Z, and 7 others. 2025. A predictive machine learning force-field framework for liquid electrolyte development. Nature Machine Intelligence 7:543–52.

Kononova O, He T, Huo H, Trewartha A, Olivetti EA, Ceder G. 2021. Opportunities and challenges of text mining in materials research. iScience 24(3):102155.

Kumar R, Vu MC, Ma P, Amanchukwu CV. 2025. Electrolytomics: A unified big data approach for electrolyte design and discovery. Chemistry of Materials 37(8):2720–34.

Lee S, Scanlan K, Reed S, Manthiram A. 2025. Cost-effective layered oxide—olivine blend cathodes for high-rate pulse power lithium-ion batteries. Advanced Energy Materials 15(5):2403002.

Li W, Erickson E, Manthiram A. 2020a. High-nickel layered oxide cathodes for lithium-based automotive batteries. Nature Energy 5(1):26–34.

Li W, Lee S, Manthiram A. 2020b. High-nickel NMA: A cobalt-free alternative to NMC and NCA cathodes for lithium-ion batteries. Advanced Materials 32(33):2002718.

Lombardo T, Duquesnoy M, El-Bouysidy H, Årén F, Gallo-Bueno A, Jørgensen PB, Bhowmik A, Demortière A, Ayerbe E, Alcaide F, and 7 others. 2022. Artificial intelligence applied to battery research: Hype or reality? Chemical Reviews 122(12):10899–969.

Manthiram A. 2020. A reflection on lithium-ion battery cathode chemistry. Nature Communications 11(1):1550.

Manthiram A, Goodenough JB. 1987. Lithium insertion into $Fe_2(MO_4)_3$ frameworks: Comparison of M = W with M = Mo. Journal of Solid State Chemistry 71(2):349–60.

Manthiram A, Goodenough JB. 1989. Lithium insertion into $Fe_2(SO_4)_3$ framework. Journal of Power Sources 26(3–4):403–8.

Manthiram A, Gopalakrishnan J. 1984. Lower-valence molybdenum oxides: Crystal chemistry and electronics properties. Reviews in Inorganic Chemistry 6:1–68.

Manthiram A, Yu X, Wang S. 2017. Lithium battery chemistries enabled by solid-state electrolytes. Nature Reviews Materials 2:16103.

Masquelier C, Croguennec L. 2013. Polyanionic (phosphates, silicates, sulfates) frameworks as electrode materials for rechargeable Li (or Na) batteries. Chemical Reviews 113(8):6552–91.

Merchant A, Batzner S, Schoenholz SS, Aykol M, Cheon G, Cubuk ED. 2023. Scaling deep learning for materials discovery. Nature 624:80–5.

Miret S, Krishnan NMA. 2025. Enabling large language models for real-world materials discovery. Nature Machine Intelligence 7:991–8.

Mizushima K, Jones PC, Wiseman PJ, Goodenough JB. 1980. Li_xCoO_2 ($0 < x < 1$): A new cathode material for batteries of high energy density. Materials Research Bulletin 15(6):783–98.

Padhi AK, Nanjundaswamy KS, Goodenough JB. 1997. Phospho-olivines as positive electrode materials for rechargeable lithium batteries. Journal of the Electrochemical Society 144:1188–94.

Szymanski NJ, Rendy B, Fei Y, Kumar RE, He T, Milsted D, McDermott MJ, Gallant M, Cubuk ED, Merchant A, and 6 others. 2023. An autonomous laboratory for the accelerated synthesis of novel materials. Nature 624:86–91.

Thackeray MM, David WIF, Bruce PG, Goodenough JB. 1983. Lithium insertion into manganese spinels. Materials Research Bulletin 18(4):461–72.

The Research Insights. 2025. Lithium ion battery market. Online at https://www.theresearchinsights.com/reports/lithium-ion-battery-market-998.

Wang Y. 2025. Application-oriented design of machine learning paradigms for battery science. npj Computational Materials 11:89.

Wang Z, Chen A, Tao K, Han Y, Li J. 2024. MatGPT: A vane of materials informatics from past, present, to future. Advanced Materials 36(6):2306733.

Ward L, Babinec S, Dufek EJ, Howey DA, Viswanathan V, Aykol M, Beck DAC, Blaiszik B, Chen BR, Crabtree G, and 18 others. 2022. Principles of the battery data genome. Joule 6(10):2253–71.

Whittingham, MS. 1976. Electrical energy storage and intercalation chemistry. Science 192(4244):1126–7.

Xu K, Hannah D, Zhang Y, Hu Q. 2025. Spotlight: Accelerating the discovery of new battery materials with SES AI's molecular universe. May 8. Online at https://developer.nvidia.com/blog/spotlight-accelerating-the-discovery-of-new-battery-materials-with-ses-ais-molecular-universe.

Yang Z, Wu Y, Han X, Zhang Z, Lai H, Mu Z, Zheng T, Liu S, Pu Z, Wang Z, and 3 others. 2025. A unified predictive and generative solution for liquid electrolyte formulation. arXiv. Online at https://doi.org/10.48550/arXiv.2504.18728.

Yoshino A, Sanechika K, Nakajima T. 1987. Secondary battery. US Patent 4668595 and Japan Patent 1989293.

Zhang H, Lai T, Chen J, Manthiram A, Rondinelli JM, Chen W. 2024. Learning molecular mixture property using chemistry-aware graph neural network. PRX Energy 3(2):023006.

Zhong P, Deng B, He T, Lun Z, Ceder G. 2024. Deep learning of experimental electrochemistry for battery cathodes across diverse compositions. Joule 8(6):1837–54.

An Interview with . . .

Ainissa Ramirez, materials scientist, writer, and science communicator

RONALD LATANISION: I'd like to welcome everyone back to the National Academies' *Bridge* interview series. Today we're joined by Ainissa Ramirez, a writer and science communicator with a background in materials science and engineering. Also here is Kyle Gipson, editor of *The Bridge*.

Ainissa, it's great to see you. I know you hold a PhD in materials science, and it's always a pleasure to speak with someone who bridges the worlds of science and storytelling. To get us started, could you tell us a little about your background like where you grew up, where you went to school, just to give our readers some context?

AINISSA RAMIREZ: Sure. First of all, I'm delighted to be here. I'm really looking forward to talking about our beloved field of materials science.

I was born in New York City but grew up in New Jersey, where I attended Catholic schools. I always loved science, but it wasn't exactly a popular subject in those environments. Fortunately, I had some fantastic teachers who encouraged me early on. And that is what motivated me to eventually apply to schools that were outside of New Jersey, which was a little unusual back in the day.

I did my undergrad at Brown, and that was probably the best decision I ever made. The liberal arts environment allowed me to study engineering while exploring broader interests, and I think that experience shaped who I am today. I'm an engineer, but also now a writer, and I believe that foundation was forged there.

After Brown, I earned my PhD in materials science from Stanford, then went on to work at Bell Laboratories for several years. Following that, I spent about a decade as a professor at Yale. Eventually, I made what I like to call the leap into science evangelism, spreading the good word that science is for everyone. These days, I do that primarily through books, but also through speaking, podcasts, and other media.

DR. LATANISION: What was the focus of your doctoral work?

DR. RAMIREZ: I worked on amorphous carbon, specifically as it relates to data storage. If you think about a hard disk, there's a thin protective layer on its surface, that's amorphous carbon. When a hard disk winds down, a small stylus-like object actually lands on that surface. So when someone says "my hard disk crashed," it's because that stylus made an unwanted contact. My research focused on that top protective layer, how to strengthen it and make those crashes less damaging.

DR. LATANISION: Did you go directly to Bell Labs from Stanford?

DR. RAMIREZ: Yes, I was very lucky. Bell Labs hadn't been hiring for some time, but when I was finishing up at Stanford, they had some openings. They came to campus to interview, and I thought, "Well, I'll give it a try." Honestly, I wanted to stay in California. Once you experience life there, you never want to leave. Returning to New Jersey wasn't in my plans—I'd even promised myself I wouldn't go back. But then Bell Labs offered me a position and you don't say "no" to Bell Laboratories. So, I

went back and it turned out to be a fantastic experience. I had a great time there.

