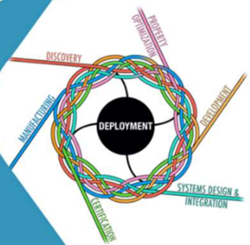
Accelerating Materials Solutions to Meet National & Global Challenges



A Workshop in Support of the MGI Strategic Plan

Subcommittee on the MGI

Accelerated Materials Experimentation Enabled by the Autonomous Materials Innovation Infrastructure (AMII)
A Workshop Report

Date:	June 10th-11th, 2024
Time:	8.00 AM – 5.00 PM
Venue:	National Science Foundation (NSF) Room 2020/2030 2415 Eisenhower Ave Alexandria, VA 22314

Organized by:
Materials Genome Initiative (MGI) Autonomous Materials Innovation Infrastructure Interagency Working Group (AMII-IWG) in support of the MGI 2021 Strategic Plan.

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Federal Agencies

Advanced Research Projects Agency - Energy (ARPA-E)
Air Force Research Laboratory (AFRL)
Defense Advanced Research Projects Agency (DARPA)
Department of Commerce (DOC)
Department of Energy (DOE)
National Aeronautics and Space Administration (NASA)
National Institute of Standards and Technology (NIST)
National Institutes of Health (NIH)
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Industry and Other

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IBM Research
Johns Hopkins Applied Physics Laboratory
Lam Research
Lockheed Martin
Merck & Co., Inc.
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DISCLAIMER: Summaries and suggestions within this report represent the discussions during the meeting and do not necessarily reflect the views of specific individuals, institutions, or government agencies involved in the workshop. Inventories and gaps are derived from inputs collected at the workshop based on the knowledge and experiences of different participants. They are not comprehensive and do not reflect the opinion of all attendees. Inclusion of specific programs or resources, including commercial products, are provided for informational purposes and reflect the conversation during the meeting and do not indicate endorsement in any way.

*Some representatives from federal agencies attended as observers, others as participants.

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Executive Summary

The Materials Genome Initiative's Interagency Working Group on Autonomous Materials Innovation Infrastructure (AMII-IWG) held a workshop hosted by the National Science Foundation Division of Materials Research on June 10-11, 2024 to develop a baseline of current capabilities and gaps in the United States (U.S.) Autonomous Materials Innovation Infrastructure (AMII). The AMII includes Autonomous Experimentation (AE), a revolutionary new way of doing research which accelerates advances and multiplies researcher effort in materials research and development (R&D) by exploiting advances in artificial intelligence (AI), autonomous systems, and automation.

Advances in materials are key to realizing significant improvements in diverse areas such as human health and welfare, energy and environment, global economic competition, and national security. AE has the potential to significantly benefit these national priorities by accelerating the insertion of new materials from decades to years.

Overall, AE is at an early stage of development, with key demonstrations of accelerated research and productivity. The first workshop breakout session focused on the landscape of the current AMII, identifying important existing resources by materials class. Summaries of the resources identified, and the corresponding breakout conversations are provided for each materials class within this report. A full list of resources identified, including in the pre-meeting information gathering process, is provided in the Appendices.

The afternoon breakout sessions focused on gaps in the current infrastructure. There were several common themes for gaps in the AMII across the breakout sessions and panel discussions. Foremost, the workshop participants saw a clear need for significant development of infrastructures for autonomous experimentation for materials R&D. Automation in experimental hardware was identified as needing development for materials synthesis, characterization, testing and sample exchange. Additionally, new AI decision methods for materials research are needed, along with standardized data structures and representations, as well as better sharing and reproduction of data and results. Finally, workforce development was uniformly identified as a critical gap for AI-Driven AE materials research.

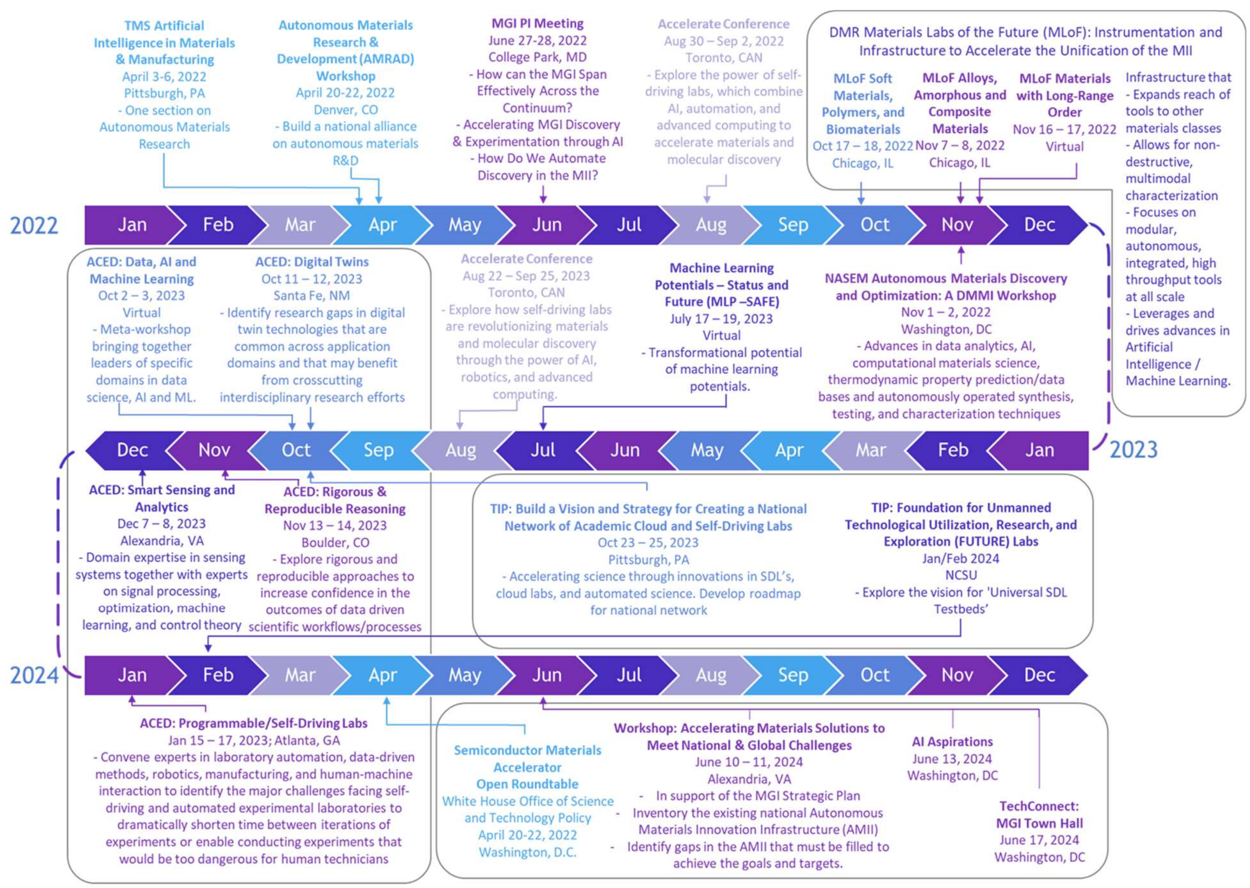
Finally, the workshop participants emphasized the importance of strong industry, university, government collaboration and suggested potential public/private partnerships or consortia to advance the U.S. Autonomous Materials Innovation Infrastructure in the United States.

Introduction and Motivation

Purpose of the Workshop

Materials are ubiquitous and pervasive. They form the critical building blocks that technology and innovation rely upon, and their development and deployments unleash new capabilities and fuel economic growth. Advanced materials are key elements for the entire range of innovation demands, from solving societal challenges to developing national security related capabilities. The Nation's ability to develop and deploy advanced materials rapidly and cost-effectively is a key component to advancing U.S. competitiveness and national security. The materials development and innovation enterprise is often rooted in and springs from fundamental materials research, i.e., materials research that, initially, may not necessarily target a specific device or application, but is also fueled by application-driven needs. The materials enterprise spans the entire technology development pathway from fundamental research through scale up and commercialization. The agencies participating in the Materials Genome Initiative (MGI) use their respective roles and responsibilities to span this entire spectrum to accelerate materials design through deployment. The United States is home to a robust industrial market investing in translating fundamental to applied research either in-house, or by leveraging federally funded research advancements to increase their national and global competitiveness.

The rapid emergence of digital tools, ranging from artificial intelligence/machine learning (AI/ML), and other data analytics methods, coupled to robotics and automation, can yield AE workflows. AE holds tremendous potential to revolutionize materials R&D. Federal agencies and private enterprises have been investing in developing the necessary infrastructure to accelerate this process - the Materials Innovation Infrastructure (MII) as outlined in the 2021 MGI Strategic Plan. Over the course of the last several years, there has been an increase in the number of workshops, conferences, and other activities related to these emerging techniques. A small subset of these activities is outlined in the figure below (not an exhaustive list.)



The Accelerating Materials Solutions to Meet National and Global Challenges Workshop was organized to complement these workshops with a focus on understanding the current U.S.

landscape of capabilities. Over 80 participants representing academia, industry, and 16 federal agencies, identified more than 500 activities ranging from small groups to broad multi-organization initiatives. Activities spanned all types of materials and tools throughout the material development and maturation process.

Organized by the Autonomous Materials Innovation Infrastructure Interagency Working Group (AMII-IWG) of the Material Genome Initiative (MGI), this workshop aimed to catalog existing efforts, primarily in the United States, to provide a baseline for follow-on MGI efforts—both among the participating agencies and in collaboration with the private sector. The outputs of this workshop can be leveraged to assess the progress of MGI activities to create an interoperable MII, for critical gap analyses and road mapping to focus the efforts of agency, interagency, and public-private partnerships, and for additional landscape surveys to identify additional opportunities for collaborative efforts.

Overview of MGI and the MII

The Materials Genome Initiative (MGI) was launched in 2011 with the recognition that there were profound advances in materials R&D that were being enabled by the tight integration of experiment, computation, and data that comprise the “Materials Innovation Infrastructure” or MII. While there were demonstrated successes that inspired the MGI, they were isolated, and barriers to widespread application of these approaches were substantial. The MII had the potential to dramatically accelerate the discovery, design, development, and deployment of new materials into manufactured products, with consequent impacts on the diverse areas where materials innovation is often the crucial technology needed for progress. Clean energy, improved human health, enhanced national security, and any number of critical emerging technologies could all be made more accessible by application of MGI principles.

At its founding, a significant motivator for the MGI was the recognition that computational methods and hardware had progressed to the point where modeling could and should be viewed as an equal partner in the materials R&D enterprise. Capitalizing on these advances required the R&D community to embrace materials simulation as a first-class research product, and to more tightly integrate such simulations into materials research. Thus, the early days of the MGI were dominated by discussions on how to best realize proven (but not-widely adopted) approaches like integrated computational materials engineering (ICME) and similar paradigms for accelerating materials R&D.

In tandem with this focus on computation was an acknowledgement that integration of computation and experiment would require a significant focus on data. Whether the data came from experiment or computation, the flows of the data were the underlying raw material of the MII. Thus, while the ultimate goal of the MGI is the synthesis of new materials for deployment into manufactured goods, the data was the means to this end. This focus on data infrastructures was quite new to materials R&D, requiring significant changes in incentives for the research community, including the need to protect intellectual property and export-controlled information.

The focus on data implied an exciting possibility, namely the advent of ubiquitous "data-driven" materials R&D. This was first suggested in the context of the MGI very near its inception and is called out in the 2014 MGI strategic plan. This recognition presaged the imminent rise of machine learning/artificial intelligence that has captured the public imagination and, perhaps more importantly, risen to significant prominence in the materials R&D endeavor.

The advent of AI approaches to materials R&D is enormously promising, with the potential to both provide models of materials systems where no models were currently available, and also to massively accelerate modeling where physics/chemistry models are well understood. However, to achieve this end, there is a need for far more data than is currently available, although databases of computed data were an excellent beginning to resolving this conundrum. What is now needed is a way to substantially lower the cost for experiments while accelerating the rate of such experiments. Thus, the MGI has turned its focus to experiment. The development of autonomous experimentation (AE) methodologies (the autonomous materials innovation infrastructure or AMII) is the key to unlocking the door to vast troves of materials data, rapidly designing new materials with fit-for-purpose properties, and thereby realizing many of the goals of the MGI.

Accelerated Materials R&D Enabled by Autonomous Experimentation

Autonomous experimentation (AE) is the coupling of automated experimentation and in situ or in-line analysis of results, with artificial intelligence (AI) to direct experiments in rapid, closed-loops to speed the research process. AE is enabled by several technological advances coupled to existing techniques that need to be integrated into the AMII. The basic elements are

1. Rapid/automatic characterization enabled by AI-trained pattern recognition
2. Based on the results of characterization, decision algorithms (like Bayesian optimization) enable tradeoffs between exploration and goal-seeking behavior in the search for desired performance characteristics, and
3. Automation, enabling robots to carry out the experimental tasks prescribed by the decision algorithms.

These steps can be carried out in a closed loop, yielding AE workflows. What follows below is a more detailed look at the elements of AE, and some of the supporting infrastructures.

High-throughput screening methods allow rapid and parallel testing of large numbers of materials or synthesis methods to identify best-fit-for-purpose for an R&D goal.

Computational models employ physics and chemistry knowledge to provide predictions on the relationships between materials composition, internal structure (microstructure), properties and performance. Incorporating the knowledge embedded in such models into AE workflows can accelerate the R&D process by reducing the search to only include regions mandated by the laws of nature. The best methods to join computational modeling and simulation with AE is an active area of research.

Artificial intelligence is defined in 15 U.S.C. 9401(3) as a machine-based system that can, for a given set of human-defined objectives, make predictions, recommendations, or decisions influencing real or virtual environments, and **machine learning (**ML**)** is a subset of AI associated with algorithms that enable systems to identify patterns and make decisions, and, importantly, to learn through the acquisition of more data. It is not uncommon for practitioners in materials R&D to use the terms AI and ML interchangeably.

Automation is a key element of AE, enabling robots and other machines to do repetitive tasks that would otherwise be performed by human researchers.

Autonomy is the delegation of decision authority to act by a higher-level authority (i.e., human researcher) to a delegee (i.e., the AE system). This authority to act is bounded and revokable and does not absolve the human researcher of responsibility for actions by the delegee.

Characterization is a broad term that captures methods for determining what material has been made, including its compositional makeup (which likely varies from point-to-point) and the internal structures and interfaces at a range of scales from nanometers to macroscale. ML techniques have dramatically improved R&D practitioners' ability to rapidly identify patterns, enabling accelerated characterization.

FAIR is an acronym for findable, accessible, interoperable, and reusable data. It is a useful suite of concepts for determining whether a data resource and the workflows of an R&D operation have been optimized to reduce the friction in their use of data, and to allow collaborators to make maximum use of other data. Data is housed in data repositories, which can be assessed against the FAIR rubric to see if it meets the demands of the R&D community.

Benefits of Accelerated Materials Experimentation

Continued investment in the next generation of scientific infrastructure is needed for the United States to maintain its leadership position in scientific innovation. Strategic leadership is not conferred solely through new infrastructure, but through the new paradigms of scientific discovery that come with technological advances and the community that forms around this infrastructure. AMII combines a number of technological advances: incredible advances in AI, affordable, sufficiently reliable robotics, and advances in characterization and high throughput synthesis. The synthesis of these technological shifts helps realize new paradigms of scientific discovery and enables greater speed and effectiveness of scientific exploration, reduces cost and human effort in experimentation, accelerates the innovation to manufacturing pipeline, and democratizes science for researchers. This transformative set of technologies, integrated together as AMII, serves to continue advancing the development of materials innovation as a core strategic advantage and national capability for the U.S.

One of the key benefits of realizing AMII is greatly increasing the pace at which scientific experiments are executed. Autonomous experimentation allows for asynchronous workload scheduling and continuous experimental campaigns, rather than being limited by human working hours or other constraints. The increase in speed of scientific experimentation not only allows more experiments to be performed but shifts from a paradigm of probing the frontier of materials through individual experiments to enabling comprehensive mapping of the materials frontier. Increasing the speed of scientific experimentation does not just linearly increase the number of experiments but fundamentally shifts how scientific exploration is enabled through prioritized and automated experimentation.