DR. LATANISION: Your recent writing is related to Jim West's history. Did you work with him or meet Jim when you were at Bell Labs?

DR. RAMIREZ: I did get to meet Jim West. Jim West is an African American inventor who created the microphone that is one of the most used microphones in the world. He was in a different department—I was in the materials department, and he was more in the acoustics part of Bell Laboratories. We did not really interface directly, but I knew of him. So I emailed him and asked if we could do lunch. I don't remember what we talked about, because I think I was just enamored the whole time—he is such a star.

I made what I like to call the leap into science evangelism, spreading the good word that science is for everyone.

DR. LATANISION: You went from Bell Labs to Yale and you taught materials science for a few years. What led you to transition from being an academic in science and engineering to writing?

DR. RAMIREZ: I think it was a gradual process. When I was a graduate student at Stanford, the women in the materials science program would organize an event for middle school girls called *Expand Your Horizons*. We put together demonstrations to explain materials science concepts using everyday objects like rubber bands and paper clips. I remember thinking, "This is fascinating." I believe that that experience planted a seed in me.

Later, when I joined Bell Laboratories, they had a program too—I believe it was called *World of Science*. It was a free lecture series where anyone who could get to their auditorium could hear talks by Bell Lab scientists. I thought, "Wow, what a great concept."

At Yale, we were all expected to contribute to broader impacts, so I created a lecture series called *Science Saturdays*. It took place each October and April, four Saturdays in a row. The format was based on what I call the three Ds: donuts, dynamic talks, and demonstrations. And we drew in kids and families for any one of those reasons.

DR. LATANISION: The donuts...

DR. RAMIREZ: The donuts would bring you in. You didn't have to worry about breakfast. There were demonstrations, and they were often given by undergraduates because we targeted middle schoolers and we wanted people who were closer in age to our audience. There were also dynamic talks that were given by professors—fantastic, high-caliber people.

I noticed that in October and April, my energy was off the charts. I was so excited to go to work. And then afterward, my energy would go down. So I enjoyed my work, but my energy was highest during the *Science Saturdays* months. Now, after 7 years of doing this, I said, "What kind of scientist are you? You're getting data!" I observed that what I really loved was being a shepherd, bringing science to the general public.

After my time at Yale was done, I could have made the change to go to another academic position. But I decided instead to take a leap and see what this science evangelism thing is. I was fortunate because right away, I got a book deal to write about football. It just kind of took off from there.

DR. LATANISION: You wrote about football?

DR. RAMIREZ: Yes. It talked about how the questions on the gridiron are some of the same questions that we're answering in the laboratory—so things like chaos theory, the butterfly effect, game theory. It wasn't about mechanics. It wasn't the physics of collisions. There are books about that already. But it was more about exploring how people make decisions about plays. That's very scientific as well.

MR. GIPSON: You talked about transitioning into shepherding scientific topics and materials to a broad audience. I'd like to hear you talk a little more about why you think that's so important, or where you think that energy comes from for you. Has there been a guiding or overarching mission underlying how you've approached communicating science to a broad audience, including younger audiences? Where do you think this energy comes from?

DR. RAMIREZ: That is such a good question, and I want to thank you for asking that. I was one of those kids who used to ask a lot of questions and take things apart. Back in Jersey City in the '70s and '80s, I didn't see any scientists but there was a program on PBS called *3-2-1 Contact* and they had a repeating segment about kids solving problems. It featured this group called the Bloodhound Gang. One of the characters was an African American girl. I saw her asking questions and I asked my mom, "What is she doing?" My mom responded, "she's doing science." I was like, "That's what *I'm* doing!" That put me on the road to becoming a scientist.

Out of all the classes I took in grammar school, science was the one that spoke to me the best. It spoke to me the most. My science teachers were so nerdy and they made it okay for me to be nerdy too. I think that exposure—of seeing my reflection—is what put me on the path to wanting to create other reflections for kids.

So, Jim West is an African American scientist who is now in his 90s. He created a technology that is one of the most used in the world. He invented it in the 1960s and it became popular in the '70s and '80s. And here we are in the 21st century. This is when I asked: "Where is Jim West's book?" That's what motivated me. I said, "Somebody ought to write this." And then I realized—I think that person is me.

DR. LATANISION: That's an interesting point. I have grandchildren who spend most of their time, it seems to me, with their phones in their hands, playing games or communicating with their friends. How do you interact with young people on that level? Do you think that we are somehow abusing young people by making our technology too available to them?

DR. RAMIREZ: I am definitely of the generation before all this technology existed and I certainly do miss my analog brain. I'm easily distractable now because of technology. All I can say is that children will evolve. They will do creativity differently because technology will assist them in new ways. Do I personally like it? Not really. But there's nothing I can really do.

What I *can* ask is that children sometimes do things without technology and see how that goes. This happens in conversations. I could be talking with someone and then they cannot recall a person's name. They'll want to look it up but I'll tell them "no" because once you look it up, you'll go down that rabbit hole and that will be the end of this conversation. My thinking is to keep this conversation going because it's not important that you do not know it. I try and make occasions where we can separate from that technology and have more human interactions.

DR. LATANISION: Frankly, I worry a little bit about it. I remember when I was a kid before we had all the electronics that are available today. We used to go out in the streets and do things. I really wonder whether technology is a little bit too advanced or maybe this is a parental issue. Maybe parents need to be more involved in making sure that kids don't overextend their time on their laptop or their cell phone.

DR. RAMIREZ: You raise good points. The other impetus for *Spark*, the book about Jim West, is my nephew. My nephew is a tinkerer. I wanted him to see another tinkerer so he'd know that who he is is okay. And I wanted this book to be for those who are STEM-minded so they could see that it was okay to be the way you are because here's a guy who was just like that and he went on to create something fantastic.

DR. LATANISION: Could you tell us a little bit more about *Spark* and your interaction with Jim?

DR. RAMIREZ: Jim created this microphone called the foil electret microphone. People often know it as a condenser microphone. He did this when he was an intern at Bell Laboratories.

Before that, Jim was a very rambunctious little boy. He used to take a lot of things apart. We would say he was naughty, but he was just curious. Jim really wanted to know how things worked. He wanted to go to college to learn more about science, but his parents actually tried to talk him out of it because this was happening in the 1950s and '60s. There weren't many Black scientists. His father told him that's a waste of money—that it is not going to happen.

But Jim wasn't just precocious; he was driven. He said "I will figure out how to go to college." He repaired televisions and he stayed with some relatives to keep the costs down. He went to Temple University and that's where he studied physics.

Now, he needed to raise some money so over the summer, he saw that Bell Laboratories were looking for interns. At Bell Labs, he landed on an interesting project. There were some psychologists who were doing studies on sound and they wanted him to make special headphones for their tests on detecting a short pulse of sound.

He didn't know anything about that but he went to the library and learned that there was a strange material that could be used to make these headphones. He learned that if you put Mylar on a disk with another piece of metal above it, you can kind of create a capacitor. And if you can change the polarity—positive and negative—of this piece of metal, then the Mylar will move in and out and that will create a sound. He was like, "Okay, great. This is wonder-ful. I'm going to use this to make my headphones."

DR. LATANISION: He is an intern.

DR. RAMIREZ: He is an intern. He is a fantastic intern. We should bring in interns because interns can do fan-tastic things.

So he needs a battery to create the positive and negative charge for the Mylar to flex. It needs to have its own circuit. One day he's in the laboratory and he has discon-nected the circuit but he finds that he's still able to hear a beep. It ends up that this material can store a charge and store it for decades. He doesn't need that battery and he's now able to make those headphones. That's also when he has a great insight. If this material can make headphones, perhaps it can make a microphone because microphones and headphones work the opposite way. And when he tries that, the microphone works!

Now, what makes this so powerful is that he discovered a material that doesn't require a power supply to sustain a charge, which means the device can be consolidated. It can be used as an earpiece for people who are hard of hearing and in many other ways. The thing that is crazy is that electret, that material, that can store charge.

DR. LATANISION: Did you talk to Jim when you were writing the book?

DR. RAMIREZ: Oh yes. I talked to Jim a couple of times because I needed to understand what he did. I had never heard about this material that stores a charge but it has been known for a long time. If you look at books from the 1600s, they talk about a strange wax that was able to store charge. It was more of a curiosity then and no one knew what to do with it. However, Jim stumbled on it serendipitously with Gerhard Sessler, his collaborator.

DR. LATANISION: It's a great story. To start with a parent who was not very enthusiastic about education and then to achieve what he has achieved is really pretty amazing.

MR. GIPSON: That is fascinating. I have another question about *Spark*, your first children's picture book. Can you talk a little bit about the difference in the process of writing this, or how you have approached this for younger audiences compared to your earlier books that might be for older audiences? Was it more challenging in some ways or less challenging in some ways?

DR. RAMIREZ: I think that I have evolved to the point where I could write a science children's book. It's challenging because you are trying to explain things to the youngest citizens in our country.

In order to explain how that microphone works, which is a little on the complicated side, I had to introduce underlying concepts like electricity first. When Jim West was young, he had a book about electricity and in it he learned that Ben Franklin had done this experiment where he flew a kite in a storm and learned that lightning was electricity. I talk about that in the book.

Later on, Jim West finds a radio and so I describe how a radio works. There is a speaker that moves in and out. I'm able to get concepts of sound established earlier in the book and build up to more complicated things. I found it very challenging but I found it challenging in a rewarding sense. I have to figure out how to explain this so that people are going to get it. It's formidable, but it shapes me and makes me a better writer, too.

DR. LATANISION: Do you meet with students and groups of students to talk about your interest in science and your history and so on?

DR. RAMIREZ: I have been doing that for years. For a while, I was on a speaker's track where I would go to different schools and libraries and talk about my path in science. More recently, I have been beta testing how to explain what Jim West did. I did some activities at some libraries. With children, we would make megaphones. We would get pieces of paper and roll them up. And I would say, "What can we do with this?" It can make the sound louder. And then I could say, "We can put it to our ear and we can hear sounds." Next, I am having them learn about different types of sounds.

Then we learn about vibrations. I will put their hands on a table and then I will smack the table a couple of times and they will feel the vibration. That's when I explain that that's what is going on in your ear. And then I will make the jump: "How do I make an electronic ear?" That is a microphone.

You have them make the megaphone so that they feel connected to the concept of sound, and then you just march slowly to the main concept that I want to get to: the microphone.

DR. LATANISION: That is very cool. You previously mentioned a book focused on football. What was that?

DR. RAMIREZ: That was called *Newton's Football*. That came out in 2013.

DR. LATANISION: I have a technical question for you. Do you remember Deflategate?

DR. RAMIREZ: I was very much involved in Deflategate. For me, this great story came out and I was waiting for Bill Nye and Neil Tyson to show up. They're going to figure this out and they are going to explain it. But then nobody showed up.

NPR reached out to me and I ended up being on with them and Fox Business News, explaining Deflategate and ideal gas law. At the time, people wanted to know if someone did it on purpose or is it possible for it to happen on its own because of the cold temperatures. I focused on the cold temperature concept.

DR. LATANISION: The reason I ask is there is a lot of science in all of that. It could be PV = nRT. That would be a good illustration to kids that science has a meaning to something that is important to them.

DR. RAMIREZ: Absolutely. I agree. That is why I thought, "This is a missed opportunity. Where is everyone?" And I think textbooks could be rewritten. They could just start off with Deflategate and explain what happened. People will be like, "What? Football?" And then the events are explained, and then you go into PV = nRT.

DR. LATANISION: There you go. Tell me about the podcast. What do you do on your podcast?

DR. RAMIREZ: The podcast—it's not sunsetted, but I haven't done it for a while. It was called *Science Underground* and it was a two-minute science explainer. I would explain things like the football spin and why snowflakes are white. It was designed to help teachers when they start a lesson. Teachers would ring a bell and say "let's start off with this 2-minute podcast and learn a little bit about science." This could be an introduction to a certain topic. That is what I did with *Science Underground*.

From that, I went on to a program on PBS called *SciTech Now*. I would talk about different topics. Some of them were provocative like "Space Suit Secrets." In that episode, we talked about how astronauts wear a diaper but there are multiple layers to their suits, too.

I think that I have evolved to the point where I could write a science children's book. It's challenging because you are trying to explain things to the youngest citizens in our country.

DR. LATANISION: One of the concerns I have personally is that I have a sense that the public is beginning to maybe lose a bit of trust in technology. I say that it is largely associated with artificial intelligence. I'm wondering if you get questions from kids about AI. For example, it is not just that you can train a computer, a machine, to give back human-like text. We're talking about artificial general intelligence so that computers and bots and agents can think and even more extensively, artificial super intelligence, which would lead to the vision of something like humanoid robots walking the streets, for example.

Do kids question you about this and ask if it makes sense that we are heading in this direction? What kinds of concerns do they have, if you have any interaction of that kind?

DR. RAMIREZ: When I talk to kids, they ask me if I am concerned about AI. The question they ask is: "Should I be concerned about it?" I will say, "Yes, you should be concerned about it."

I also will tell them this is the reason why I wrote *The Alchemy of Us*. *The Alchemy of Us* looks at older technologies: the telegraph, the light bulb, the computer, and the clock. And it shows that these technologies have shaped us. These technologies are easy to wrap our brains around. The telegraph, for example, is just turning electricity on

and off. And clocks—we kind of know how they work. We may not be able to take one apart, but we know how they work.

I treat *The Alchemy of Us* as a gym where you are working on smaller weights. If audiences recognize how older technologies have shaped us, they can also understand that AI will inevitably shape us too and they'll be ready to ask questions, just as they did about earlier technologies.

There are debates about AI. "Is this snake oil and what will it do?" People want to know whether they should be concerned and my response is "yes, you should be concerned and you should feel empowered to ask questions."

When you write books that use stories, you write differently.

MR. GIPSON: You were talking about the importance of *The Alchemy of Us*, your book. Can you help us understand what makes a particular book topic a good topic?

DR. RAMIREZ: It was part of my own evolution. I had to step away from academia for a couple of years for my brain to go through a transformation to figure out how to write this book. I wanted to write about my beloved field of materials science but the way that I learned materials science was not going to work for general audiences. That is the first thing that I had to learn. As enthusiastic as I might be about the field, people have their own baggage about science.

Interestingly, there was a materials science book that came out that was similar to what I was thinking about doing. Originally—and this is part of my evolution—I was going to have several different chapters about different materials. I was going to tell you everything I knew about that material. "Let me tell you everything about carbon, about aluminum, and you're going to like it." That is the posture that you have as an academic.

DR. LATANISION: Your vision was for the book to be written for the general public.

DR. RAMIREZ: That was the original vision. However, that other book came out as I was writing my book proposal and I knew that it was not going to work. So I said what I'm going to do is shape my book differently. I'm going to use stories because stories are a billion-dollar industry. It is called Hollywood! I'm going to tell the story of these inventions and how they shaped us. I chose eight different materials and for each material I needed a vignette from history—something that happened because of this material or because this material was absent. Then there is going to be an origin story. Who made this material or who was impacted by this material? And then I was going to talk about the impact on society.

Also, I start off the book with something that will hook you. The first person that you meet in *The Alchemy of Us* is a woman named Ruth Belville. In 1890, she had a crazy job: she lived in England and she sold time. No one knew what the precise time was back then and people who owned banks or had factories needed to know the time. She would go around with her pocket watch, which was a very precise chronometer. She'd stop at the Royal Observatory first, collect the actual time from them and then go to different parts of London, showing her watch. That was her job—she sold time. When I first heard that I thought "this is incredible." She's the first person you meet in the book and then that chapter discusses timekeeping. So you learn about her job, who made the original clocks and how time shaped us.

All this is to say that I had to evolve as a materials scientist in order to write this book. I had to embrace stories to do that. When you write books that use stories, you write differently. There was a tremendous amount of research, too. I travelled all over the world to get the materials I needed to "rehydrate" these people. That was part of my own evolution. Writing this book was an adventure of a lifetime.

DR. LATANISION: Is your target audience largely young people, or how do you decide what audience you want to reach?