AMII can also deliver enhanced effectiveness of discovery at reduced fiscal and labor cost. AMII amplifies human effort and agency by reducing menial, repetitive tasks which can burn out early career researchers in the lab today. Instead, AMII enables more seamless manifestation of human-generated scientific ideas through autonomously generated experimental results, while improving labor productivity of the materials development and innovation enterprise, reducing the cost of scientific experimental campaigns, and magnifying the impact of research funding.

Traditionally, scientific discoveries of new materials take over a decade to scale to commercialization, even in successful cases. Developing AMII can shrink the valley of death from translating laboratory research into commercialized technology as automation brings the lab one step closer to the manufacturing line. Incorporating automation equipment and robotics improves reproducibility and ensures that the experimental synthesis pathways being explored are already automation-ready to scale towards manufacturing. Developing AMII can help the United States translate its historical strategic advantage in basic discoveries into domestic, commercial applications and internationally competitive industries.

Similar to how cloud computing democratized access to computing infrastructure, AMII is capable of democratizing and broadening researcher access to unified MII platforms, independent of location. Digital twins and cloud-based laboratory operations allow researchers across the country to remotely schedule workloads and view experimental campaign results in real time. Integrating existing characterization and synthesis equipment into AMII can improve the equipment utilization rate, for example by allowing instrumentation to run autonomously 24/7 without human intervention. Continuous operation not only lowers capital cost for facilities but also enables more users to leverage existing user facilities and improves researcher access to equipment and facilities that may otherwise be at capacity.

Workshop Description

What follows below is a description of the workshop, as well as a discussion of the analysis performed to develop the graphical representations of the outputs of the landscape exercises (detailed agenda found in **Appendix A**). The workshop was attended by over 80 participants across academia, industry, and government (see attendee list in **Appendix B**) and was split into four components: two panel discussions and two breakout discussion sessions.

Panel 1: The Autonomous Materials Innovation Infrastructure (AMII) and Global Challenges

The first panel on "The AMII and Global Challenges" was moderated **Jim Warren** (NIST) and included panel members **Jae Hattrick Simpers** (University of Toronto)**, Milad Abolhasani** (NCSU), **Rob Moore** (ORNL), **Shijing Sun** (University of Washington), **Javier Read de Alaniz** (BioPACIFIC MIP), and **Theresa Mayer** (CMU). This panel focused on the following discussion points:

Discussion Points

- Scientific challenges that are ripe for the application of the AMII
- Status of developed infrastructures to meet demands/requirements of identified challenges
- Areas/capabilities/mechanisms that are under-resourced, reasons for under-resourcing, and potential solutions to address this
- Potential immediate stakeholders and possible engagement models
- Ideal ways for the MGI community to collaborate and coordinate as a part of the publicly supported autonomous experimentation (AE) community
- Opportunities to keep the momentum going at the Federal level

During the panel, several key scientific challenges emerged as ripe for the application of the AMII. The convergence of the data age with the industry age presents both opportunities and challenges in terms of enabling infrastructure. Bridging the gap between these realms is essential for accelerating scientific progress. To achieve progress, there is a need for autonomous instrumentation / experimentation capable of generalizing to novel datasets and ensuring interoperability across different systems. This interoperability would not only multiply the effectiveness of researchers and speed up discoveries, but also enable access to reliable and high-quality data. Participants emphasized the need for knowledge-sharing and discussed the specific hardware required for discovery. Participants also highlighted the importance of robust data management and how better understanding capabilities can help build effective bridges between fields. A critical aspect discussed was the importance of not relying on big data abstractly but focusing on the specific data representations of materials in fundamental workflows, and autonomously acquiring the most valuable data.

Reflecting on the current status of the AMII, the discussion noted the significant excitement and successes already achieved. Investments in robotics and materials have led to the creation of numerous autonomous laboratories, embracing the automation of science and moving towards its democratization. However, it was acknowledged that more needs to be done, particularly in choosing specific areas to delve deeper and developing infrastructure sharing to accelerate progress. The importance of cross-disciplinary efforts and workforce training was emphasized. Participants called for the democratization of knowledge, drawing parallels with the development of cloud-computing democratizing access to software, requiring both better access to experimental instruments and to others' data. The participants advocated for building new communication channels between universities, national labs, and industry. Additionally, restructuring data to achieve vertical integration was identified as a crucial need in the future.

The discussion also explored why certain areas are under-resourced. Key points included the necessity of ensuring investments in security from the outset and addressing the lack of training in building, operating, and maintaining autonomous labs in the United States. Participants stressed the importance of starting conversations now to address these gaps. While many tools have been developed independently, there is a need to connect them and enhance data management through more effective coordination of efforts. Collectively defining incentives and identifying a form of rewards programs was suggested as a potential solution to encourage participation and investment in these areas. The panel highlighted the need for a concerted effort to ensure that the necessary resources, training, and infrastructure are in place to support the burgeoning field of autonomous experimentation.

Working Session 1: Inventory of the Existing National Autonomous Materials Innovation Infrastructure (AMII)

To achieve the goals of the workshop, the MGI AMII-IWG identified 10 breakout groups to represent the materials domains: Structural Metals, Structural Ceramics, Structural Soft Matter, Structural Composites, and Structural "Other", as well as Functional Metals, Functional Ceramics, Functional Soft Matter, Functional Semiconductors, and Functional "Other".

It was recognized that these bins are not perfect representations of the entire materials universe, but organizers decided these categories would be adequate to cover a large proportion of materials research (with the “Other” categories provided to help capture additional important infrastructures). Participants were asked to self-select between the 8 categories (excluding other) during the registration process, and two breakout leads were recruited to facilitate and capture the discussions. Given preferences of participants, teams were assigned to the following 7 topics, as there were not enough participants selecting Structural Composites. Both groups Functional Ceramics and Functional semiconductors garnered enough interest to necessitate splitting into two parallel but collaborative groups:

Structural Metals	Functional Metals
Structural Ceramics	Functional Ceramics A
	Functional Ceramics B
Structural Soft Matter	Functional Soft Matter
	Functional Semiconductors A
	Functional Semiconductors B

Additionally, the materials development continuum was divided into 6 broad segments: Discovery & Experimental Design, Synthesis, Characterization, Scale-Up/Manufacturing, Certification/Qualification, and Recycling/End-of-Use. Each existing infrastructure or capability was assigned to one (or multiple) segments, and further categorized by the following topics within each segment: Models, Data and Information Handling, Autonomous Instrumentation, Software, Sample Handling / Handoff, and Decision Tools with the following broad definitions:

A. Models: In the realm of materials development, models refer to mathematical or computational representations of physical processes, properties, or phenomena. These models can range from simple empirical equations to complex simulations based on fundamental principles of physics and chemistry. They are used to predict material behavior under various conditions, optimize material properties, and guide experimental design.

B. Data & Information Handling: This category involves the collection, storage, organization, and analysis of data and information related to materials development. With the advent of high-throughput experimentation and advanced characterization techniques, large amounts of data are generated at every stage of the materials development process. Effective data handling involves ensuring data integrity, accessibility, and security, as well as employing techniques such as data mining and machine learning to extract meaningful insights from the data.

C. Autonomous Instrumentation: Autonomous instrumentation refers to the use of automated or self-regulating instruments and systems in materials R&D. These instruments can perform tasks such as synthesis, characterization, and testing with minimal human intervention. Examples include robotic sample handling systems, automated microscopy platforms, and self-calibrating sensors. Autonomous instrumentation accelerates the pace of materials discovery by enabling high-throughput experimentation and continuous operation.

D. Software: In materials development, software plays a crucial role in facilitating data analysis, modeling, simulation, and experimental control. This includes both commercial software packages tailored for specific tasks (such as finite element analysis or molecular dynamics simulations) and custom-developed software tools designed to address the unique challenges of materials research. Software enables researchers to visualize complex data, simulate material behavior, and optimize experimental parameters, ultimately accelerating the development of new materials and processes.

E. Sample Handling/Handoff: Sample handling refers to the processes involved in preparing, transporting, and transferring material samples within the materials development workflow. This includes tasks such as sample synthesis, preparation for characterization, and distribution to different research groups or facilities. Efficient sample handling is essential for ensuring reproducibility, minimizing contamination, and maximizing the throughput of experiments.

F. Decision Tools: Decision tools encompass a variety of techniques and methodologies used to support decision-making throughout the materials development process. These techniques include methods for experimental design, optimization, risk assessment, and resource allocation. Decision tools may range from simple heuristic guidelines to sophisticated algorithms based on statistical analysis and optimization theory. By providing quantitative insights into the trade-offs and uncertainties associated with different options, decision tools help researchers make informed decisions and prioritize their efforts effectively.

In Breakout Session 1, the individual groups were asked to identify current capabilities across the entire materials development continuum for each of the 9 groups. For example, in Structural: Metals, participants were asked to discuss, identify, and fill in existing capabilities on the following graphic via sticky notes that capture relevant information on hard-backed posters at their table:

	Discovery & Experimental Design						Synthesis					
	Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools	Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Metals	1A	1B	1C	1D	1E	1F	1G	1H	1I	1J	1K	1L
	2A	2B	2C	2D	2E	2F	2G	2H	2I	2J	2K	2L
	3A	3B	3C	3D	3E	3F	3G	3H	3I	3J	3K	3L
	4A	4B	4C	4D	4E	4F	4G	4H	4I	4J	4K	4L
	5A	5B	5C	5D	5E	5F	5G	5H	5I	5J	5K	5L

	Characterization						Scale-Up / Manufacturing					
	Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools	Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Metals	1M	1N	1O	1P	1Q	1R	1S	1T	1U	1V	1W	1X
	2M	2N	2O	2P	2Q	2R	2S	2T	2U	2V	2W	2X
	3M	3N	3O	3P	3Q	3R	3S	3T	3U	3V	3W	3X
	4M	4N	4O	4P	4Q	4R	4S	4T	4U	4V	4W	4X
	5M	5N	5O	5P	5Q	5R	5S	5T	5U	5V	5W	5X

	Certification / Qualification						Recycling / End-of-Use					
	Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools	Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Metals	1Y	1Z	1AA	1BB	1CC	1DD	1EE	1FF	1GG	1HH	1II	1JJ
	2Y	2Z	2AA	2BB	2CC	2DD	2EE	2FF	2GG	2HH	2II	2JJ
	3Y	3Z	3AA	3BB	3CC	3DD	3EE	3FF	3GG	3HH	3II	3JJ
	4Y	4Z	4AA	4BB	4CC	4DD	4EE	4FF	4GG	4HH	4II	4JJ
	5Y	5Z	5AA	5BB	5CC	5DD	5EE	5FF	5GG	5HH	5II	5JJ

In the individual cells, participants were asked to populate information that they considered relevant, including but not limited to:

Name of project or platform with associated URL **for more information**

Materials Class: Identify the specific types of materials or materials systems the instrumentation is designed to analyze or test.

Level of Autonomy: Determine the degree to which the instrumentation operates autonomously. The level of autonomy could range from manual operation by researchers to fully automated systems controlled by algorithms or AI.

Funding Source: List where the funding for the instrumentation came from. Sources could be government grants, private investments, institutional funds, etc.

User Access Model: Define how researchers access and utilize the instrumentation. The access model could involve scheduling systems, user permissions, and training requirements.

Collaborative Opportunities: Identify any opportunities for collaboration or shared use of the instrumentation with other research groups or institutions.

Performance Metrics: Assess the performance metrics of the instrumentation, such as accuracy, precision, throughput, and sensitivity.

Maintenance Requirements / Sustainment Models: Share the maintenance and sustainment plans for the infrastructure and identify the long-term opportunities.

Data Output and Analysis Tools: Explore the types of data outputs generated by the instrumentation and the tools available for data analysis. Tools could include software packages, data visualization tools, and computational resources.

At the conclusion of the breakout session, breakout leads were asked to transfer sticky notes to a very large-scale printout of the landscape as seen in the graphics below which was split between structural and functional materials.

		Discovery & Experimental Design						Synthesis					
		Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools	Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Functional Materials	Metals	1A	1B	1C	1D	1E	1F	1G	1H	1I	1J	1K	1L
		2A	2B	2C	2D	2E	2F	2G	2H	2I	2J	2K	2L
		3A	3B	3C	3D	3E	3F	3G	3H	3I	3J	3K	3L
		4A	4B	4C	4D	4E	4F	4G	4H	4I	4J	4K	4L
	Ceramics	5A	5B	5C	5D	5E	5F	5G	5H	5I	5J	5K	5L
		6A	6B	6C	6D	6E	6F	6G	6H	6I	6J	6K	6L
		7A	7B	7C	7D	7E	7F	7G	7H	7I	7J	7K	7L
		8A	8B	8C	8D	8E	8F	8G	8H	8I	8J	8K	8L
	Soft Matter	9A	9B	9C	9D	9E	9F	9G	9H	9I	9J	9K	9L
		10A	10B	10C	10D	10E	10F	10G	10H	10I	10J	10K	10L
		11A	11B	11C	11D	11E	11F	11G	11H	11I	11J	11K	11L
		12A	12B	12C	12D	12E	12F	12G	12H	12I	12J	12K	12L
	Semicond.	13A	13B	13C	13D	13E	13F	13G	13H	13I	13J	13K	13L
		14A	14B	14C	14D	14E	14F	14G	14H	14I	14J	14K	14L
		15A	15B	15C	15D	15E	15F	15G	15H	15I	15J	15K	15L
		16A	16B	16C	16D	16E	16F	16G	16H	16I	16J	16K	16L
	Other	17A	17B	17C	17D	17E	17F	17G	17H	17I	17J	17K	17L
		18A	18B	18C	18D	18E	18F	18G	18H	18I	18J	18K	18L
		19A	19B	19C	19D	19E	19F	19G	19H	19I	19J	19K	19L
		20A	20B	20C	20D	20E	20F	20G	20H	20I	20J	20K	20L

		Characterization						Scale-Up / Manufacturing					
		Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools	Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Functional Materials	Metals	1M	1N	1O	1P	1Q	1R	1S	1T	1U	1V	1W	1X
		2M	2N	2O	2P	2Q	2R	2S	2T	2U	2V	2W	2X
		3M	3N	3O	3P	3Q	3R	3S	3T	3U	3V	3W	3X
		4M	4N	4O	4P	4Q	4R	4S	4T	4U	4V	4W	4X
	Ceramics	5M	5N	5O	5P	5Q	5R	5S	5T	5U	5V	5W	5X
		6M	6N	6O	6P	6Q	6R	6S	6T	6U	6V	6W	6X
		7M	7N	7O	7P	7Q	7R	7S	7T	7U	7V	7W	7X
		8M	8N	8O	8P	8Q	8R	8S	8T	8U	8V	8W	8X
	Soft Matter	9M	9N	9O	9P	9Q	9R	9S	9T	9U	9V	9W	9X
		10M	10N	10O	10P	10Q	10R	10S	10T	10U	10V	10W	10X
		11M	11N	11O	11P	11Q	11R	11S	11T	11U	11V	11W	11X
		12M	12N	12O	12P	12Q	12R	12S	12T	12U	12V	12W	12X
	Semicond.	13M	13N	13O	13P	13Q	13R	13S	13T	13U	13V	13W	13X
		14M	14N	14O	14P	14Q	14R	14S	14T	14U	14V	14W	14X
		15M	15N	15O	15P	15Q	15R	15S	15T	15U	15V	15W	15X
		16M	16N	16O	16P	16Q	16R	16S	16T	16U	16V	16W	16X
	Other	17M	17N	17O	17P	17Q	17R	17S	17T	17U	17V	17W	17X
		18M	18N	18O	18P	18Q	18R	18S	18T	18U	18V	18W	18X
		19M	19N	19O	19P	19Q	19R	19S	19T	19U	19V	19W	19X
		20M	20N	20O	20P	20Q	20R	20S	20T	20U	20V	20W	20X

		Certification / Qualification						Recycling / End-of-Use					
		Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools	Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Functional Materials	Metals	1Y	1Z	1AA	1BB	1CC	1DD	1EE	1FF	1GG	1HH	1II	1JJ
		2Y	2Z	2AA	2BB	2CC	2DD	2EE	2FF	2GG	2HH	2II	2JJ
		3Y	3Z	3AA	3BB	3CC	3DD	3EE	3FF	3GG	3HH	3II	3JJ
		4Y	4Z	4AA	4BB	4CC	4DD	4EE	4FF	4GG	4HH	4II	4JJ
	Ceramics	5Y	5Z	5AA	5BB	5CC	5DD	5EE	5FF	5GG	5HH	5II	5JJ
		6Y	6Z	6AA	6BB	6CC	6DD	6EE	6FF	6GG	6HH	6II	6JJ
		7Y	7Z	7AA	7BB	7CC	7DD	7EE	7FF	7GG	7HH	7II	7JJ
		8Y	8Z	8AA	8BB	8CC	8DD	8EE	8FF	8GG	8HH	8II	8JJ
	Soft Matter	9Y	9Z	9AA	9BB	9CC	9DD	9EE	9FF	9GG	9HH	9II	9JJ
		10Y	10Z	10AA	10BB	10CC	10DD	10EE	10FF	10GG	10HH	10II	10JJ
		11Y	11Z	11AA	11BB	11CC	11DD	11EE	11FF	11GG	11HH	11II	11JJ
		12Y	12Z	12AA	12BB	12CC	12DD	12EE	12FF	12GG	12HH	12II	12JJ
	Semicond.	13Y	13Z	13AA	13BB	13CC	13DD	13EE	13FF	13GG	13HH	13II	13JJ
		14Y	14Z	14AA	14BB	14CC	14DD	14EE	14FF	14GG	14HH	14II	14JJ
		15Y	15Z	15AA	15BB	15CC	15DD	15EE	15FF	15GG	15HH	15II	15JJ
		16Y	16Z	16AA	16BB	16CC	16DD	16EE	16FF	16GG	16HH	16II	16JJ
	Other	17Y	17Z	17AA	17BB	17CC	17DD	17EE	17FF	17GG	17HH	17II	17JJ
		18Y	18Z	18AA	18BB	18CC	18DD	18EE	18FF	18GG	18HH	18II	18JJ
		19Y	19Z	19AA	19BB	19CC	19DD	19EE	19FF	19GG	19HH	19II	19JJ
		20Y	20Z	20AA	20BB	20CC	20DD	20EE	20FF	20GG	20HH	20II	20JJ

Subsequently, all participants were asked to gather first at the structural poster then at the functional poster and breakout leads reported out to the entire workshop group. Participants were encouraged to ask questions and contribute additional capabilities.