DR. RAMIREZ: The *Alchemy of Us* is a popular trade book. But when I wrote it, I structured it so that a smart 12-year-old could understand it. That came from my experience at Yale. I told the professors who gave *Science Saturdays* lectures to target it for smart 12-year-olds because I had talked to some folks in education and they told me that middle school is where kids get turned off from science. So I said, "Okay, explain things in a way that a smart 12-year-old could understand."

What's fascinating is that book received a young adult award but has also done well in older adult reader categories.

DR. LATANISION: If you were to look 5 years forward, what kind of books are you thinking of writing next? Do you have a list of topics that are on your mind?

DR. RAMIREZ: I have beta testers—my family members. I also stumble onto stories. My mom lives in Florida and there is a fort there called the Castillo de San Marcos. The walls are made out of coquina, a sedimentary rock made from crushed shells. When the British attacked the Spaniards there, they shot at it with cannonballs for almost a month. If the walls had been made of brick, they would have shattered and crashed to the ground. But that's not what happened. The walls swallowed the cannonballs, burrowing into them like earthworms. When I learned this, I said, "What?!" Here I am as a materials scientist and am learning about this for the first time. I wanted to buy a book about it but there wasn't one in the fort store. So that is how I decide what to write about.

You asked me what I'll be doing in 5 years. I have a whole bunch of picture books in me. I've written about 20. They haven't all found homes yet so I think that some of my time will be creating my own press to get some of these things out.

DR. LATANISION: You cannot build any engineering system, no matter what it is, without materials.

DR. RAMIREZ: Materials are everywhere. I have a couple of picture books that are on the horizon, but I also have another book for older readers that I'm starting to work on.

DR. LATANISION: I think you're at least the third writer we've had as part of this series— Henry Petroski and Andy Weir, who wrote *The Martian*, are the others. It's always interesting to me, because somewhere deep inside, there must be a pent-up urge to write on my part. I've never written anything like what you folks have written, but writing is something I just find interesting.

Were you always interested in writing, or is it something you had to cultivate?

DR. RAMIREZ: I think you have it in you, Ron because if you're saying that, it's true. When I was a professor, I was a writer because I was doing experiments so I could write about them. You might have been focusing on the experiment. I was focused on, "I can't wait to share this part." I think that professors are naturally writers. Some scientific journals are dry, but others contain beautiful language. You have to write things concisely to get a lot of information across and make sure someone else can repeat the process. It's really a craft. I knew that craft well, but I had to learn a new one. Writing for the public is very different from writing for journals.

DR. LATANISION: That's what I was about to say. What kind of research did you do when you were at Yale?

DR. RAMIREZ: I worked on shape-memory alloys, specifically, nickel-titanium alloys. The reason I found them fascinating was that I could heat a wire with a match and it would change shape. I was interested in looking at those phase changes.

We did a lot of work with electron microscopy to learn about how the transformation happens when we make thin films of it. When you have a metal wire, it operates one way. But when it's a thin film, it operates differently. We did a lot of work to figure out how to explain what that mechanism was on a small scale.

But probably the most important work I did was with a theorist. We were able to figure out how to predict the structure that starts from an amorphous material. You can heat it up, and we can tell you what the grain size will be ahead of time. As you know, being able to predict something is always fantastic.

Toni Morrison said, "If there's a book you really want to read but it hasn't been written yet, then you must write it."

MR. GIPSON: Listening to you talk about the way that your books develop and the way that book ideas come to you, reminds me of something that Toni Morrison said: "If there's a book you really want to read but it hasn't been written yet, then you must write it."

DR. RAMIREZ: I have that quote in *The Alchemy of Us*. It's in there because I would've loved to have read my book that as a kid—I'm not propping myself up, but there are other ways to understand materials science.

Ron, how many textbooks about materials science do you have?

DR. LATANISION: It is a huge number. I'm not sure.

DR. RAMIREZ: Are they all very different from each other?

DR. LATANISION: Materials science is a pretty broad field. I have books on physical metallurgy. I have books on electrochemical properties and materials and so on. It is a huge, long list.

DR. RAMIREZ: It's a huge field, but once we figure out what physical metallurgy is or what the introduction to materials science is, there is not a whole lot of variation in terms of how we explain it. I think I would have liked to have seen a little bit more. I would have liked to have known more about who the people behind materials science were. Who is Henry Bessemer? What is his story? And J.J. Thomson? When I found out that Henry Bessemer had severe bouts of seasickness, he became very interesting to me. And when I found out that J.J. Thomson was so absent-minded that one day his wife chased after him because she thought he didn't have his pants on because he had left pants on the bed and decided to wear another pair. I would have liked to have seen some more depth to these folks.

So again, as Toni Morrison said, "If there's a book you really want to read but it hasn't been written yet, then you must write it."

DR. LATANISION: One thing that you have done in your career that I think is really difficult is to have written effectively for expert audiences and non-expert audiences, including young readers. That is such a broad range. For *The Bridge* readers—for people in engineering and who are wondering, "How can I make my writing more accessible?" or who are interested in reaching broader audiences—what advice would you give to them?

DR. RAMIREZ: I think when I was a person who was a professor, I had to eat a lot of humble pie. When you're a professor, you think you know everything because the whole system tells you that you know everything. If I want to write for children and I'm not an expert in that, then I have to be willing to go to people who write in this field and say, "Does this work?" Writers use these things called critique groups. In the humanities, they do this all the time. You write something. You workshop it. You bring it to another group of people. They look at it and they tell you what could be enhanced and what the strengths are.

In the sciences, we do that in peer review, but it's very distant from the creative process because we use it after we have written things. In the humanities, it's done in the early stages. As such, I had to learn a new culture. I had to embrace being a beginner. I don't know everything. I'm smart, but I have to be willing to try new things and realize that another culture has a way to do this.

I guess I would say to the folks reading *The Bridge*: If you are moving into a new field, you have to be a beginner, but you have to be a good beginner. You cannot go in saying, "I know everything." You will miss things if you come from a posture of not being receptive and flexible.

DR. LATANISION: Obviously you enjoy writing and you're good at writing. But it strikes me that you need to reach kids who are a target audience. Do you speak to groups routinely? How do you manage that?

DR. RAMIREZ: I have been on speaking tours, and that put me in front of a lot of kids. For this new book that's coming out, I have scheduled talks at a lot of local libraries and a couple of schools as well. I'll also be on some podcasts. What I hope to do is get librarians excited about the book, because if they're excited about it, they'll put it on their shelves and that's how it will reach kids. For me, the pathway is through librarians.

DR. LATANISION: That's a good point. Again, thinking of my grandchildren, I wrote a book for them. It's a personal biography, with a little bit of history. I grew up in a household where I couldn't speak to my grandparents. They were Polish and Ukrainian, and they never learned to speak English. And I thought, I wish I had known more about them. I wrote a book for my grandchildren based on that beginning. I had a lot of fun doing it.

DR. RAMIREZ: Wonderful.

DR. LATANISION: One of the things that has always interested me is the avenues for people to write things like that, especially for academics. You get so involved in academia. When I was teaching at MIT, I didn't have time to write anything except proposals and books. How do you instill in professional engineers and scientists the wisdom that you have shown us today—trying to reach out to young people, encouraging and inspiring them. I'm thinking about your book on Jim West, *Spark*. It's a very inspirational book. How do you get to the point

where you can choose a topic that you feel will make that happen? How did you do that?

DR. RAMIREZ: For the folks reading *The Bridge*, I understand that they have lots of time constraints, so maybe they can't write a book on their own. But I do know that children's book authors need consultants. They want to make sure the science is accurate.

If someone reaches out, then be willing to work with them. This is how you can change how children relate to science because if they have your credibility and your expertise, the book is going to be better. That's one thing they can do.

When people go on sabbatical or after they're done with their professional careers and want to retire, they can also explore children's books.

Henry Petroski—he was just so prolific. He would write articles for *American Scientist*, and then those things became part of his books. He found some time to do that. Maybe he just took a couple of hours on Friday to do it. If it's important to you, carve out time for it.

DR. LATANISION: It's interesting. I knew Henry pretty well. He and I served on the US Nuclear Waste Technical Review Board for about 10 years together. We traveled the world together. It was while he was writing some of these books. He was a charming fellow; a brilliant writer and a great human being.

I sense in our conversation today that we've met another one who qualifies for some of those characterizations. Ainissa, I want to thank you for joining us. I've enjoyed this enormously. I have a great fascination for watching kids. The people I taught at MIT in my lab are like an extended family. I appreciate what you're doing. I just want to give you a round of applause for taking that initiative. You are a real credit to the engineering profession.

DR. RAMIREZ: Thank you. It is so touching, because I have to say, when I first left academia, I felt like I might be making a mistake. But now I feel that I am doing the work that I was designed to do.

NAE News and Notes

NAE Newsmakers

Kenneth E. Case, Regents Professor Emeritus, Oklahoma State University, has been posthumously named a **2025 Distinguished Alumni Award** recipient of Oklahoma State University. Dr. Case was widely regarded as one of the top industrial engineers in the world.

Robert C. Cohen, president, Digital, Robotics and Enabling Technologies, Stryker Corporation, received a **Science and Technology Medal** from the Research and Development Council of New Jersey in recognition of his leadership in surgical device and robotics innovation.

Avelino Corma, professor, Instituto de Tecnología Química, has received the BBVA Foundation **Frontiers of Knowledge Award in Basic Sciences** for fundamental advances in the catalysis field that have made it possible to "control and accelerate chemical reactions" and obtain products across multiple industrial processes, thereby "improving efficiency and reducing energy consumption." He shares the honor with John F. Hartwig, University of California, Berkeley, and Helmut Schwarz, Technical University of Berlin, Germany.

Birol Dindoruk, director, Interaction of Phase Behavior and Flow (IPB&F) Consortium, University of Houston, has been named a **Senior Member of the National Academy of Inventors**. NAI Senior Members are active faculty, scientists, and administrators from NAI member institutions who have "demonstrated remarkable innovation producing technologies that have brought, or aspire to bring, real impact on the welfare of society." They also have exhibited success in patents, licensing, and commercialization, while educating and mentoring the next generation of inventors.

John L. Anderson concluded his 6-year term as president of the NAE on June 30, 2025.

Bonnie J. Dunbar, John and Bea Slattery Chair Director, Aerospace Human Systems Laboratory AHSL, Texas A&M University, and **Vicki Ann Hollub**, president and CEO, Occidental Petroleum Corporation, have been **inducted into the Texas Woman's Hall of Fame**. Those inducted are honored in recognition of their exceptional achievements and lasting contributions to the history of Texas. Dr. Dunbar is acknowledged for her meaningful contributions to engineering design solutions for human space flight and for her leadership in STEM education. Ms. Hollub is acknowledged for her outstanding business leadership in a career spanning 40 years and three continents.

Liang-Shih Fan, Distinguished University Professor and C. John Easton Professor in Engineering, The Ohio State University, is the **first recipient of the Pierre Agostini Prize**, Ohio State's most prestigious honor for scholarly and artistic achievement. The award will be given annually to a faculty member whose research or creative work is recognized by peers as so groundbreaking and influential that it deserves to be called "world-class." Dr. Fan's

research focuses on creating cleaner, more efficient ways to produce energy, fuels, and chemicals while reducing pollution. In addition, Dr. Fan has been honored by the American Institute of Chemical Engineers with the creation of a new Institute-level high honor, the **L.-S. Fan Award for Advancing Fundamentals of Chemical Engineering**, which will recognize significant and new contributions to fundamental practice in chemical engineering. The inaugural award presentation is slated for the Fall 2026 AIChE Annual Meeting.

Dan M. Frangopol, Inaugural Fazlur R. Khan Endowed Chair of Structural Engineering and Architecture Emeritus, Lehigh University, is the inaugural recipient of the **Distinguished Service Award** presented by the International Association of Structural Safety and Reliability (IASSAR). Although the award was established in 2013 to recognize an IASSAR member who has provided long and sustained service to the organization, it was awarded for the first time to Dr. Frangopol at ICOSSAR'25 in June.

Anil K. Jain, University Distinguished Professor, Michigan State University, and **Michael I. Jordan**, Pehong Chen Distinguished Professor, University of California, Berkeley, have been awarded the BBVA Foundation **Frontiers of Knowledge Award in the Information and Communication Technologies**. They were chosen for their core contributions to machine learning by teaching computers to recognize patterns and make predictions based on large data sets used to power the development of biometrics and artificial intelligence.

Jay D. Keasling, senior faculty scientist at Lawrence Berkeley National Laboratory and CEO of the Joint BioEnergy Institute, University of California, Berkeley, was presented the second annual "OTC/NAI Innovator of the Year" Award. The award is presented annually to one individual selected from across the entire DOE complex. Professor Keasling received the award on June 24 during the 14th Annual Meeting of the National Academy of Inventors held in Atlanta.

Stephen R. Quake, Lee Otterson Professor, Stanford University, has been welcomed as a **Nonresident Fellow of the Salk Institute**. He joins a group of eminent scientific advisors who guide Salk's leadership. Dr. Quake will contribute his innovations in DNA sequencing technologies, diagnostic tools, and noninvasive prenatal testing to the Salk Institute.

John A. Rogers, Louis Simpson and Kimberly Querrey Professor of Materials, Northwestern University, has been elected a **Fellow of the Royal Society**. Professor Rogers becomes one of only three individuals in the world with membership in all three US academies (National Academies of Science, Engineering, and Medicine) and in the Royal Society.

Terrence J. Sejnowski, head of the Computational Neurobiology Laboratory and holder of the Francis Crick Chair, Salk Institute for Biological Studies, has been **elected to the Royal Society and the American Philosophical Society**. These prestigious elections recognize his outstanding leadership and extraordinary achievement in computational neuroscience.

Henry I. Smith, emeritus professor of electrical engineering, Massachusetts Institute of Technology, has received the **SPIE Frits Zernike Award for Microlithography** in recognition of outstanding accomplishments in microlithographic technology, as well as highly influential achievements in liquid-immersion lithography, achromatic-interference lithography, and zone-plate array lithography.

Molly Morag Stevens, John Black Professor of Bionanoscience, University of Oxford, has been elected a **Fellow of the Academy of Medical Sciences**, recognizing her contributions to advancing medical science. Her multidisciplinary research spans diagnostics, advanced therapeutics, and regenerative medicine, influencing global healthcare innovation.

2025 Japan-America Frontiers of Engineering Held at UCSD

The 2025 Japan-America Frontiers of Engineering Symposium (JAFOE) was held at the University of California, San Diego, on June 1–4. NAE partners with the Engineering Academy of Japan (EAJ) to carry out JAFOE symposia, which started in 2000. The conference organizing committee was co-chaired by NAE member Dr. **Christopher Schuh**, dean of the Robert R. McCormick School of Engineering and Applied Science at Northwestern University, and Dr. Chiharu Tokoro, professor in the Department of Sciences, Resources and Engineering at Waseda University.

The 2025 JAFOE symposium brought together approximately 60 early-career engineers from US and Japanese universities, companies, and government labs, where leading-edge

JAFOE attendees gather for a group photo in UCSD's Franklin Antonio Hall. Photo by: David Baillot/UC San Diego.

developments in four engineering topics—resurgence in fusion science and engineering, heterogeneous integration in semiconductors, clinical-grade wearable sensors, and sustainable ocean engineering—were discussed.

The "Resurgence in Fusion Science and Engineering" session provided an overview of obstacles that must be overcome in the development of future fusion power plants, focusing on the critical areas of plasma confinement, heating and current drive, materials science, and tritium fuel cycle. Speakers focused on the technological limitations and prospective development of current systems from advanced supercomputing magnets to actuators able to heat and sustain plasma efficiently. They also addressed the considerable challenges posed by extreme operating environments, such as neutron damage to structural materials and the need for effective tritium breeding. These techniques, participants said, should be integrated into a reliable, scalable energy system that emphasizes the role of innovative design concepts, advanced diagnostics, and computational modeling in accelerating fusion power plant development.