Panel 2: Building a Community to Realize the Autonomous Materials Innovation Infrastructure (AMII) – An Industry Perspective

The second panel was titled "Building a Community to Realize the AMII – An Industry Perspective" and was moderated by **Benji Maruyama** (AFRL). Here, **Richard Gottscho** (LAM), **Tim Erdmann** (IBM), **Carol Handwerker** (CHIPS Program Office), **John Lockemeyer** (Shell Global Solutions US), and **Michael Glavicic** (Rolls-Royce) discussed the following points:

Discussion Points

- Industry's needs from the larger community for best engagement
- Modes or paths for industry engagement with community
- Company requirements to enable robust interactions and partnerships
- Mechanisms and incentives needed to "sell" the investment to industry leadership

The panel highlighted the indispensable role of industry in realizing the full potential of the AMII. Participants underscored that robust industry involvement is crucial not only for capital investment but also for workforce development and providing the unique tools necessary for realizing the societal benefits unlocked by discoveries and innovations from the AMII. To transition from theory to practical application, industry must actively participate in the development of AMII to help bridge between scientific innovation and real-world implementation.

One need from the community identified by these industry leaders was for graduates equipped with critical thinking skills capable of bridging autonomous experimentation and materials R&D. Graduates should possess the ability to analyze where processes have succeeded or failed and think critically about the implications. Additionally, there is a pressing data problem that necessitates a comprehensive and well-defined data structure driven by community incentives. The challenge of communicating across different technical languages, particularly between AI/ML experts and experimental scientists, was noted. Additionally, it is difficult to find graduates with the combination of AI/ML coding skills and the specific specialization in their respective materials field. For example, the combination of a Ph.D. Chemical Engineering graduate who studied catalyst development usually does not have experience or exposure to coding or language skills for AI/ML algorithms. The inverse is also true—coders do not possess in-depth knowledge or expertise in chemistry or engineering. Expecting the latter to learn chemistry or engineering is likely less practical than having chemists or engineers use AI/ML tools while pursuing their respective disciplines. Presumably this will change, as these students are beginning to use the digital tools more often in their discovery/development protocols, but an intentional and possibly formal changes to the curricula could be considered. For successful collaboration, new scientists need training that encompasses both domains. Furthermore, industry emphasized the essential role outside researchers play in supporting industrial development and aligning fundamental research with broader industry goals, such as carbon neutrality and manufacturability within realistic timeframes.

The panel discussed several pathways to foster industry engagement. Early engagement with a company champion is vital for testing concepts and ensuring the materials developed are both useful and applicable. Identifying realistic points in the design phase and involving federal agency support can positively impact project success. Passionate scientists or engineers within companies are crucial to drive projects forward; without their commitment, projects risk falling apart. Management support is also essential, and this requires clearly explaining the project's value. Choosing significant, impactful problems that align with industry interests can facilitate this support.

Robust interactions and partnerships necessitate specific company requirements. These requirements include aligned objectives and a clear business case demonstrating how collaboration will improve production, reduce costs, or expedite market entry. Pre-competitive collaboration on fundamental science is possible, provided there is trust between parties. Companies need assurance that their collaborators understand their key needs and are bringing a comprehensive solution to the table.

Persuading industry leadership to invest requires a compelling vision and demonstrated long-term value. The potential for collaboration with national labs and other institutions can serve as a significant recruiting tool and a means to leverage applied research funding effectively. Additionally, structured agreements outlining terms of engagement can facilitate management buy-in and commitment.

Audience comments emphasized the potential for academic-industry consortia, such as those forming around digital twins, sustainability, and circular chemistry. The importance of early engagement with companies to discuss scaling and pilot testing was highlighted. Companies need assurance that proposed technologies are robust and scalable to mitigate the risks associated with commercialization efforts. Engaging in detailed conversations early and understanding company needs can foster a collaborative environment and help build trust.

An example of impactful academic discovery involved a collaboration where a student developed a diagnostic technique that solved a significant problem for the company. This example highlighted the potential for academic partnerships to drive innovation and address real-world challenges. Overall, the panel underscored the importance of communication, early engagement, and alignment of objectives to build a successful community that can realize the goals of the AMII.

Working Session 2: Identify Gaps in the Autonomous Materials Innovation Infrastructure (AMII)

Similar to Breakout Session 1, breakout groups reconvened to work together to discuss and capture specific gaps in the AMII for their materials topic of focus. Participants were asked to consider gaps concerning, but not limited to:

• **Sensors and Data Collection**: Identify the types of sensors required to gather relevant data about the material being tested. This type could include temperature sensors, pressure sensors, strain gauges, etc.

• **Automation and Control Systems**: Explore how automation can be implemented to control the experimentation process. Automation involves programmable logic controllers (PLCs), microcontrollers, or even AI-driven systems.

• **Data Analysis Techniques**: Determine the analytical methods and algorithms needed to process the data collected from the sensors. Techniques might involve statistical analysis, machine learning algorithms, or other computational techniques.

• **Feedback Mechanisms**: Implement feedback mechanisms to adjust experimental parameters in real-time based on the data collected. Mechanisms could involve closed-loop control systems or adaptive control algorithms.

• **Safety Protocols**: Ensure that appropriate safety protocols are in place to prevent accidents or damage to equipment during autonomous experimentation.

• **Integration with Laboratory Equipment**: Consider how the autonomous instrumentation will integrate with existing laboratory equipment such as furnaces, mechanical testers, or spectroscopy devices.

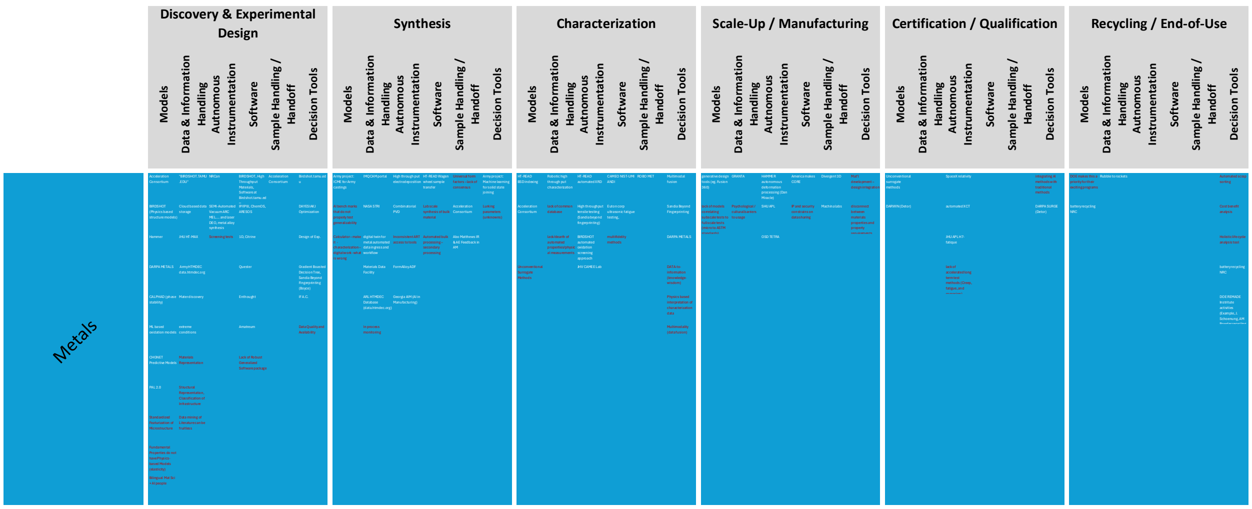
• **User Interface and Accessibility**: Design a user-friendly interface for researchers to interact with the autonomous instrumentation system. Options include a graphical user interface (GUI) or a command-line interface (CLI).

• **Data Storage and Management**: Develop a system for storing and managing the vast amounts of data generated during experimentation. Systems could involve database management systems or cloud-based storage solutions.

As in breakout session 1, breakout leads presented their findings to the larger group.

Landscape Data Analysis

To provide a visual representation for a comparison between the status of the AMII of each materials domain considered during the breakout sessions, the following procedure was performed to develop sunburst charts. First, the collected workshop data found on sticky notes were transcribed and digitized by NSF staff with identified gaps being differentiated to capabilities by using red font. Each entry of a capability was counted as 1, and no qualitative assessment was made. For example, for the structural metals table, the digitized table is shown below:



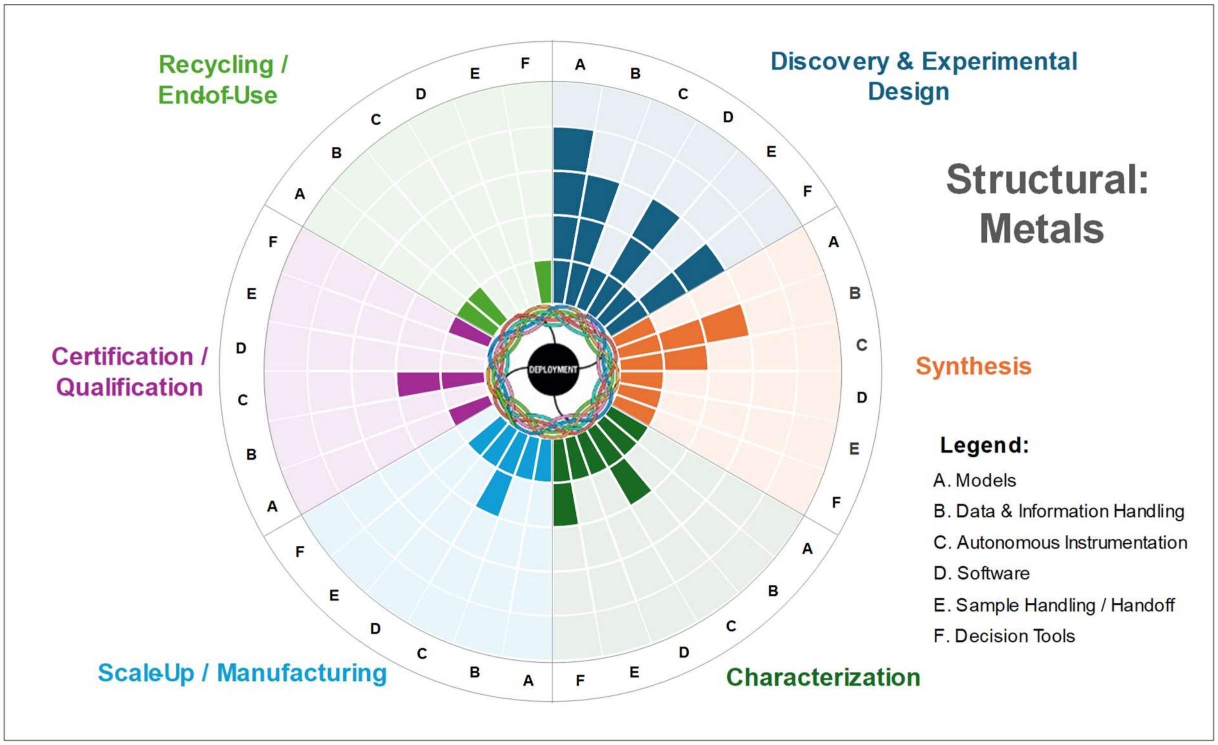
This process resulted in the following capability counts for Structural Metals:

	Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Discovery & Experimental Design	8	6	2	6	1	6
Synthesis	2	5	4	1	2	2
Characterization	2	1	4	2	1	3
Scale-Up / Manufacturing	1	1	3	1	2	0
Certification / Qualification	2	0	3	0	0	1
Recycling / End-of-Use	1	1	0	0	0	2

Across all materials domains, the highest number of entries identified was 11, which was subsequently used for scaling. Therefore, each of the 36 numbers above was divided by 11 to give a percentage. Using this percentage, each section was assigned a numerical value between 0 and 5 using the following scale:

0%	→ 0
< 20%	→ 1
20-40%	→ 2
41-60%	→ 3
61-80%	→ 4
81-100%	→ 5

For example, Discovery and Experimental Design: MODELS has 8 entries in the Structural Metals landscape. Therefore, it would be assigned 8/11 = 72% and therefore a 4. These assignments were then used to develop a sunburst chart, with the number determining the number of fields of darkened color (see below for Structural Metals example.) The full array of data gathered and digitized as described above is provided in **Appendix C.**



While this does not provide a quantitative assessment of the readiness of the AMII in a given domain to fulfill the promise of autonomous experimentation, it gives a comparative indicator of how far developed the community is for each material domain.

AMII Landscape, Gaps, and Opportunities

The confluence of AI, robotics, high-throughput screening along with the foundational capabilities established over the past decade of the MGI provide an opportunity to accelerate, and fundamentally change, how the materials community conducts research into the future. It is first necessary to understand the current infrastructure landscape and identify both the existing capabilities and the key gaps. Because the infrastructure requirements depend in part on the materials class, the workshop participants were split into the following groups to dive more deeply into this topic: structural metals, structural ceramics, structural soft matter, structural composites, functional metals, functional ceramics, functional soft matter, and functional semiconductors. The participants in each group were asked to use sticky notes to identify existing capabilities and gaps in models, data and information handling, autonomous instrumentation, software, sample handling/handoff, and decision tools in the following categories: discovery and experimental design, synthesis, characterization, scale up/manufacturing, certification and qualification, and recycling/end of use. The content gathered with these sticky notes is summarized in the starburst chart for each section and detailed further in **Appendix C**. The groups were also asked to provide a short summary of the discussion that took place throughout the day. These narratives developed by the facilitators are provided below and reflect the discussions during the meeting. They do not reflect the view of specific individuals, institutions, or agencies, but rather are intended as a basis for further discussions and engagement. Additional detail captured in PowerPoint format in **Appendix D**.

This landscaping exercise is intended to enable better understanding of current infrastructure capabilities. The inventories and gaps discussed below are derived from inputs collected at the workshop based on the knowledge and experiences of different participants. They are not comprehensive and do not reflect the opinion of all attendees. Also, the specific resources listed throughout the document were identified by the participants and should not be taken as an endorsement in any way or considered to be complete. The community will be provided with additional opportunities to contribute resources to this landscaping exercise.