Semiconductor devices have long been miniaturized in two dimensions to improve performance and multifunctionality. While the 3-nm generation is already in mass production, it is expected to reach the limit of miniaturization soon. The alternative miniaturization technique, Heterogeneous Integration (HI), aims to improve performance, multifunctionality, and power saving by combining chips with various functions such as memory, communication, microelectromechanical systems (MEMS), and sensors into a single package, and is being actively researched. Speakers in the "Heterogeneous Integration in Semiconductors" session discussed the future of HI and the technological challenges to its realization. While HI has already been introduced in image sensors and uses a memory technology suitable for an AI called High Bandwidth Memory (HBM), these represent only a small part of HI's potential and the breadth of its possible applications.

Clinical-grade wearable sensors have become increasingly important in healthcare for real-time monitoring and early disease detection. These devices measure various parameters such as heart rate, oxygen levels, and blood glucose, providing non-invasive continuous tracking. Speakers in the "Clinical-Grade Wearable Sensors" session described the challenges wearable sensor technology faces. These include ensuring accuracy and reliability, particularly as factors like body movement and skin conditions can affect measurements. Talks in these sessions covered wireless wearable sensing for subsurface physiological fluid flow, next-gen wearable optoelectronics, mechanochromic polymers for developing wearable colorimetric force sensors, and architectures of smart contact lenses.

Oceans cover 70% of the Earth's surface and contain substantial renewable energy resources in the form of tidal currents, waves, surface winds, solar irradiance, and temperature gradients. Renewable energy in the oceans could satisfy global energy demands multiple times over. In the

final session, "Sustainable Ocean Engineering," presenters explored the engineering challenges and opportunities associated with ocean technologies, as well as advancements in sensing and forecasting technologies that will enhance our understanding of the marine environment and our impact upon it. Talks focused on offshore wind and marine energy, ocean carbon capture, advancements in sensing technology for monitoring the aquatic environment, and forecasting ocean conditions using multiscale meteorological analysis.

NAE president **John Anderson** opened the meeting with welcome remarks, followed by a video message from EAJ president Yuichiro Anzai and welcome messages from dean of the Jacobs School of Engineering at UCSD and NAE member, **Al Pisano**, and the symposium co-chairs, Chris Schuh and Chiharu Tokoro. This was followed by flash poster presentations and the symposium's two poster sessions, which served as an icebreaker and an opportunity for all participants to share information about their research and technical work. The posters were displayed throughout the meeting, which facilitated further discussion and exchange during coffee breaks.

The meeting's dinner speaker was SONE Kenko, Consul General of Japan in Los Angeles. [See https://www.linkedin.com/in/kenko-sone-00250217.] SONE is a career diplomat who focuses on supporting Japanese businesses, promoting environmental collaboration—particularly in clean technologies—and advancing the country's food exports. He spoke about his career path since coming to the United States in 1990 and how his mission is to deepen the enduring US-Japan alliance through friendship, cooperation, and proactive consular service.

After the second day's sessions and lunch, UCSD staff led groups on tours of their choice of either UCSD's Center for Wearable Sensors, Center for Wireless Communications, Supercomputing Center, or the Nanoscience, Nanoengineering, or Nanomedicine Research Facility (NANO3). The symposium wrapped up on the morning of day three with the final technical session.

The Grainger Foundation and the National Science Foundation provided funding for the meeting. The next JAFOE meeting will be held in 2027 in Japan.

In addition to the Grainger Foundation Frontiers of Engineering US-based symposia, NAE has other bilateral Frontiers of Engineering programs with Germany, China, and the European Union. FOE meetings bring together outstanding engineers from industry, academia, and government at a relatively early point in their careers, typically within 12 years of receiving an advanced degree. They provide an opportunity for participants to learn about developments, techniques, and approaches at the forefront of fields other than their own, something that has become increasingly important as engineering has become more interdisciplinary. The meeting also facilitates the establishment of contacts and collaboration among the next generation of engineering leaders. For more information about this activity, go to www.naefrontiers.org or contact Vernon Dunn at vdunn@nae.edu.

Artificial Intelligence in Engineering: NAE Regional Meeting at UC Berkeley

Engineers are harnessing the power of artificial intelligence (AI) to build a safer, more efficient tomorrow. Partnering with UC Berkeley, Lawrence Berkeley National Laboratory, and NVIDIA, the NAE's 2025 Regional Meeting gathered leaders from academia, industry, and research on May 15 to examine AI's transformative potential and the complex challenges that accompany its rise. The event explored the topic of Artificial Intelligence in Engineering through keynote talks, lightning sessions, and panel discussions.

The day began with a welcome session in UC Berkeley's Jarvis Auditorium. **Tsu-Jae King Liu**, dean of the College of Engineering at UC Berkeley and incoming NAE president, and Carol Burns, deputy laboratory director for research at Lawrence Berkeley National Laboratory, opened the meeting. Their opening was followed by a welcome video message from NVIDIA CEO **Jensen Huang** and an address from NAE President **John L. Anderson**, which emphasized the NAE's role in addressing engineering challenges and opportunities.

The opening keynote session focused on AI's role in infrastructure. **Kenichi Soga**, Donald H. McLaughlin Professor in Mineral Engineering and a distinguished professor of civil and environmental engineering at UC Berkeley, discussed how AI can revolutionize the way civil engineers approach aging infrastructure. Soga explained how engineers are designing machine learning models that

can detect weak points in systems like urban water pipes, predicting failures before they occur. These models could prevent damage and save thousands of dollars.

In the second keynote, Tianzhen Hong, senior scientist at Lawrence Berkeley National Laboratory, described how AI is helping make building operations more energy efficient, resilient, and demand flexible. Hong introduced the use of surrogate models that combine engineering and data-driven insights to deliver more accurate predictions across the building lifecycle, from planning to demolition.

In the afternoon keynote, Tejas N. Narechania, professor of law at UC Berkeley, raised critical concerns about AI's concentration of power and its implications for democracy, resilience, and equality. He cautioned that many AI models are designed with a preference for self-optimization, creating scenarios where systems could fail if dominated by a single provider that is unable to deliver. This creates tight supply constraints that make critical infrastructure vulnerable. He offered mitigating solutions, including establishing public options for data and cloud services and enacting nondiscrimination rules for AI model owners to ensure fair access and competition.

In her keynote, **Kristin Persson**, Daniel M. Tellep Distinguished Professor in Engineering at UC Berkeley, reflected on how engineering data collection has evolved from the time of Thomas Edison to today's AI-driven landscape. She highlighted the leaps in technological capability over hundreds of years and underscored that AI could streamline these leaps. Persson showcased how AI has enabled the discovery of innovative materials, including an alkaline cathode developed using AI-guided data analysis, and emphasized that we will continue innovation through AI.

In the closing keynote, Pieter Abbeel, professor in AI and robotics at UC Berkeley, dubbed the current era "the humanoid summer," describing how AI is driving rapid progress in humanoid robotics. Abbeel highlighted the use of tele-creating methods, where robots learn from human video demonstrations, and encouraged engineers to get involved in using simulation tools, even without physical robots. He noted that there is currently no clear consensus on how best to build AI for humanoids, making this an open frontier ripe for innovation.

A series of lightning talks showcased how AI is driving innovation across diverse disciplines, from scientific discovery and electron microscopy to healthcare, robotics, and data analysis. Speakers included Aditi Krishnapriyan, Mary Scott, Alane Suhr, Emma Pierson, Dani Ushizima, and Angjoo Kanazawa. The talk ended with a video of the Lawrence Berkeley National Lab.

The meeting closed with a panel discussion featuring Bryan Catanzaro, vice president of applied deep learning research at NVIDIA, and UC Berkeley professors **Ion Stoica** and Dan Klein. Moderated by Tsu-Jae King Liu, the conversation explored professional perspectives on the future of AI and its implications for engineering disciplines.

Panelists reflected on the ethical challenges posed by AI, including bias in data, the risks of centralization, and the importance of ensuring AI systems are transparent and trustworthy. They emphasized that as AI continues to accelerate, so too must industry, academia, and policymakers collaborate to ensure its responsible and inclusive deployment.

The discussion also addressed the pressures of keeping up with AI's pace of change and the need for cross-sector ecosystems that democratize access to AI tools and resources, particularly for small and mid-sized enterprises navigating rapid technological shifts.

The NAE Regional Meeting at UC Berkeley's central theme was that while AI transforms engineering disciplines, its future will depend on the ways we choose to govern, deploy, and scale it. Whether it's embedding sensors in aging infrastructure, designing ethical frameworks for AI models, or exploring the frontiers of humanoid robotics, the meeting highlighted the need for engineers to lead with curiosity, caution, and a commitment to equity.

Transforming Healthcare at the Intersection of AI and Medical Devices: NAE Regional Meeting with University of Minnesota and Medtronic

The NAE's final regional meeting of 2025 took place at Medtronic's Mounds View campus on May 21. The theme, "Transforming Healthcare at the Intersection of AI and Medical Devices," brought together leaders and innovators across fields to explore how artificial intelligence is a promising new tool in health outcomes, medical tools, and care systems.

The day opened with a keynote from **Omar Ishrak**, former chairman

and CEO of Medtronic, who delivered a high-level view of AI's transformative potential in medicine. Framing AI and the human body as "ever-changing frontiers," Ishrak emphasized that healthcare AI is just beginning but, if developed correctly, could lead to huge benefits in lifetime health.

The morning continued with a series of rapid-fire talks spotlighting applied innovation in neurology, implantables, and machine learning-enhanced therapy.

Zhi Yang, associate professor at the University of Minnesota, introduced Fasikl, an AI platform powering next-generation neurotech devices. Current products include a wearable for neural therapy and a brain-computer interface that enables real-time system interaction. Fasikl's cloud-based model allows for scalable signal interpretation and personalized neurological support.

Paul Gerrish, VP of technology development and Medtronic Fellow, pushed the audience to rethink conventional metrics for pain and healing. Challenging the limitations of the 1-to-10 pain scale, he outlined the development of smaller, smarter, and simpler implantable devices, moving toward less invasive, more intuitive technologies that integrate seamlessly with both patients and health systems.

Tay Netoff, professor at the University of Minnesota, shared information on an AI-driven neuromodulation device used to treat spinal cord injuries. By building patient-specific "preference maps," the system adjusts wave stimulation protocols to optimize therapeutic effects. In one compelling case, the approach enabled a patient to regain bladder function after 21 years, an outcome Netoff cited as evidence of AI's power to customize and transform neurological care.

David Rhew, global chief medical officer and VP of healthcare at Microsoft, delivered the afternoon keynote, calling for a paradigm shift from reactive to proactive healthcare. Rhew described the present-day system, which largely responds to symptoms only after they appear, and challenged attendees to envision a future in which AI enables earlier detection, targeted prevention, and continuous care. Rhew emphasized AI's role in bridging access gaps, especially for two vulnerable populations: undiagnosed individuals, who are often overlooked due to systemic inequities, and diagnosed patients, who face challenges managing chronic conditions consistently. By embedding intelligence into workflows and clinical pathways, Rhew sees a future healthcare system that is not only smarter but also more equitable and resilient by design.

The meeting concluded with a multidisciplinary panel featuring voices from Ecolab, Cargill, and 3M. Though representing different sectors, the panelists found common ground in the shared promise—and shared obstacles—of integrating AI into regulated medical environments.

Panelists discussed AI's ability to streamline processes, improve patient safety, and drive human-centered innovation. But they also pointed to persistent challenges, including cultural resistance, regulatory ambiguity, and the need for strong internal education around AI tools. One panelist summed up the moment this way: "This is the slowest time in innovation for the rest of our lives."

As healthcare AI accelerates, the panel underscored that collaboration across disciplines and industries will be essential to ensure progress is thoughtful, inclusive, and safe.

The 2025 NAE Regional Meeting with University of Minnesota and Medtronic made one thing clear: the future of healthcare will be shaped not just by algorithms or devices, but by the people who guide them. As AI continues to evolve, so must our ethical frameworks, regulatory systems, and collaborative networks. By placing patient needs at the center of innovation, the engineering community has the opportunity to build a healthcare future that is not only more advanced but more human.

EngineerGirl 2025 Writing Contest Winners

On June 25, the NAE announced the winners of its 2025 EngineerGirl Writing Contest. This year's contest prompt, "Innovating Smarter," asked students in elementary through high school to write an essay about a common object they would make "smart," and then consider what it would do, what it would need to function, and what could go wrong. Prizes were awarded to students based on grade level.

"Congratulations to the 2025 EngineerGirl Writing Contest winners for their inventive and thoughtful essays imagining smart innovations from everyday objects," said NAE President **John L. Anderson**. "These students demonstrated a strong grasp of both the possibilities and challenges of engineering design,

reflecting the curiosity and creativity that drive real-world innovation."

NAE congratulates the following first place winners:

- Olive Monrad, a fifth-grade student at Indian Springs Middle School in Keller, Texas, placed first among elementary school students for her essay "The Backpack of Tomorrow."

- Kendall Wilkerson, an eighth-grade student at the Academy of International Studies at Rosemont in Norfolk, Virginia, placed first among middle school students for her essay "The Smart Wardrobe."

- Aleena Shaji, a twelfth-grade student at Sandra Day O'Connor High School in Helotes, Texas, placed first among high school students for her essay "The Smart Solution to Hair Care Confusion."

Awards for contest winners are $1,000 for first place, $750 for second place, and $500 for third place. Winning entries, along with honorable mention entries, are published on the EngineerGirl website. Additional winners are listed below.

Elementary Winners:

- Second Place: Milana Kurpad, "Smart Plate: Safe and Enjoyable Eating Experience"

- Third Place: Vrinda A. Iyengar, "Smart Wearable Audio Recorder (SWAR)"

- Honorable Mention: Kiran B., "My Dumb Tongue"

- Honorable Mention: Sophia Tong, "The Future of Trash: The Smart Garbage Can"

Middle School Winners:

- Second Place: Minlu Wang-He, "Introducing iFridge"

- Third Place: Aaila Howard, "Medicine's BFF: How the Biometrics of Facial Rec and Fingerprints Improve Compliance"

- Honorable Mention: Aydina Johnson, "The SmartDesk: The Desk That Knows You're Brilliant!"

High School Winners:

- Second Place: Vivian Foutz, "Luna the AI Fridge: Revolutionizing Food Intelligence, Smart Living, and Global Sustainability"

- Third Place: Chloe Ko, "The Smart Playmat: Future of Language Learning"

- Honorable Mention: Seoyeon Shim, "Stepping Forward"

- Honorable Mention: Stephanie Wang, "Bringing the World Together: How AI Can Reinvent the Globe"

The NAE extends its congratulations to all this year's winners and participants in the 2025 EngineerGirl Writing Contest for their creativity and thoughtful contributions.

New Staff

The NAE Membership team welcomes Rachel Amhaus as a senior membership assistant. Rachel recently served as a program assistant for the Ocean Studies Board in the Division on Earth and Life Studies at the National Academies of Sciences, Engineering, and Medicine. In this role, she supported a range of studies and initiatives focused on coastal and marine environments and resources, managing logistics and contributing to programmatic efforts. Prior to her time at the National Academies, Rachel held two internships with the US House of Representatives, where she worked alongside congressional staff on legislative recommendations and policy development. She earned her bachelor's degree in business management with a minor in political science from Texas Tech University.

In her free time, Rachel enjoys reading, trying new restaurants, and spending time with her friends, family, and her cat, Norman. Originally from New Mexico, she also takes every opportunity to spend time outdoors and enjoy the sunshine.

Calendar of Meetings and Events

September 12	How Artificial Intelligence Is Reshaping Engineering Education and Practice Virtual Forum
September 14–17	The Grainger Foundation Frontiers of Engineering 2025 Symposium University of Pennsylvania
September 17	Frontiers of Engineering's 30th Anniversary Gala Penn Museum, Philadelphia
September 18	NAE Member-Led Event: Enabling Materials for Clean, Renewable and Sustainable Energy Virtual
October 3	NAE Council Meeting
October 5–6	NAE Annual Meeting
October 20–23	2025 EU-US Frontiers of Engineering Bordeaux, France
October 25	NAE Member-Led Event: Materials for Microelectronics Virtual
November 4–5	NAE Member-Led Event: Innovative/ Blue-Sky Ideas for Noise Control

In Memoriam

David Vernon Boger, 85, Emeritus Laureate Professor, University of Melbourne, died July 5, 2025. Professor Vernon was elected in 2017 for discoveries and fundamental research on elastic and particulate fluids and their application to waste minimization in the minerals industry.