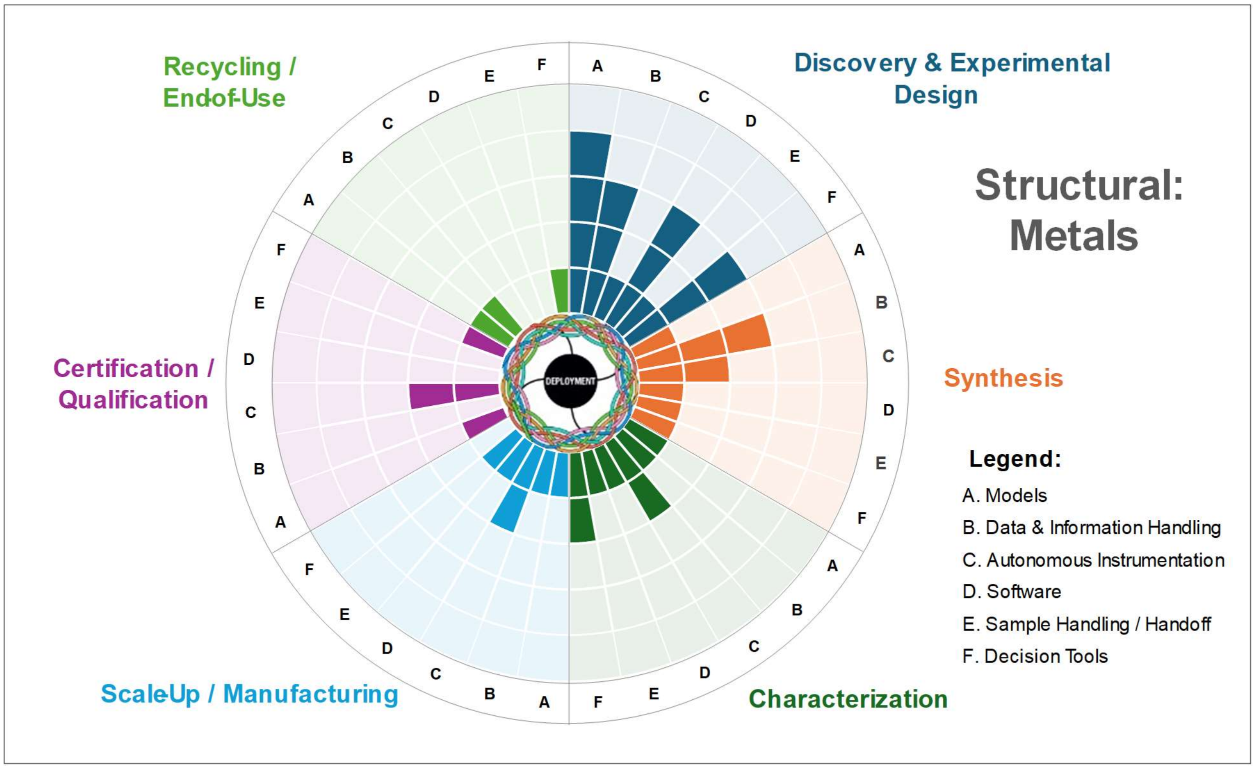
Structural Materials

Structural Metals

Facilitators: Dan Miracle (AFRL), Brad Boyce (SNL), Jae Hattrick-Simpers (University of Toronto, Acceleration Consortium)
Participants/Observers: Ibrahim Karaman (Texas A&M), Andrew Detor (DARPA), Robert Hart (U.S. Army DEVCOM Ground Vehicle Systems Center), Harry Partridge (NASA), Eddie Gienger (JHU Applied Physics Lab)

Current Landscape

Structural metals are relatively new to combinatorial and autonomous experimentation (AE) methods, so the infrastructure and facilities are less well established than for other materials such as polymers and thin film materials. Nevertheless, new capabilities are being established and validated for this distinct class of materials. Existing software packages and databases are available to drive innovation in structural materials, examples include ARES OS, Enthought, and products from companies such as Citrine and QuesTek. Limited infrastructure exists for the rapid and robust primary synthesis and characterization of bulk metals in a manner that is consistent with AE methods. In most cases, these are one-of-a-kind facilities at a low technology readiness level/manufacturing readiness level (TRL/MRL) that have not yet been adequately reduced to practice. Further, all of the infrastructure needed for the full AE cycle is generally not available at a single facility. Several large efforts are currently underway to develop and validate AE infrastructure and methods for structural metals, exemplar programs include BIRDSHOT, HT-READ (both funded by HTMDEC), Georgia AIM, OSU HAMMER and P2P, other programs may also exist.



Identified Gaps and Opportunities

Major gaps exist for structural metals under the topics of: synthesis; characterization; design-relevant properties; legacy facilities; workforce; and certification and qualification. AE methods require rapid, on-demand synthesis of bulk (≥100 g) metal alloys. None of the current lab-scale primary synthesis methods (arc or induction melting, additive manufacturing) are sufficiently rapid and robust, but the aggressive use of automation (especially in arc melting) and innovative redesign (including bulk ingot melting using lasers) are expected to make major advances in this area. Additive manufacturing (AM) is already strongly automated, but gaps in metal AM include availability of powder feedstock in the preferred spherical form, and the ability to rapidly determine deposition parameters that can avoid the formation of common material defects. AE approaches to rapidly evaluate the effect of microstructure on properties requires new thermomechanical processing methods that in most cases have not yet been conceived or validated. Characterizing composition and microstructure is currently sufficiently automated to be used in an AE workflow, but some aspects of quantifying the results (for example, microstructure classification and diffraction indexing) are still bottlenecks. Work is currently underway to solve these gaps. Many high-throughput techniques have been validated to measure properties, but most have not yet been automated or reduced to practice. Characterizing materials under representative service conditions remains a gap. Drastically reducing the time between measuring lab-scale properties and input to design-relevant models is a major issue. New efforts are just underway to begin tackling this need, for example, the DARPA METALS program. Replacing legacy facilities with digital equipment remains a barrier, along with training a competent workforce that is facile in materials science as well as data science, artificial intelligence methods and mechatronics-robotics. Finally, accelerated materials design and deployment via AE will necessitate new policies and procedures for certification and qualification.

Structural Ceramics

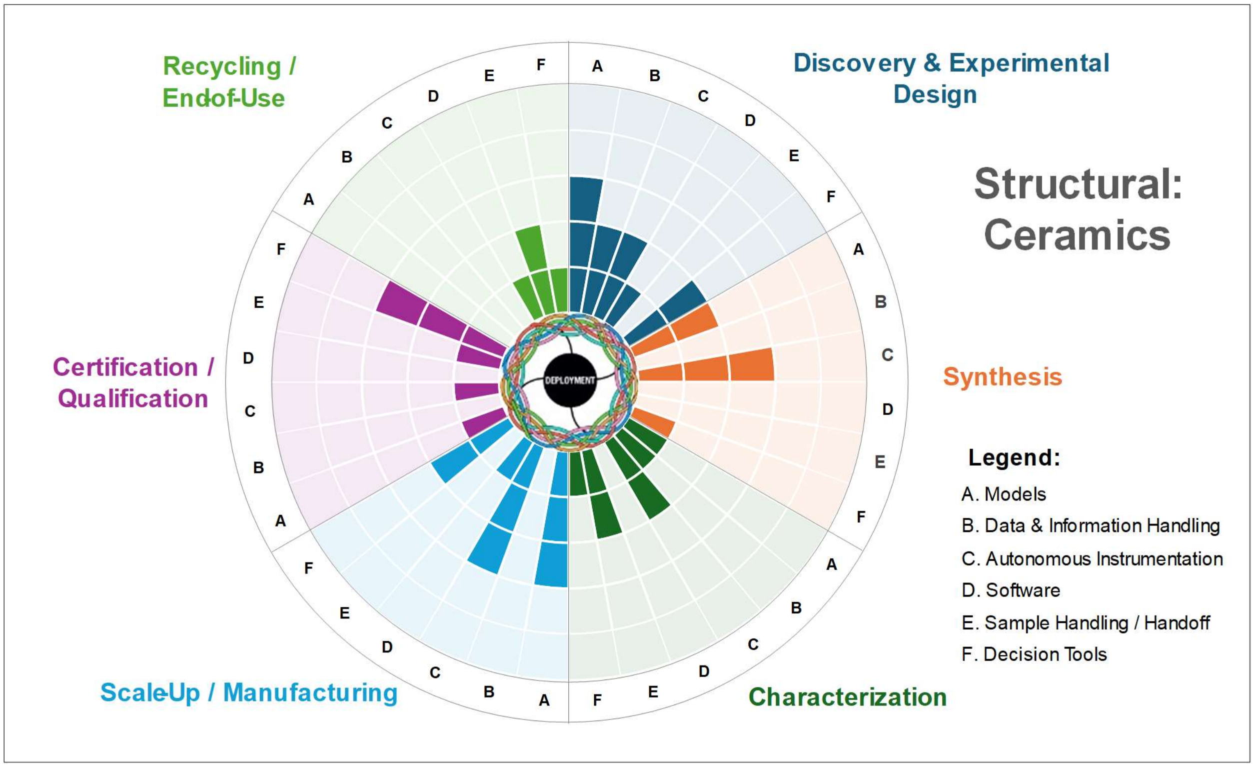
Facilitators: Joshua Schrier (Fordham University), Sergei Kalinin (UT Knoxville/Pacific Northwest National Laboratory)
Participants/Observers: James Dorman (DOE), Stu Miller (ULRI), Chris Haines (ARL)

Current Landscape

Structural ceramics—non-metal, non-organic materials that can withstand high mechanical, thermal, and tribological stresses, often in corrosive environments and at high temperature—are a broad category that span high-tech, low-volume materials applied as electronic elements (capacitors, dielectrics, circuit boards), coatings in specialized applications (such as thermal protection tiles in hypersonic, aerospace, and nuclear technologies) to bulk commodity materials such as glass and cement. The range of production scales, compositions, and wide variety of synthesis and processing conditions make authoritative general statements about the current state of the field elusive; the below text should be considered as illustrative examples at the different scales.

At present, most aspects of *experimental design* rely upon heuristics and experience. Current computational approaches build upon the foundation of past MGI computational database infrastructure (AFlow, OQMD, Materials Project); in practice these databases of physics-based (density functional theory, DFT) simulation results are a necessary—but insufficient—part of a computational design of new structural ceramics. For example, recent work used a combination of DFT and machine-learned descriptors to predict (and subsequently experimentally validate) the synthesizability of high-entropy carbonitrides and borides by hot-press sintering[i]. Real materials are considerably more complex than pure chemical formulas, and both microstructure and dopants can play a significant role in the emergence of properties. Recent work on experimental design of high-performance cementitious materials uses data-driven approaches trained on experimental data,[ii] to treat these properties. One exciting area is the use of large-language model (LLM) design tools for providing decision support in the design of novel alkali-activated concrete mixes as environmentally friendly alternatives to conventional Portland cement-based concrete.[iii]

Participants emphasized that the state of synthesis, characterization, and scale-up for structural ceramics generally lags that of other materials. For example, whereas additive metal and polymer fabrication are now well-established, additive techniques are still an emerging research area in ceramics, in part because the necessary processing steps (power handling, debinding, sintering) are less amenable to automation, and in part because the chemical diversity of binders and ceramic powders. The state of additive manufacturing of ceramics has been recently reviewed.[iv] Some exemplar projects discussed in the panel included efforts at HT-Max project at Johns Hopkins University on extrusion-based additive manufacturing for high-temperature ceramics[v], and work at the Underwriters Laboratory Materials Discovery Research Institute (MDRI).[vi] Autonomous systems for cementitious materials development have been proposed,[vii] but not yet implemented. A small number of commercial vendors, such as Cerion Nanomaterials,[viii] provide scaled-up nanomaterials for advanced ceramics. Additionally, while it is appreciated that recycling and end-of-use management is important, the economies of scale for the commodity applications make it challenging (for concrete), require strong social involvement (glass), or require special handling (nuclear).



Existing standards for certification and qualification of structural ceramics are typically conducted on length- and timescales that are incompatible with miniaturization and rapid-turnaround required for feedback in autonomous experimentation. One way these issues are being addressed is by using non-destructive proxy measurements to intelligently plan traditional certification experiments. A notable example is work at Army Research Laboratory on non-destructive, high-throughput dielectric-based testing of armor ceramics which is used to intelligently plan ballistics testing to maximize information gain.[ix]

Identified Gaps and Opportunities

Discovery & Experimental Design. The MGI created a strong foundation of computational/theoretical pipelines; the AMII has the opportunity to connect these models to experimental data, especially with theory-data integration, experimental validation of data and theory-based prediction, and updating theory based on experimental data. As in the other materials areas, there was general support for ML/AI serving as more of a human-in-the-loop assistant tool rather than hands-off automation.

The integration of experimental data with theory provides an opportunity to improve the underlying ***fundamental theory of materials formation***. Nascent efforts include understanding the interplay of thermodynamics and kinetics for ceramic synthesizability[x]and uncovering the microscopic mechanisms of crystallization in cementitious materials.[xi] Simulating the length- and time-scales needed to understand nucleation processes will benefit from ongoing developments in machine-learned interatomic potentials.[xii] The AMII would have a synergistic value in generating high-quality/high-quantity experimental data from automated/autonomous laboratories to provide constraints that would enable development of better theories, beyond just empirical input-output relations to ML models. Similar advances are anticipated with the broad deployment of phase field models for microstructure formation, including both numerical schemes and physics-informed neural network and neural operator accelerated schemes. It is important to note that key aspect of these techniques is not only forward modeling of materials microstructure evolution, but capability to discover governing equations from the experimental data.

A critical gap is the need for ***improved data repositories***, especially for experimental data. For example, the NIST Structural Ceramics database[xiii] has not been updated since 2002. Nascent efforts to construct databases for cementitious materials development[xiv] should be encouraged and will be enabled by rapidly improving LLM-based literature extraction tools.[xv] Direct integration with new automated/autonomous laboratories would enable the capture of negative results from methodologically correct experiments, which are not typically reported (but highly valuable for machine learning model development). The heterogeneity of methods and equipment used in this field is a challenge, and there is a need to develop appropriate ontologies. Although in principle the "pull" of added value from machine learning is high, there will be some need for "push" requirements from funders and journals to make sure that these data are deposited in reusable ways.

Workforce development is another challenge. There are only a limited number of ceramic engineering programs in the United States, so this is an opportunity that suggests that a large impact can be made by focusing efforts on a few sites. Programs that help build stronger partnerships between academia and industry—such as funding faculty sabbaticals, student internship/co-op placements—can have a disproportionate impact. It is important to analyze the underpinning driving forces in this field. For classical ML applications, since the introduction of personal computers in the early 1980s, there has been a continuous evolution of the IT and computing workforce. The computer builders and software developers of the 1980s laid the foundation by creating companies like Microsoft and developing key software horizontals. More recently, the emergence of deep learning in 2012 has attracted skilled professionals from fields such as density functional theory, molecular dynamics, and finite element analysis. These experts, now armed with deep learning experience, are founding companies focused on applying deep learning to theoretical domains. Examples include Schrödinger and InSilico, alongside hundreds of startups dedicated to theoretical drug and materials discovery. This convergence of expertise in traditional computational methods and deep learning is driving innovation and creating new opportunities in these advanced scientific fields.

The incorporation of automated experiments cannot be expected to benefit from the same evolutionary process that transformed IT and computing in the past. This shift introduces fundamentally new challenges and creates a need for diverse tasks, ranging from instrument development and workflow design to new types of machine learning for experimental design and cloudification. Currently, we lack a trained workforce equipped to tackle these multifaceted demands. Therefore, it is of utmost priority for current domain experts to adopt and integrate machine learning expertise. However, the challenge is compounded by the scarcity of qualified individuals capable of training these experts—only a small number of pioneers in the field are available to lead this transformation. This gap underscores the urgent need for educational initiatives and professional development programs to build the necessary skills and knowledge base.

High-throughput synthesis of structural ceramics is challenging and would benefit from investments in both basic and applied research. A challenge for automation and autonomy is the wide variety of materials and processes, and the high temperatures and long times involved. Developing high-throughput experimental methods for structural ceramics has many different methods, each with their own challenges (hydrothermal, powder synthesis, molten salts, etc.), and many methods present challenges for common high-throughput instruments (such as the use of corrosive acids). As noted above, additive manufacturing methodologies for structural ceramics lag developments for additive metal manufacturing; there is an opportunity both for investment and innovation to design new processes. Predictive modeling for additive manufacturing of structural ceramics is under-developed. Large opportunities would be unlocked by new accelerated synthesis for powders, development of novel binders, and formulation methodologies (each of which themselves would benefit from automation/autonomous operation). In relation to the need for improved data repositories (noted above), the creation of an “Additive Structural Ceramics Data Repository” containing information needed to reproducibly synthesize and characterize powders, ink formulations, and processing conditions would be a powerful demonstration of AMII methodologies.

High-throughput characterization is another challenge, because many structural applications require large samples which are incompatible with the typical high-throughput miniaturization approaches often used for other materials classes. Similarly, their mechanical and functional properties are often non-local, and are determined by subtle details of the structure, composition, and strain variability within the part. These issues limit the potential use of purely data-based multifidelity methods and require physics-based models. Typical characterization modalities are slow, and so there is also a need for low-cost and fast proxy measurements which can be used for preliminary evaluation or optimally planning traditional characterization approaches. One example is the use of machine learning to generate simulated SEM micrographs using laser spot brightness during laser sintering of ceramics.[xvi] These efforts in turn necessitate the development of ML algorithms that act as proxies and establishing their predictive power. Strongly connected to this is the general dearth of the instrument control APIs and interfaces that allow direct deployment of ML agents on the autonomous tools, and tools for building active characterization workflows given specific exploratory goals. While the efforts in these areas have been initialized, or the time being they lack systematic support and broad community acceptance. A closely related need for *Certification /Qualification* was discussed, and participants emphasized the need for automated certification and mechanisms for sharing samples across laboratories for trusted characterization.

In parallel to developing new synthesis and characterization methods and machines (“hardware”) is the need to develop appropriate ***software abstractions*** and “hyperlanguages” to represent possible operations in the laboratory (which can be “compiled” to work with particular instruments), orchestration of multiple parallel experimental processes, and conduct multi-step workflows to achieve desired reward functions. Currently, there is a mixed landscape of home-built solutions, vendor-specific application programming interfaces (API), and lab-driven modifications. Development of standardization consortia would be helpful, especially if linked to purchasing requirements of customers. Consortia would also provide an opportunity to improve traceability of the experimental workflows. A set of agreed upon monitoring indicators from the processing and in-situ materials processing side can be a step towards capturing and tracing experimental workflows. Current examples may be RHEED during PLD growth.

Scale-Up and Manufacturing could be supported in a variety of ways. One model would be the creation of user facilities that would enable small companies or academic groups to develop and scale novel ceramic materials faster and cheaper. This model might take the form of services which can synthesize and formulate new powder and binders for ceramic additive manufacturing or prototyping of novel materials. These efforts could initially be developed and operated as user facilities with the goal of data collection and prototyping—along the lines of the National

Nanotechnology Initiative User Facilities[xvii] —before technology transferring to commercial operation.

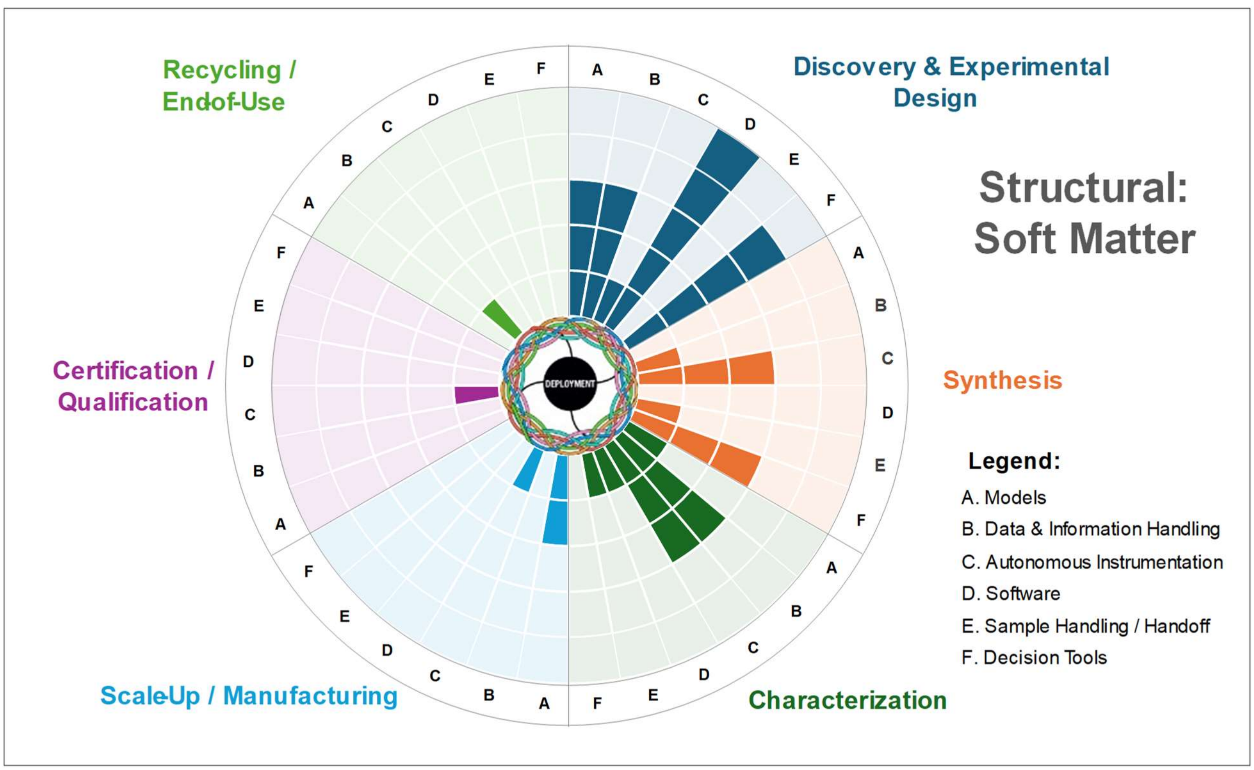
Recycling/end-of-use would be advanced by the creation of easily accessible computational models of lifecycle analysis, techno-economic evaluation, and environmental impact which allow for incorporating these as design constraints earlier in the development process. At present, this type of analysis is highly challenging and requires significant expertise which makes it largely unavailable. Even approximate—but easily computable—versions would help development, by allowing optimization algorithms to incorporate the applied research outcomes into the immediate experimental result or goal in the early-stage research lab to develop more sustainable processes and materials. Another important and promising research direction is the use of recycled ceramics as aggregate materials in structural concrete.

Structural Soft Matter

Facilitators: Keith A. Brown (Boston University), Vicky Nguyen (JHU)
Participants/Observers: Sanket Deshmukh (Virginia Tech, GlycoMIP), Chinedum Osuji (UPenn), John A Schlueter (NSF), Rich Vaia (AFRL)

Current Landscape

The full range of topics we discussed is documented on the sticky notes (see **Appendix C**). This summary focuses on the conversation during the brainstorming session as well as items not explicitly noted on the stickies.



We began this session by listing the largest efforts in this space with noteworthy examples being CMU's cloud lab, relevant MIPs, and CHIMAD. While listing these, we noted that many efforts are likely occurring within industry, namely the large-scale manufacturers of structural polymers. There are limited examples of relevant academic and national lab autonomous experimentation systems and so we broadened our discussion to cover all facets of AI-accelerated work in this space. We also included discussion of wide-ranging tools for accelerating research including very general ones (e.g. ChatGPT) and software platforms that are shared between many materials types (e.g. python packages like BoTorch or ChemOS). It is also worth highlighting the advent of software tools (e.g. CRIPT) specifically designed to capture the multidimensional parameter sets (e.g. topology; molar mass dispersity, end-group functionality) needed to properly describe macromolecular materials.

One additional point was that there was discussion about the specific role of each category. For instance, should discovery include the synthesis and characterization of new materials, or is it simply the identification of candidates with their synthesis and characterization being relegated to their respective sections? We ultimately opted to think about the synthesis section as including making materials during the discovery process (rather than just being synthesis during development or manufacturing).

Identified Gaps and Opportunities

As a grand challenge, we noted that AMII could allow for the **true inverse design of materials with multiple properties that are perhaps commonly thought of as being in conflict**. For example, materials that are stiff and tough or materials that are stiff and sticky. We thought that the techniques embodied in AMII could allow for this vision to be realized.

Most of the conversations during lunch focused on the questions relevant to the industrial panel. We speculated that a major need from industry are trained people and the know-how related to emerging AI tools. An advantage of the academy is our critical mass of technical expertise, which can be uncommon in industry. That said, industry has many more resources than the academy, albeit with the full-time equivalent cost being much higher.

A key method of engagement we discussed were consortia with discussion focusing on 'America Makes' as an exemplar. We noted that industrial players have many reasons to participate in such consortia including developing relationships across the supply chain and managing contracts. We noted that a major need is for industry to communicate their problems to the academy - perhaps through a consortium - to guide our research. A consortium can also help set the community roadmap, which we felt was critical to align the effort of the community.

A fundamental problem with structural soft matter is that properties depend on structure across scales and that this structure depends strongly and often unintuitively on processing. We do not even have a structural language or ontology to describe this structure in a compact way. The critical missing piece is **reliable** data that connects processing-structure-property across the relevant scales.

Addressing these needs would require a number of advances including: (1) Clear definitions of *material properties* and data reporting as polymers can exhibit large strains, tension/compression asymmetry, and anisotropic properties, (2) *Reference materials* and data, (3) In situ and in line measurements to determine properties, (4) *Surrogate properties* and processes for connecting properties to certification/qualification (e.g. melt flow index). It is crucial that such surrogates are developed alongside knowledge about limitations and boundaries. (5) An interoperable polymer database, perhaps run by a national facility, but with good and verified data. (6) Standard modular workflows for processing history - *what is a* 96 *well plate equivalent for materials testing*, and (7) Sufficiently complex robotic handling.

We noted that we need **better simulation tools.** Current models are not sufficient because of the wide range of time and length scales needed to describe the behavior of these inherently nonequilibrium materials. Digital twins are particularly important as thermal, chemical, and mechanical factors are so strongly coupled, particularly to describe chemical aging or the effects of humidity on the thermomechanical properties. This complexity means that the community needs better models.

We discussed a few additional open challenges. For instance, in order to have full relevance to industrial manufacturing, the academy needs access to a full-scale processing line and enough materials to make it work. We noted that there is no one funding people looking at the reliability of data and discussed the example of the Journal of Organic chemistry as an example of an entity putting money into reproducibility. There was also discussion about whether autonomous experimentation systems should be one-off systems developed by the academy or commercial products. The transition seen in the use of AFM from custom to commercial was an illuminating example as these systems have many parallels.

Finally, we discussed the open questions related to the end of life of materials. We noted that there was a lack of metrics for -bilities (recyclability, sustainability, manufacturability). This lack compounds with the fact that recycling is hard. We shared the goal of making recycling cheaper, but also discussed how doing this could substantially narrow the scope of polymer engineering.

Structural Composites

Current Landscape

The integration of AI and automated experimentation in the development of new structural composite materials is still in its early stages, but current applications include utilization of AI to optimize material composition (i.e. reinforcement and matrix materials) and to predict material properties of high-performance fiber-reinforced composites. Current software tools leveraging AI to accelerate material discovery include commercial tools like Granta Materials Intelligence AI+ (Granta MI AI+) and research tools using TensorFlow-based custom models. These tools utilize machine learning algorithms and data-driven approaches to simulate and predict the mechanical, thermal, and chemical properties of composite materials based on their composition, fiber orientation, and processing conditions and to gather insights on process-property relationships. These commercial and research tools are typically limited to solving discrete problems and require significant human oversight. There are no concrete examples of programs enabling full automated experimentation of new structural composites connecting discovery to manufacturing to characterization to end of life recycling. As far as government funded programs, the Institute for Advanced Composites Manufacturing Innovation (IACMI) has invested in programs focused on automated/high-throughput inspection technology for certification and validation of automotive composites as well as high throughput recycling processes. Additionally, autonomous experimentation efforts focused on polymers under programs like DMREF translate well towards the discovery of new polymer matrix materials to be used in structural composites.

Identified Gaps and Opportunities

The existing infrastructure in automated experimentation of structural composites remains immature due to some significant gaps in areas such as: characterization methods, modeling &

simulation, qualification, and recycling. Characterization methods for structural composites are currently based around manual methods that require human interpretation, making automation difficult. Failure of a composite in tension, compression, or shear is a micro-level failure that is being measured through a macro-level test specimen, and currently humans must visually inspect the failure mode to interpret the quality and validity of the numerical test data. Digital methods (Digital Image Correlation, Virtual Fields Method, and others) are available for determining local material response, but these methods do not currently work well with many established ASTM tests and fixtures, which require strain gauges or extensometers. Industry and academia have developed their own specialty fixtures for compression and shear property testing and there is not widespread agreement on the best fixture or test methods used for measuring a particular property. In addition, a significant amount of labor goes into developing test specimens and processing them through current ASTM test standards, therefore automating experimental characterization will require alternative test methods and models that can correlate those test results to material properties relevant to designs. Qualification processes for structural composites are highly regulated, particularly in aerospace, however in other industries like automotive and sporting goods, high production volume manufacturing environments may be more conducive to accelerated qualification through automation, particularly in non-critical structural applications. Similar to challenges with characterization methods, process modeling and finite element structural modeling are done at a macro level scale, requiring full mechanical characterization on the composite laminate level. Discovery of new composite materials involves discovery of new matrix materials (polymers), new reinforcements (fibers), and/or new combination of these constituents. Multi-scale models are available for finite element models and can be used to optimize the material constituents, but physics are often idealized, especially regarding fiber-matrix interface interactions, and these models do not account for process-dependent effects. Accelerating the discovery of new composite materials will require improved multi-scale models and correlations between small scale experimental coupons and macro-level properties needed for design. Recycling of thermoplastic composites is far ahead of recycling for thermoset composites. To improve sustainability of composites, there is a need for full lifecycle models and understanding for how structural composites can be recycled at end-of-life and utilized as a useful structural feedstock rather than viewed as a waste product.

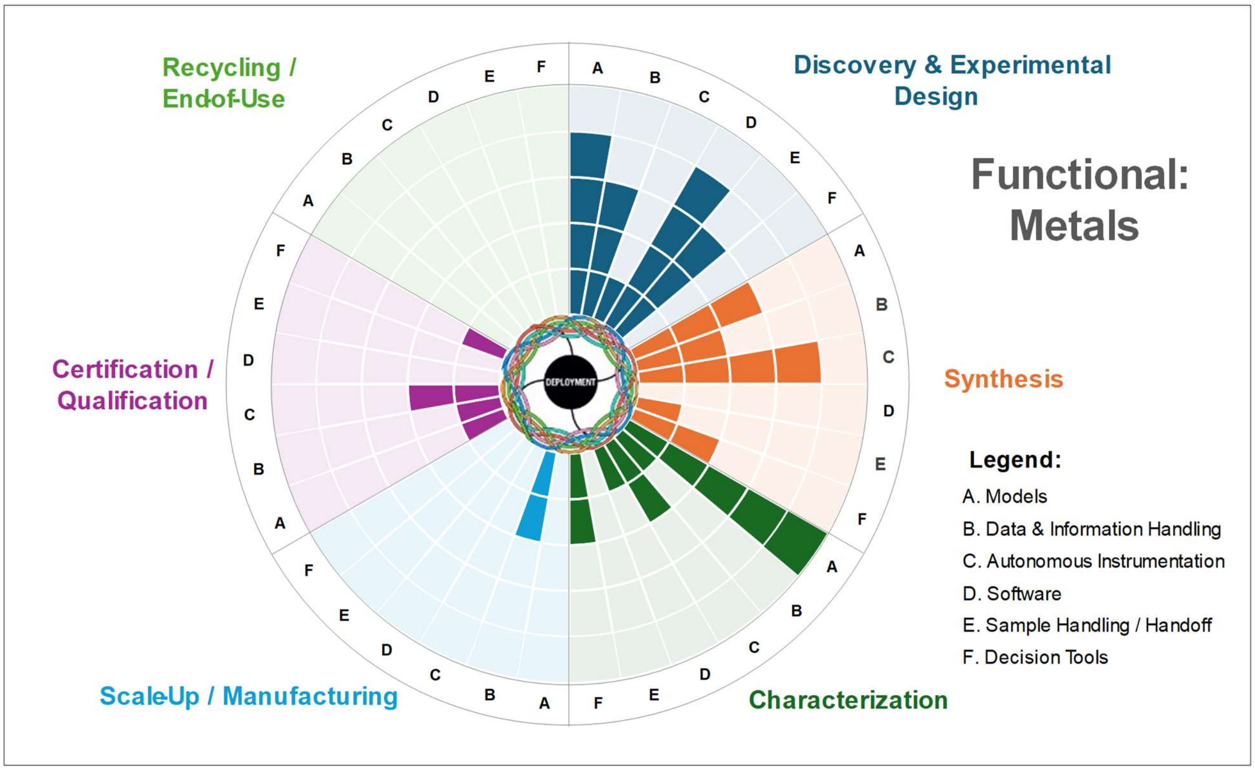
Functional Materials

Functional Metals

Facilitators: Francesca Tavazza (NIST), Philseok Kim (ARPA-E)
Participants/Observers: Mike Glavicic (Rolls-Royce), Aisha Haynes (OUSD(R&E)), John Lockemeyer (Shell Global Solutions US), Rob Moore (ORNL), Mitra Taheri (JHU), Leslie Hamilton (JHU APL), Jeffrey Aguiar (Lockheed Martin Corporation)

Autonomous experimentation applied to the research and development of functional metals is at its early stages and still presents many challenges. In a pipeline that starts from Discovery & Experimental Design, then covers Synthesis, Characterization, Manufacturing, Certification and ends with Recycling/End-of-Use, most of the current work covers the first three steps, especially the discovery and experimental design, while very little is done in the last three steps.