John R. Casani, 92, special assistant to the director (retired), NASA Jet Propulsion Laboratory, Caltech, died June 19, 2025. Dr. Casani was elected in 1989 for pioneering systems engineering of planetary spacecraft and for leadership of spacecraft engineering and science teams.

Ivar Giaever, 96, chief technical officer, Applied BioPhysics Inc., died June 20, 2025. Dr. Giaever was elected in 1975 for contributions in the discovery and elaboration of electron tunneling into superconductors.

Barry M. Horowitz, 82, professor of systems engineering, University of Virginia, died July 20, 2025. Dr. Horowitz was elected in 1996 for contributions in the field of military and civilian aeronautical and information systems engineering.

Pradman P. Kaul, 78, president and CEO (retired), Hughes Communications Inc., died May 3, 2025. Mr. Kaul was elected in 2004 for leadership in the development of satellite communication networks.

George Leitmann, 99, professor emeritus of engineering science and professor in the Graduate School, University of California, Berkeley, died May 19, 2025. Dr. Leitmann was elected in 1982 for contributions to the theories of optimal control and dynamic systems, and the applications of these theories to engineering, biological, and social systems.

Benjamin Y. Liu, 90, retired CEO and president, MSP Corporation, died June 30, 2025. Dr. Liu was elected in 1987 for pioneering research on the design of novel aerosol instrumentation, and for contributions to the understanding of fine particle behavior and to the prediction of availability of solar radiation.

Hani S. Mahmassani, 69, William A. Patterson Distinguished Chair in Transportation and director of the Transportation Center, Northwestern University–Evanston, died July 15, 2025. Dr. Mahmassani was elected in 2021 for contributions to modeling of intelligent transportation networks and to interdisciplinary collaboration in transportation engineering.

Shiro Matsuoka, 95, adjunct full professor, Columbia University, died May 18, 2025. Dr. Matsuoka was elected in 1989 for pioneering contributions to the methodology for prediction and explanation of the aging and strain history of mechanical properties of solid engineering polymeric materials.

Nelson L. de Sousa Pinto, 93, retired consulting civil and hydraulic engineer and independent consultant, died June 8, 2025. Dr. Pinto was elected an international member in 1995 for solutions to resolve cavitation from high-velocity flows, together with contributions to and international leadership in hydropower design.

Robert A. Pucel, 99, retired consultant, RCP Consultants, died July 24, 2025. Mr. Pucel was elected in 1994 for contributions to semiconductor device theory, integrated circuit technology, and microwave system applications.

George E. Smith, 95, head, MOS Device Department (retired), AT&T Bell Laboratories, died May 28, 2025. Dr. Smith was elected in 1983 for the invention of the charge-coupled device and contributions and leadership in the field of electron devices.

Alejandro López Valdivieso, 71, profesor investigador area de ingenieria de minerales, Universidad Autónoma de San Luis Potosí, Mexico, died October 27, 2024. Professor Valdivieso was elected an international member in 2021 for contributions to the processing of complex sulfide ores and educational leadership.

Ward O. Winer, 88, Eugene C. Gwaltney, Jr. School Chair Emeritus, Georgia Institute of Technology, died May 25, 2025. Dr. Winer was elected in 1988 for significant contributions to the understanding of lubricant rheology and thermal phenomena in tribology, and for advancement of tribology education.

John A. Young, 93, retired president and CEO, Hewlett-Packard Company, died May 26, 2025. Mr. Young was elected in 1991 for leadership in the electronics industry.

Invisible Bridges

When AI Dies

Guru Madhavan is Norman R. Augustine Senior Scholar and senior director of programs at the NAE.

A brush with death sharpens our focus. When the Supreme Court forced TikTok to choose between sale and silence, 170 million Americans glimpsed the loss of a dopamine-driven feed powered by an artificial intelligence (AI) moving billions in commerce. That fragility reminds us that a world built on intelligent systems can vanish suddenly, leaving little trace.

The tech industry celebrates each AI birth—sharper reasoning, smoother conversation, slicker images—but it rarely acknowledges AI mortality. This culture of disposable intelligence carries, though, both market and moral costs. Microsoft's Tay lived and died in a feverish 24-hour cycle. Google's Duplex withered after early promise. IBM's Watson for Oncology faded without a eulogy, forcing hospitals to adapt. Tesla's shift from radar to vision unsettled its systems, demanding reconfiguration. These departures seldom appear in investor presentations; they are obituaries written in invisible ink.

When AI dies, it follows three patterns:

First: abrupt termination. Core systems shut down and leave vacuums. When platforms vanish, digital communities scatter and the algorithms that powered commerce or secured transactions disappear. Adobe's Flash discontinuation, although not AI, left agencies scrambling for alternatives for a utility once thought permanent. When DeepMind retired AlphaGo, access ended to a system that had reshaped a 2,500-year-old game. Microsoft folded Bing Chat into Copilot, altering how users accessed its tools. Google's Gemini restructuring stirred unease. Each shift required rapid consumer adjustments, often amid uncertainty about continuity.

Second: gradual obsolescence. Systems that once seemed indispensable lose relevance as conditions shift. Legacy COBOL programs still anchor core banking workloads, carried forward by necessity. These aging sentinels, still guarding billions in transactions, grow increasingly blind to sophisticated threats. IBM's punch cards once powered entire industries before fading into obsolescence. The telegraph, once as vital as AI today, disappeared as a mainstream service, leaving rusted wires as its epitaph. Without planning for graceful exits, AI risks the same fate.

Third: residual influence. The mark of defunct technologies lingers long after they disappear. Despite detailed documentation, much of NASA's Apollo know-how lived in engineers' minds. When they retired, gaps opened and vital knowledge was lost: why certain materials were used, how systems were backed up. The rotary telephone is long silent, yet its echoes remain in the dial tone and in the way we still "hang up" a call. AI systems, too, leave embedded assumptions. Even updated facial recognition models inherit biases from predecessors, quietly embedding vulnerabilities long after their code has gone cold.

Services like Gmail reflect all three patterns. Abrupt termination: a cyberattack could erase emails and authentication histories (indeed, in 2011 a software bug wiped some accounts before Google restored them from tape, and in 2020 global outages underscored operational dependence). Gradual obsolescence: outdated software may misclassify malicious emails and files as legitimate. Residual influence: algorithm-optimized text prediction

erodes individual voices and creates patterns that can be exploited. We have stored our thoughts on platforms we neither own nor replace, leaving us as digital hostages vulnerable to risks we barely understand.

The designer Joe Macleod coined *endineering* to describe how products and services should be designed for closure. The same principle belongs in AI. Systems that die should not leave voids but relay knowledge forward, like fallen trees whose decay fosters seedlings, passing on ecological knowledge. Applied here, endineering means designing for continuity and treating intelligence as enduring knowledge rather than disposable technology. When IBM retired Watson for Oncology, its underlying methods and data informed other medical research efforts—showing how even endings can contribute to new beginnings. Dead systems should nourish successors rather than vanish, ensuring that decline becomes preparation for growth.

Forward-thinking organizations have considered this issue and implement critical practices to address it: they document institutional knowledge beyond technical specifications, track how teams adapt to technology, and conduct premortems to anticipate failures. This discipline fuels a competitive edge during transitions.

We have built AI into a dazzling but deficient genius, a machine of vast memory with no legacy. TikTok's fragility demonstrates how regulation, political considerations, or other shocks can unravel years of algorithmic craft in a moment. As our dependence on it deepens, the challenge is no longer how we give life to AI, but how we prepare for its afterlife.

Future-proofing requires more than continuity. It calls for blueprints that transfer knowledge, threat models that account for transitions, and designs that compost old systems into nutrients for what comes next. Good engineering has always understood that knowledge is meant to endure and guide in practice. If we abandon that precept, we risk deleting brilliance: all processing, no posterity.

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