Current capabilities related to Discovery and Design include a wide range of models, some physics-based and some purely phenomenological, covering length scales from atomistic to continuum. A few, key models are still missing, though, as, for instance, one for ductility predictions. Some ML algorithms are available too, as surrogate models. Predictive software tools also exist, at least as a starting point. Substantial data is available, as are data handling tools, but they come with pressing open questions. Among those: how to put together legacy data and new ones? How to restructure data and data capturing to work better with AI and autonomous systems? What are the needed metadata? There is a large agreement in the community on the need for negative data, which are currently not usually available. What infrastructure is needed to share negative data? Lack of interoperability and standardization in data handling is another substantial problem that needs to be addressed as soon as possible. More work is also needed in designing full autonomy and real-time control in instrumentation, multi-workflow orchestration and intelligent decision-making from sparse data as well as automated sample handling strategies.



Both the synthesis and characterization steps have some AI-driven models as well as predictive tools available. Automated experimental setups also exist, a few of which actually have autonomous capabilities. Examples of such instrumentation for synthesis exist within the INTERSECT initiative ecosystem developed at ORNL, which includes autonomous flow reactor with multi-modal in situ characterization, autonomous chemistry lab with multi-modal characterization tools connected by mobile robots, and autonomous additive manufacturing for metals and composites. Additionally, it seems that the complexity of robotic synthesis is under-appreciated. Some systems are obviously more amenable to automation, but there remain many gaps. The ability to develop workflows that are robust using robotics remains a bit of a challenge. This varies, of course depending upon the system being considered (e.g. homogeneous versus heterogenous syntheses), but a robust workflow depends upon many variables which can be influenced by the individual robotics being employed. Robotics typically need to be customized for the task at hand, which makes it difficult to have reliable operation and quick support from vendors when things go wrong. Invariably experimentalists become frustrated with the machines that are supposed to alleviate their mundane or dangerous tasks and resort to human intervention. While it is clear that the one-unit-does-it-all type of approach often leads to significant problems, breaking the process into pieces also comes with challenges. Interruption of a serial process by one robotic aspect of the workflow represents a significant issue. This will be a difficult issue to resolve and will require deep connections between users and vendors to arrive at sustainable solutions.

In the characterization arena, there exist 4D-STEM, neutron beamlines, tools for thermal analysis, microscopy, and PLD with multi-modal characterization. There seems to be more software available for characterization (ex: DT of 4D-STEM at JHU, AI-driven feedback loops used in several institutions and in-line automated testing at DARPA METALS), than for synthesis. A main difference between these two steps is that synthesis is very material and condition specific, i.e., not easily generalizable, while characterization techniques can more easily be used across different domains. Ideally, in an autonomous laboratory characterization should be done in-situ and on-line, but that is not common at the moment. Additionally, the amenability of the characterization component to integration into an autonomous system depends significantly on the field being considered. For example, testing of materials for specific physical properties (e.g. conductivity, mechanical strength, breakdown voltage, etc.) can often be more easily automated than testing for physiochemical properties. The latter often involves chemical conversion testing, online analysis, and mass balanced data analysis. One specific example is that of flow testing for catalysts which is very process dependent and difficult to do in a fully automated fashion. Industry participants mention that experience has shown that the equipment necessary to collect such testing data requires significant care and feeding, but can be automated to some extent.

This is the time to rethink how experiments are conducted and, especially, how experimental facilities should be built to allow for many, if not all, instruments to be in the same place, automated sample handling, remote management of instruments and so on. In addition, achieving a seamless flow of information across facilities is challenging yet crucial for developing complex autonomous workflows. This integration of distributed experimental and computation resources is essential for effective large-scale data management and theory-driven processes. Industrial partners pointed out the importance of having automated notice of breaking down of equipment, failure analysis, defect detection, and handling of unexpected results. Obviously, this transition requires large investments, so the need for de-risking products from autonomous labs was also discussed. Instrumentation and software interoperability is critically missing, as each piece of equipment (or software) is developed independently from any other and proprietary issues also exist. Vendors should be actively involved in addressing interoperability issues and remote operations. In addition, developing common protocols, standards, and standard parameters, like already in use in the electronics industry, was suggested as a way to substantially help the transition. Lastly, as many experiments require fast time-scale response, instrument control (real time analysis and feedback) requires direct access to the instrument itself and cannot happen through an API, as APIs are usually too slow for autonomous operation. Such direct access is not currently available in most cases.

Better automated, streamlined processes for capturing synthesis and characterization data are needed, especially for such a data capture to occur in a secure manner. The need for investments in security from the beginning was noted. Currently, no uniform data representation for synthesis and characterization data is available. The option to standardize knowledge extraction instead of data format, i.e., to develop a tool able to deal with as many data formats as possible, was suggested as a possible solution to overcome the difficulty due to the variety and independence of vendors. As an example, it was pointed out how LHM moved from Granta to "Material Center."

Very few current capabilities were identified for Manufacturing, Certification and End-of-life. These capabilities included a few databases (ex. the process parameter monitoring and trending at TAMU and the database on shape memory alloys at NASA), statistical models and an example of Research Institute (JHU-CMU-led in collaboration with NASA) focused on enabling rapid certification of metal parts created using advanced manufacturing techniques. Workforce skills and mid-scale manufacturing tools, as well as standardized control messages for instruments were identified as most pressing gaps, together with the need for models for recycling pathways, autonomous disassembly and frameworks for recyclability and sustainability. The fact that, at the manufacturing level, most data and information are proprietary was also identified as a key factor hindering the development of autonomous capabilities. Lastly, the pressing need to accelerate certification was pointed out, and the hope that autonomous could help in that regard.

Across the board, a pressing issue holding back the development of autonomous laboratories was identified in the lack of a quick path for industry-government collaboration. Such types of agreement currently exist between industry and their supplier, but the standard ways industry and government collaborate (NDR, CRADAS and FTO) often require too long a time to be drafted. Issues around keeping data private and sharing them, as well as solving IP issues and export controls contribute to the challenges in these agreements.

Currently, most players in the autonomous arena have the tendency to build their laboratories and workflows without talking to anyone else. Exceptions do exist (for example, the DOE-led FASST initiative which is working across agencies), but there are too few. To advance the field of autonomous experimentation quickly and effectively in the USA, it has been suggested that what is missing is a centered consortium/institution comprised of members from government agencies/labs, academia, and industry, where companies making the materials, vendors, and industrial users are all represented.

Lastly, the education of the current and future generation was discussed. While many more students are interested in ML now than in the past, in the current workforce we are still missing experts across domains/fields. It was also suggested that education should be done in partnership with the private sector.

Functional Ceramics

Facilitators: Shirley Meng (UChicago), Shijing Sun (University of Washington)
Participants/Observers Group A: Chaitan Baru (NSF), Vijay Murugesan (PNNL), Joey Montoya (TRI), Ian Foster (Argonne/Chicago), Antti Makinen (ONR), Ankit Agrawal (Northwestern), David Elbert (JHU, PARADIM)
Participants/Observers Group B: Simon Billinge (Columbia University), Ram Seshadri (UCSB), Eric Wang (Samsung), Asra Hassan (ULRI), Tulsi Patel (ExxonMobil Low Carbon Solutions), David Darwin (NSF TIP)

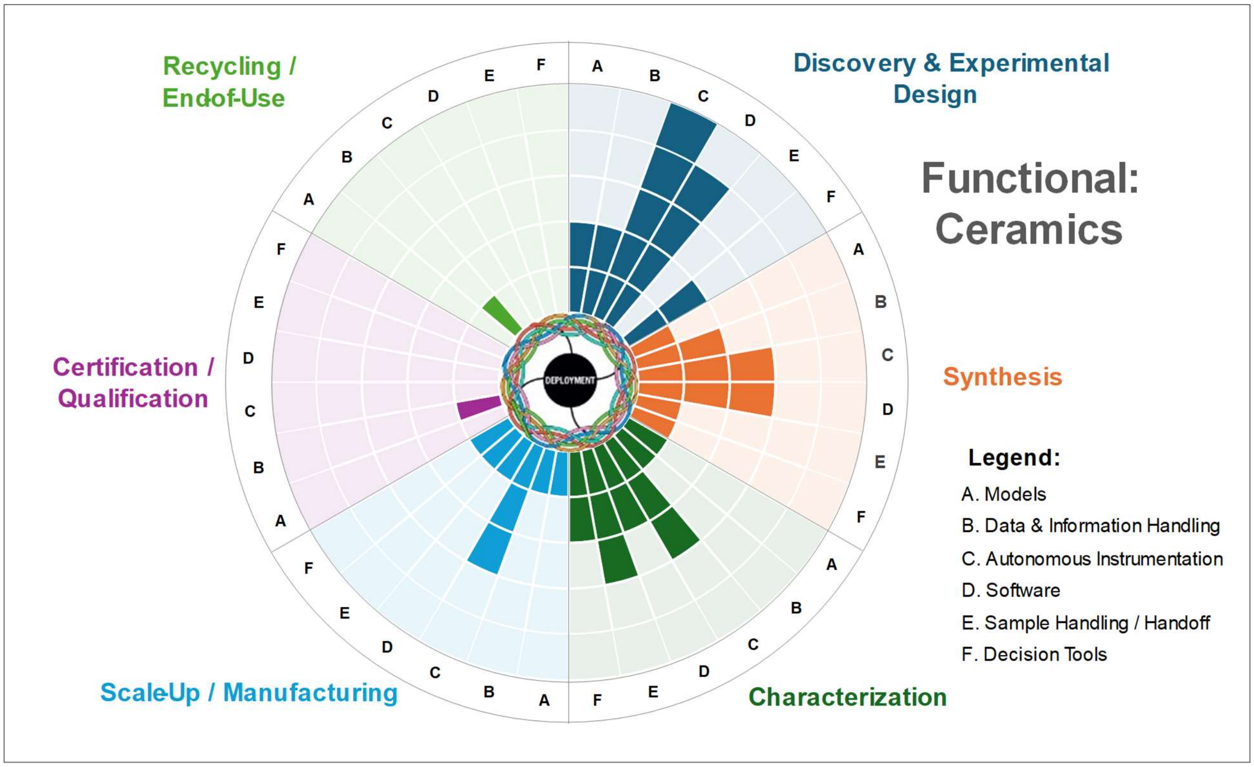
Current Landscape

Functional ceramics present unique synthesis and characterization challenges, requiring specialized capabilities such as high-temperature processing, ball milling, sintering, and pressing. These complexities make the full automation of labs challenging, underscoring the importance of a collaborative approach that integrates human expertise, AI, and robotics. Traditionally, there is often a delayed discovery of materials' key functionalities, which often emerge years or decades after the initial material synthesis. This delay highlights the need for strategic scientific alignment, where autonomous experimentation efforts must focus not only on developing advanced infrastructure and tools ("hammers") but also on identifying the right problems ("nails") that are apt for high-throughput and AI methods. Moreover, while there have been successes with automated experiments, gaining the trust of domain experts for fully autonomous experimentation remains a challenge. To overcome these barriers, it is crucial to foster a three-way collaboration between human scientists, AI systems, and robotic technologies, ensuring that the development and application of infrastructures are scientifically aligned and trusted by the broader research community. This integrated approach will be essential for realizing the great potential of autonomous experimentation in functional ceramics.

Recent infrastructure innovation for autonomous experimentation has been uneven, with a focus on computational discovery, synthetic workflow planning, and high-throughput characterization, while areas such as scale-up/manufacturing, certification/qualification, and recycling/end-of-use are overlooked. In discovery and experimental design, notable software tools include OpenMSI and AlabOS for data handling and experiment orchestration. For synthesis and characterization, key tools include the Calphad modeling platform, GEMD data processing format, PIRO synthetic planning software, reaction-network, and the PARADIM decision-making platform. Emerging software for automated characterization data analysis includes PDFitc, PDFFit, Phase Mapper, Xtal2dos, TRIXS, and autoxrd. Additional resources on accelerated materials discovery include the Materials Project database, Polybot Echembot at Argonne National Laboratory, the high-throughput synthesis, xrd characterization and electrochemistry suite by Eric McCalla at McGill, and the facilities at MDRI-ULRI. Overall, the current trend of infrastructure innovation highlights three emerging themes:

- **Central Characterization Facilities**: Increasing number of beamlines with robotic sample handling and big data analytics capabilities, such as synchrotron PXRD and GIWAXS, enhancing precision and efficiency in material analysis.
- **Community Software**: Efforts in the materials science community to develop open-source software infrastructure like the Bluesky Data Collection Framework, addressing challenges in experiment orchestration and scheduling.
- **Industry R&D efforts**: Autonomous materials discovery would attract broad industry interests, as exemplified by contributions from Google DeepMind, Microsoft Azure, Samsung Advanced Institute and Toyota Research Institute.

Furthermore, several initiatives in Europe lead this area, such as the BIG-MAP project within Europe's BATTERY 2030+ initiative and the EU-funded VIPERLAB for Perovskite solar research. AMANDA manages multiple materials acceleration platforms, while Line1 automates organic solar cell manufacturing and characterization. Spain's ION-SELF project develops an autonomous MAP for battery materials, and Finland's Synbio-MAP by VTT Technical Research Centre of Finland links synthetic biology to high-throughput screening and AI-driven modeling for protein-based materials and bioplastics. These advancements highlight the growing global landscape of tools for advancing autonomous experimentation in functional ceramics.



Identified Gaps and Opportunities

- **Autonomous setup for ceramics**: The critical role of experimental design, which humans excel at, but robots cannot fully replicate, underscores the need for dedicated robotic designs tailored for materials scientists, particularly for functional ceramics.
- **Cross-disciplinary collaboration**: Incentives are necessary to foster collaboration among computer scientists, materials experts, and robotics specialists. Students from these disciplines see vast differences in productivity, highlighting the need for better integration and cooperation.
- **Private-public partnerships**: There is a lack of collaboration between private and public sectors, with the industry holding a leading edge in AI/ML. Strengthening these partnerships could accelerate advancements in autonomous experimentation.
- **Flexible instrumentation**: Many synthesis and characterization tools lack APIs and interoperability, creating barriers in integrating the tools with AI/ML algorithms.
- **Autonomous experimentation across scales**: In functional ceramics, the method of making often differs from the method of measurement, requiring different platforms (e.g. thin-film processing vs powder synthesis) for functionality tests.
- **Innovation for manufacturing**: Beyond initial materials synthesis, there is a need for dedicated focus on scaling up, manufacturing, and recycling processes.
- **Data generation and standardization**: The absence of automatic data capture and structuring leads to labor-intensive manual organization. Following the FAIR principles and standardizing data across instruments are critical for cross-lab validation. Code standardization and comprehensive documentation are also essential to lower entry barriers for new researchers.

- **Human-in-the-loop initiatives**: Workforce development should focus on training robots to assist students rather than the reverse. Domain experts are crucial to ensure the quality and relevance of data and scientific conclusions. The strategic collaboration between human and artificial intelligence ensures that the results emerging from autonomous discovery are useful, reliable, and non-trivial.

Functional Soft Matter

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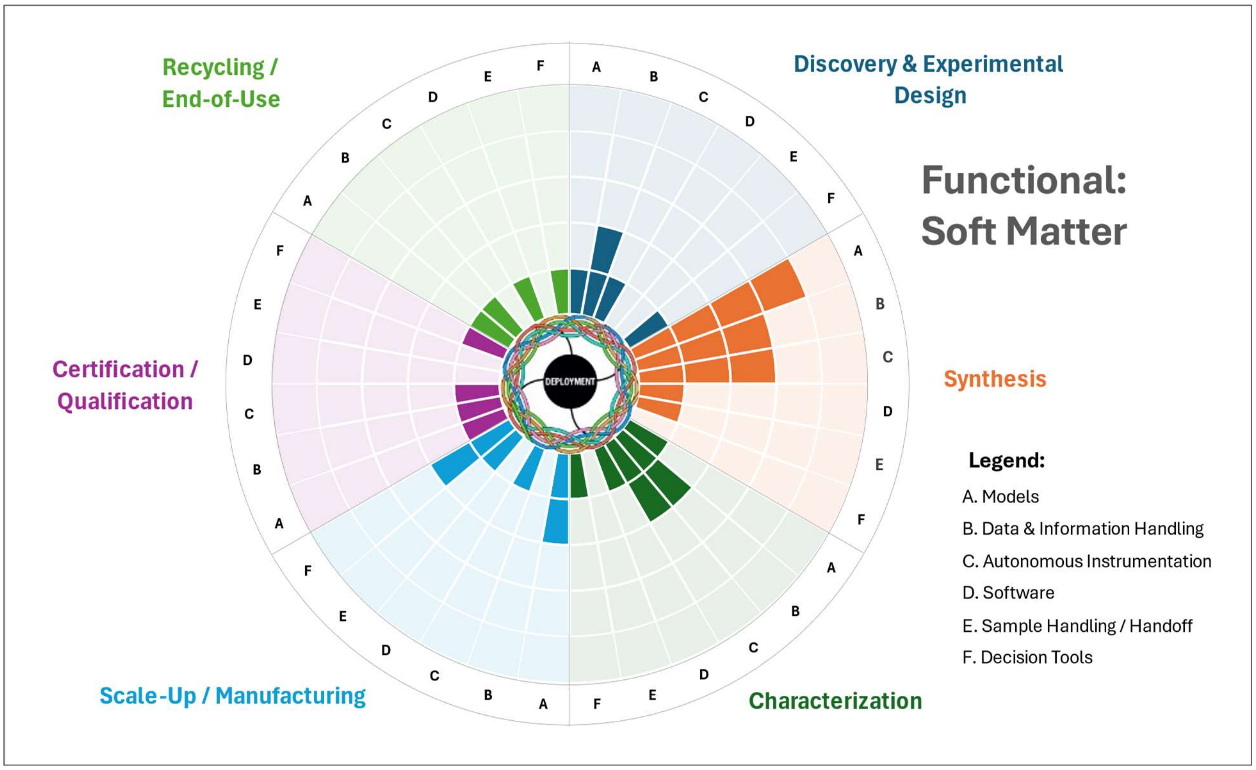
Current Landscape

The current state of accelerating materials solutions for functional soft matter (FSM) to meet national and global challenges consists of little inventory and limited access, both of which represent important bottlenecks for advancing the field. Materials innovation platforms (MIP) such as BioPACIFIC MIP, GlycoMIP, and the Molecule Maker Lab Institute support chemical and/or biochemical synthesis-based workflow protocols which have substantial promise for democratizing materials innovation, but targeted infrastructure investment is necessary to transform such platforms into broadly accessible resources. Industry and national labs, such as NIST, have developed small molecule workflow and living therapeutic foundries for cellular engineering, but in general these resources remain challenging to access for outside users. The following suggestions have been noted by the working group to fully harness the substantial untapped potential of FSM to be accelerated and elevated by autonomous and closed-loop science, and to position the nation for global impact. This white paper highlights the need for major infrastructure investments to democratize access to functional soft matter innovation, the disruptive potential of forward-thinking strategies to better harness the substantial untapped power of autonomous science in the FSM domain, and a novel fit-for-purpose “mission-oriented research” model leveraging cross-disciplinary expertise, including citizen scientists.

The current landscape for functional soft matter combines living (bio) foundries, modular chemical synthesis platforms, autonomous science platforms, self-driving labs, and infrastructure from national labs to provide some support for design and development. But major investments in infrastructure and new models for engagement (e.g., mission-oriented research models) are needed to democratize access to these powerful resources.



- ***Living Biofoundries:*** MIPs (BioPACIFIC MIP, GlycoMIP) are research platforms with highly integrated research focus teams designed to educate and advance the next generation of materials synthesis and characterization. NIST's living measurement system foundry is an automated facility that supports high-throughput measurements for engineered cellular systems; this design, build, and test model supports machine learning cycles.
- ***Modular Chemical Synthesis****:* Akin to automated peptide and oligonucleotide synthesizers, a platform for automated modular synthesis of small molecule-based functional soft matter based on MIDA/TIDA boronates has recently emerged. This platform has the potential to shatter the synthesis bottleneck that has traditionally limited access to carbon-carbon bond-based materials innovation and enable the power of closed-loop and autonomous experimentation to be practically interfaced with FSM discovery campaigns.
- ***Industrial Autonomous Platforms:*** Based on more traditional chemical approaches, IBM RoboRXN, based on Chemspeed, offers a liquid-handling, partly-sided handling synthesis platform connected to LC/MS. Merck PSW-HTE supports small-molecule and peptide libraries via experimental design, automation, analysis, and data capture. Self-driving labs, such as the Emerald Cloud Lab and Carnegie Melon Cloud Lab, also provide access to remote synthesis and telerobotic capabilities
- ***National Lab Autonomous Infrastructure:*** Automated platforms at Brookhaven for SAXS data and the autonomous chemistry labs at Oak Ridge provide examples of chemical automation in practice.
- ***Software Packages:*** Recent reports of one-shot LCMS purification/characterization platforms, such as the one recently reported at U. Toronto, have the potential to address characterization bottlenecks to enable rapid cycling through AI-guided closed-loop campaigns.

Identified Gaps and Opportunities

The call for action to improve the current state of functional soft matter toward accelerated, autonomous, and more democratized science is noted below. Of resounding concern was the need to broaden access to innovation-enabling infrastructure and ensure that quantifiable metrics focused on mission-driven projects using a fit for purpose model resonated with the group. This model supports *mission-driven* directives using team science with a finite timeline to achieve deliverables.

- ***Scope, Scale, Sustain:*** Broad support was voiced for investing in infrastructure to create multidisciplinary Centers of Emerging Chemical Technologies - dedicated research centers that bring together experts from various fields to partner with external innovators to advance and broaden access to FSM innovation projects. It was specifically mentioned that we need a CHIPS Act for small molecule synthesis. It was further recommended that the nation develop multi-directional partnerships between academic institutions, industry leaders, industry manufacturers, national labs, and policy stakeholders focused on mission-oriented research projects. Also highlighted was the need to share knowledge and resources and implement best practices and strategies for automated functional soft matter.
- ***Implement*** a well-defined materials database for all classes of materials that is streamlined and easy to populate and machine readable, with nomenclature covering the intersection of this new field.
- ***Standardization of workflow for synthesis and additive manufacturing*:** Improved liquid-sample handling and the need for reliable and scalable quantifiable measurements are desired.
- ***Hardware:*** There is a lack of transparency from equipment manufacturers in terms of automation and data sharing that prevents interoperability and ability to leverage emerging techniques necessitating a means by which to have the commercial, standard lab equipment available in some kind of "FAIR-like" manner.
- ***High Throughput Characterization and Testing*:** recommendations to streamline the workflow process from synthesis to characterization and testing would optimize this process for translational applications.
- ***Data Storage and Security***: Secure funding from public and private sources to support multidisciplinary research and development efforts.
- ***Artificial Intelligence and Machine Learning Models***: Data scientists who understand scientific jargon to support synthesis, characterization, and translation are needed.
- ***Training, Education, and Workforce Development***: There is a major need for workforce development in this emerging intersection between AI, automated synthesis, and automated testing. Emphasis was placed on recommending specialized training programs (associate degrees, certificates, and post-bac programs) to equip technicians, researchers, and engineers with the skills needed for FSM development and deployment.
- ***Technology Transfer***: Further connect technology transfer and commercialization to help facilitate the translation of research findings into commercial products through partnerships and licensing agreements.

Broad support was voiced regarding the need to invest in infrastructure that provides broad access to FSM innovation. It was also specifically mentioned that these investments should be guided by a fit-for-purpose model ensuring that FSM development is aligned with specific application needs and regulatory requirements. This model involves

- Targeted Research and Development: A Mission-Oriented Research model, focusing on key application areas such as drug delivery, diagnostics, and sustainable materials
- Interdisciplinary Teams: Establishing teams with expertise across the relevant disciplines to foster innovation and address complex challenges; Including supported access to highly-enabling infrastructure that eliminates synthesis bottlenecks are recognized as key elements for the success of such an approach
- Iterative Design Process: Employing a cyclical process of design, testing, and refinement to achieve optimal material performance
- Regulatory Alignment: Ensuring that FSM products meet regulatory standards and safety requirements from the early stages of development
- Stakeholder Engagement: Involving industry partners, regulatory bodies, and end-users throughout the development process to ensure relevance and acceptability.

Recent breakthroughs in AI, automated platforms for the synthesis of carbon-carbon bond-based materials, advances in automated testing and characterization have synergistically yielded a historic opportunity to revolutionize FSM innovation, and for the United States to lead this burgeoning Molecular Industrial Revolution. Development of systems and multidisciplinary teams that drive Mission-Oriented Research have the potential to disruptively shift the design, engineering, and translation of FSM research and democratize FSM innovations. Adopting a fit-for-purpose model and fostering cross-disciplinary collaborations can accelerate the innovation and deployment of FSM synthesis, characterization, and technologies at scale. However, realizing all of this tremendous potential will require strategic investments in infrastructure that shatter synthesis bottlenecks and bring the power of closed-loop/autonomous research to a broader scope of the scientific and broader communities.

Functional Semiconductors

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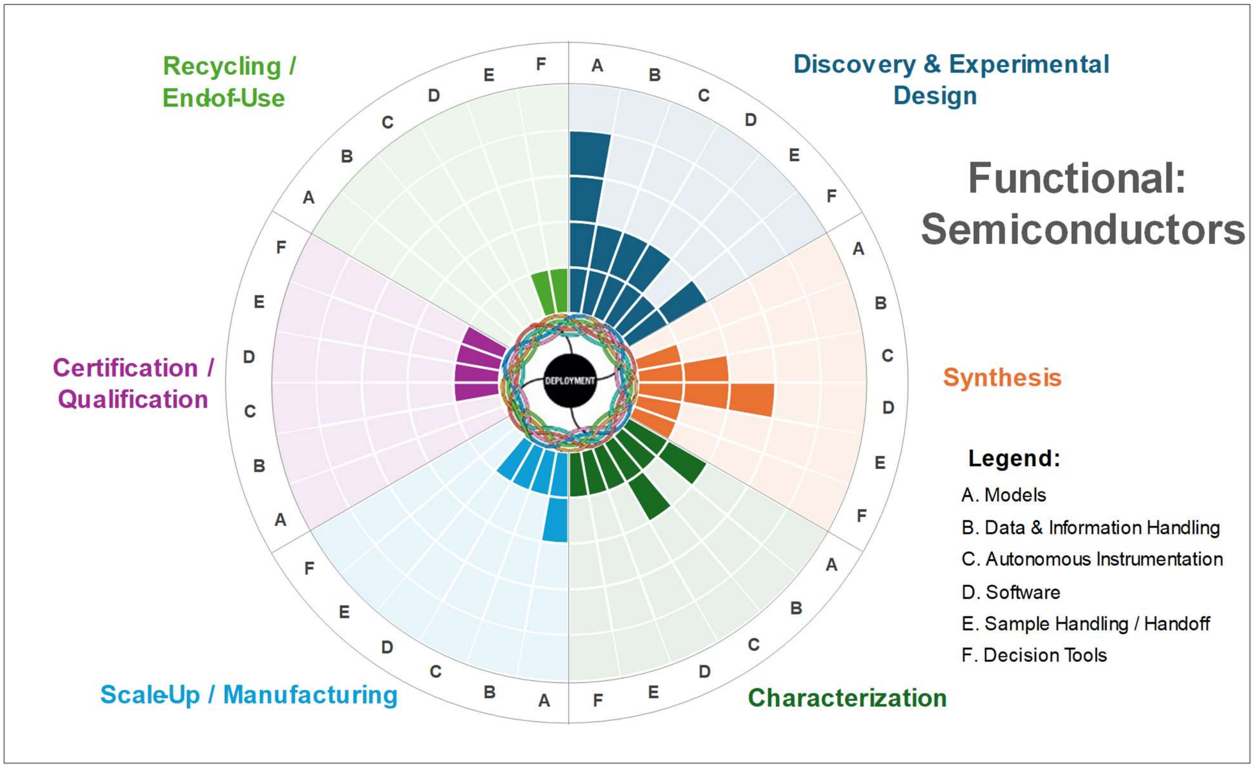
Current Landscape

Semiconductor manufacturing has been at the forefront of automation for decades driven by inherent demands for high throughput, yield, quality and reliability. The emergence of highly automated wafer fabs with robotic wafer-handling systems, advanced process control, high throughput metrology and integrated cyberinfrastructure provide a compelling platform for advanced decision-making technologies that incorporate machine learning and artificial intelligence to optimize workflows and process outcomes. Significant deviations from process parameters, however, still rely on human intervention, failure analysis and troubleshooting which reduce productivity. Similar considerations apply for laboratory scale infrastructure for semiconductor materials which, while not as highly integrated as production fabs, still commonly employ automation and adaptive control. Autonomous instrumentation, on the other hand, requires the ability to make complex decisions at the timescale of the process employed (e.g. deposition, epitaxy, etching) based on limited data from real time metrology techniques.



Identified Gaps and Opportunities

- **Autonomous instrumentation for thin films materials discovery:** Autonomous set-ups have been demonstrated for solution-based synthesis and to some extent for powder-based synthesis which are of limited applicability to semiconductors that require ultra-high purity and high vacuum processing environments. Sources available on tools are limited, constraining options for high-throughput discovery of new materials and complex multi-material systems and devices. New instrumentation designs for high throughput multi-source thin film processing with integrated in situ metrology are needed to accelerate discovery.
- **Innovation for manufacturing:** Semiconductor processing tools used in manufacturing incorporate aspects of automation (e.g. sample handling, in situ metrology, statistical process control) but rely on humans for decision making when processes deviate beyond acceptable levels. Digital twins are needed which incorporate ML/AI enabling integration of autonomous process control and troubleshooting.
- **Multi-scale physics-based models:** Approaches are needed to capture non-equilibrium and kinetic processes inherent to materials synthesis and nanofabrication to predict resulting composition, phase, microstructure and topography, specifically as these relate to materials and device performance and durability. Models must consider macroscale processing geometry which varies from vendor to vendor and also be translatable from lab-scale to manufacturing-scale equipment. Digital twins can also enable further physics-based modelling for materials qualification and development.

- **Advances in metrology:** This area includes in situ techniques and high throughput spatiotemporal methods to meet the rapid feedback timescales required for autonomous operation.
- **Metadata and data standardization:** Semiconductor manufacturing utilizes a very large number of different tools, from multiple vendors, often with proprietary data formats and limited access to metadata. Open data approaches would enable broader adoption of AE methods.

Significant additional information of key outcomes for the Functional Semiconductor group discussion can be found in **Appendix D**.

Challenges and Considerations

While this report baselines existing AMII capabilities and identifies gaps across material systems, AMII is still a relatively nascent field of practice. There are still several challenges and important considerations to building a robust community of practice and develop scalable AMII that is accessible to the broader community.

To successfully implement and realize impactful discoveries from AMII will require bringing together a diverse set of relevant stakeholders. Consortia models were brought up throughout the workshop for consideration, as they can help bring together government funders, private industry, and researchers to coordinate efforts, pool resources, and realize greater returns from investments. Consortia can help align government programs towards applied research that is relevant to critical challenges domestic industry faces. Collaborative, pre-commercial research can help demonstrate the value of AMII to practical research questions, providing value to various types of consortia members. Consortia can also act to convene practitioners and bring together a community of practice around the various aspects of development still needed to realize AMII. While other countries have established consortia for autonomous materials discovery, the United States today does not have a comprehensive consortium for AMII.

One key aspect of AMII development is the tooling required for the generation and integration of significant amounts of data, the upgrading and digitalization of scientific hardware, and orchestration and management software specifically geared towards AMII. While different researchers have developed their own implementations, open-source software and hardware can help accelerate adoption of AMII components and lower the barrier to entry for researchers interested in implementing AMII. Open-source adoption can also enhance standardization, modularity, and reproducibility of AMII infrastructure and results. Promoting adoption of these best practices can help accelerate the iteration cycles for improving AMII, reduce the timelines to further deployments of AMII platforms and help realize breakthrough innovations more quickly.

Another key consideration for AMII development is the workforce behind it. Implementing AMII will require bringing together a diverse array of skills: from building AI models to support autonomous platforms, to developing software orchestration and data management, to hardware and firmware maintenance and operations, to domain knowledge of scientific problems. Building a skilled scientific workforce capable of developing and working with AMII will be critical to realizing success from AMII investments. For national security positions, an AMII workforce that includes U.S. citizens will be critical. Conveniently, many of these skills are already recognized as critically necessary by the broader scientific community – AMII can serve as a useful leverage point to accelerate educational development in these critical skillsets. As discussed previously, AMII can also enable researchers to spend more of their time on scientific thinking and discovery and reduce the time spent on menial tasks.

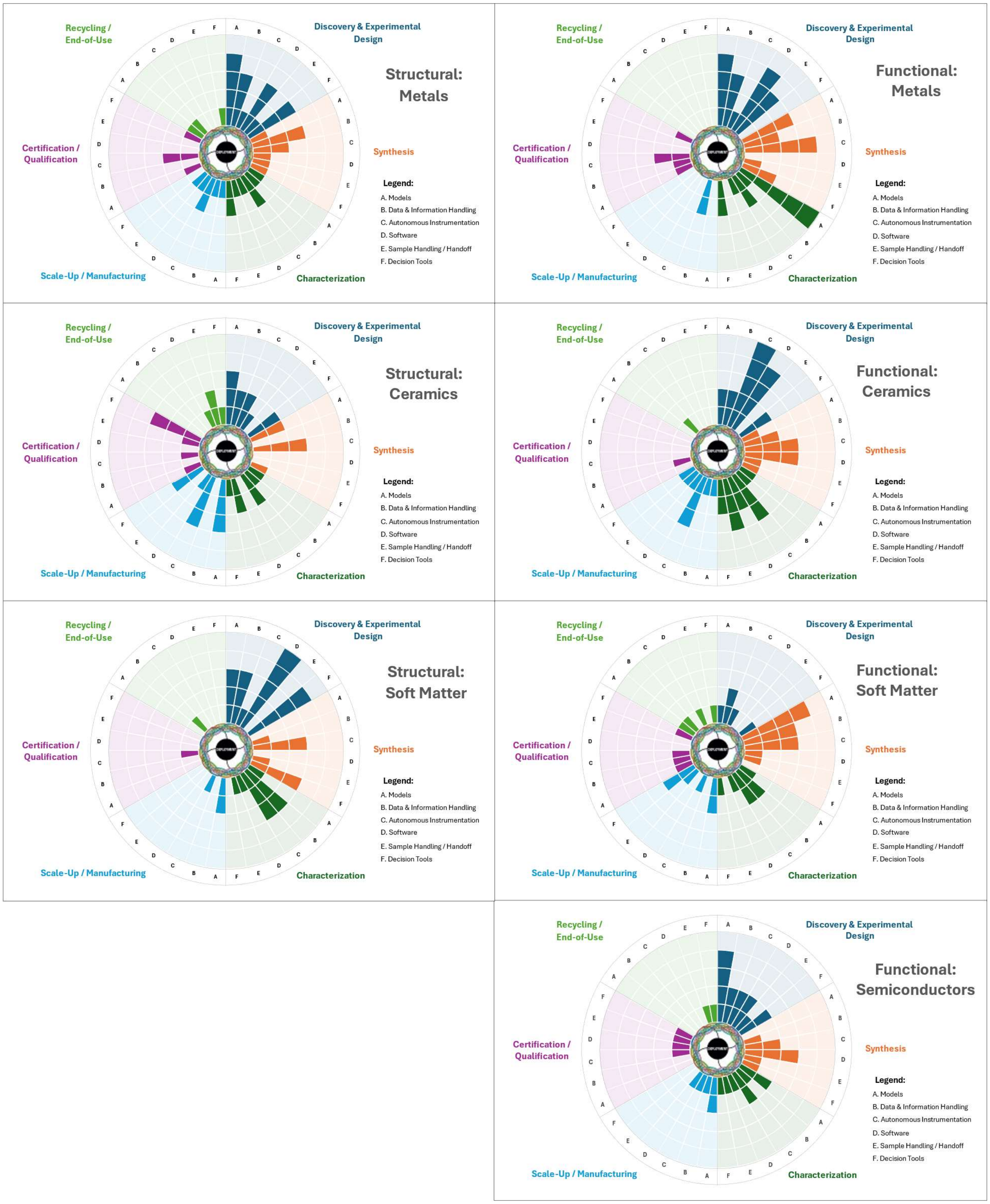
Finally, as autonomous platforms continue to expand and the AMII becomes more accessible, ethical, safety, and security considerations will become increasingly important. For classified, biologically hazardous, and other national security related research, traditional frameworks of risk assessment and assurance may need to be modified to accommodate autonomous platforms. Lab safety practices will have to incorporate robotic sensing and automated equipment, as well as notification and safety protocols for unsupervised experiments. Ethical guidelines for scientific research and disclosure may also evolve.

Conclusion

The Materials Genome Initiative (MGI) Workshop “Accelerating Materials Solutions to Meet National and Global Challenges” brought together stakeholders to help understand the landscape of the AMII, including the existing infrastructure and the gaps needed to advance Autonomous Experimentation (AE) for materials R&D. This report should provide a useful baseline for researchers, policymakers, and program managers looking to develop efforts supporting the AMII.

Overall, AE is at an early stage of development, but the community has made key demonstrations of accelerated research and productivity.

The figures below illustrate the output of the analysis of the input received for all 7 domains considered during the workshop. Clearly differences in capabilities can be seen, but there are also some trends that emerged. For example, there are generally limited capabilities identified in the certification/qualification and recycling/end of use categories. For most materials domains, the participants identified more resources in the discovery and experimental design, synthesis, and characterization categories, and also in scale-up and manufacturing, especially for the ceramic materials domain. This workshop exercise and the data captured within the appendices serve as a benchmark of the existing AMII and will help inform continued development in this area.



These starburst charts illustrate the input received for each of the materials domains during the breakout sessions, as described in more detail in the Workshop Description. Larger shaded radius indicates more existing resources identified during the workshop landscaping activity.

There were common themes for gaps in the AMII across the breakout sessions and panel discussion from the workshop participants that are highlighted here.

Common Gaps in AMII across Materials Domains:

- Significant infrastructure for autonomous experimentation for materials R&D
- Workforce development for AI-Driven AE for materials research
- Automated experimentation hardware for
    - Synthesis
    - In-line & in situ characterization
    - Testing (mechanical, electrical…)
    - Sample handling/exchange between instruments
- AI-driven autonomous decision methods tailored for materials research
- Integration of modeling & simulation into AE workflows
- Software for autonomous workflows and hardware interfaces
- Standardized data structures that improve R&D workflows (FAIR)
- Improved sharing and access to non-proprietary results & data
- Safety and security for laboratories, data
- Shared/centralized facilities to improve access
- Integration of digital manufacturing, digital twin, and scale-up for technology transition
- Consortia or Public Private Partnerships to leverage strengths of government, industry and academia

Beyond these needs, the appendices contain a valuable and insightful trove of detailed information and observations from both the working sessions and data gathered in preparation for the workshop.

In closing, the organizers are grateful to the workshop participants who have provided very important contributions to this assessment of the AMII. It is expected that this report will serve as a valuable resource to inform future efforts in autonomous experimentation.

Appendices

A. Agenda

Accelerating Materials Solutions to Meet National and Global Challenges

A Workshop in Support of the MGI Strategic Plan

Subcommittee on the MGI

Workshop Agenda – Day 1

Date:
June 10th, 2024

Time:
8.00 AM – 5.00 PM ET

Place:
National Science Foundation
Room 2020/2030
2415 Eisenhower Ave
Alexandria, VA 22314

Start	End	Time	Point of Contact - Lead
8:00 AM	8:30 AM	**Registration**	**Claire Riley** (NSF)
8:30 AM	8:50 AM	**Welcome and Opening Remarks**	**Denise Caldwell** (Assistant Directors, MPS) **Germano Iannacchione** (Division Director, DMR)
8:50 AM	8:55 AM	**Setting the Stage: The MGI**	**Lisa Friedersdorf** (OSTP)
8:55 AM	9:10 AM	**Setting the Stage: Logistics of the Day**	**Cosima Boswell-Koller** (NSF)
9:10 AM	9:55 AM	**Panel: The AMII and Global Challenges** Moderator: **Jim Warren** (NIST) Panel Members: **Jae Hattrick Simpers** (University of Toronto), **Milad Abolhasani** (NCSU), **Rob Moore** (ORNL), **Shijing Sun** (University of Washington), **Javier Read de Alaniz** (BioPACIFIC MIP), **Theresa Mayer** (CMU) **Discussion Points:** • Scientific challenges that are ripe for the application of the AMII • Status of developed infrastructures to meet demands/requirements of identified challenges • Areas/capabilities/mechanisms that are under-resourced, reasons for under-resourcing, and potential solutions to address this • Potential immediate stakeholders and possible engagement models • Ideal ways for the MGI community to collaborate and coordinate as a part of the publicly supported autonomous experimentation (AE) community • Opportunities to keep the momentum going at the Federal level	

Agenda continued on next page...

9:55 AM	10:00 AM	**Setting the Stage: Logistics Working Session**	**Cosima Boswell-Koller** (NSF)
10:00 AM	11:15 AM	**Working Session 1:** **Inventory of the Existing National Autonomous Materials Innovation Infrastructure (AMII)** **Breakout Leads:** Structural: Metals - **Jae Hattrick Simpers, Brad Boyce** Ceramics - **Sergei Kalinin, Joshua Schrier** Soft Matter - **Vicky Nguyen, Keith Brown** Composites - **Chris Haines, Benji Maruyama**	Functional: Metals – **Francesca Tavazza, Phil Kim** Ceramics - **Shijing Sun, Shirley Meng** Soft Matter - **Marty Burke, Juana Mendenhall** Semiconductors - **Joan Redwing, Eric Stach**
11:15 AM	11:30 AM	**Break**	
11:30 AM	12:30 PM	**Report Out**	**Moderator: Cosima Boswell-Koller** (NSF) **Breakout Leads reporting out**
12:30 PM	1:30 PM	**Working Lunch**	
1:30 PM	1:35 PM	**Setting the Stage: Logistics Working Session**	**Charles Yang** (DOE)
1:35 PM	2:35 PM	**Working Session 2:** **Identify gaps in the Autonomous Materials Innovation Infrastructure (AMII) that must be filled** **Breakout Leads:** Structural: Metals - **Jae Hattrick Simpers, Brad Boyce** Ceramics - **Sergei Kalinin, Joshua Schrier** Soft Matter - **Vicky Nguyen, Keith Brown** Composites - **Chris Haines, Benji Maruyama**	Functional: Metals – **Francesca Tavazza, Phil Kim** Ceramics - **Shijing Sun, Shirley Meng** Soft Matter - **Marty Burke, Juana Mendenhall** Semiconductors - **Joan Redwing, Eric Stach**
2:35 PM	2:50 PM	**Break**	
2:50 PM	3:35 PM	**Report Out**	**Moderator: Charles Yang** (DOE) **Breakout Leads reporting out**
3:35 PM	4:20 PM	**Panel: Building a Community to Realize the AMII - An Industry Perspective** Moderator: **Benji Maruyama** (AFRL) Panel Members: **Richard Gottscho** (LAM) **Tim Erdmann** (IBM) **Carol Handwerker** (CHIPS Program Office) **Discussion Points:** • Industry's needs from the larger community for best engagement • Modes or paths to industry engagement with community • Company requirements to enable robust interactions and partnerships • Mechanisms and incentives needed to "sell" the investment to industry leadership	**John Lockmeyer** (Shell) **Michael Glavicic** (Rolls-Royce)
4:20 PM	5:00 PM	**Wrap Up:** Government Next Steps	**Lisa Friedersdorf** (OSTP) **Cosima Boswell-Koller** (NSF) **Benji Maruyama** (AFRL) **Jim Warren** (NIST) **Charles Yang** (DOE)

B. Attendee List

First	Last	Institution / Organization	Group
Milad	Abolhasani	North Carolina State University	Functional Semiconductors - A
Ankit	Agrawal	Northwestern University	Functional Ceramics - A
Jeff	Aguiar	Lockheed Martin	Functional Metals
Chaitan	Baru	National Science Foundation (NSF)	Functional Ceramics - A
Simon	Billinge	Columbia University	Functional Ceramics - B
Cosima	Boswell-Koller	National Science Foundation (NSF)	
Bryan	Boudouris	University of Alabama	Functional Soft Matter
Brad	Boyce	Sandia National Labs	Structural Metals
Branden	Brough	National Nanotechnology Coordination Office (NNCO)	Functional Semiconductors - A
Keith A.	Brown	Boston University	Structural Soft Matter
Marty	Burke	University of Illinois at Urbana-Champaign	Functional Soft Matter
David	Darwin	National Science Foundation (NSF)	Functional Ceramics - B
Sanket	Deshmukh	Virginia Tech	Structural Soft Matter
Andrew	Detor	Defense Advanced Research Projects Agency (DARPA)	Structural Metals
James	Dorman	U.S. Department of Energy (DOE)	Structural Ceramics
David	Elbert	Johns Hopkins University	Functional Ceramics - A
Tim	Erdmann	IBM Research	Functional Soft Matter
Hal	Finkel	U.S. Department of Energy (DOE)	Functional Semiconductors - A
Eric	Forsythe	National Institute of Standards and Technology (NIST)	
Ian	Foster	Argonne National Laboratory & University of Chicago	Functional Ceramics - A
Lisa	Friedersdorf	White House Office of Science and Technology Policy (WH OSTP)	
Eddie	Gienger	Johns Hopkins University - Applied Physics Lab	Structural Metals
Mike	Glavicic	Rolls-Royce Corporation	Functional Metals
Rick	Gottscho	Lam Research	Functional Semiconductors - A
Chris	Haines	U.S. Army DEVCOM - Army Research Lab (ARL)	Structural Ceramics
Leslie	Hamilton	Johns Hopkins Applied Physics Laboratory	Functional Metals

Carol	Handwerker	Department of Commerce (DOC)	Functional Semiconductors - A
Robert	Hart	U.S. Army DEVCOM Ground Vehicle Systems Center (GVSC)	Structural Metals
Asra	Hassan	Underwriters Laboratories Research Institutes (ULRI)	Functional Ceramics - B
Jae	Hattrick-Simpers	University of Toronto	Structural Metals
Aisha	Haynes	Office of the Under Secretary of Defense, Research and Engineering (OUSD(R&E))	Functional Metals
Germano	Iannacchione	National Science Foundation (NSF)	
Sergei	Kalinin	UT Knoxville	Structural Ceramics
Ibrahim	Karaman	Texas A&M University	Structural Metals
Eugenia	Kharlampieva	National Science Foundation (NSF)	Structural Soft Matter
Philseok	Kim	Advanced Research Projects Agency - Energy (ARPA-E)	Functional Metals
Alex	Klironomos	National Science Foundation (NSF)	Functional Semiconductors - A
Shane	Krska	Merck & Co., Inc.	Functional Soft Matter
Alexis	Lewis	National Science Foundation (NSF)	
John	Lockemeyer	Shell Global Solutions U.S., Inc.	Functional Metals
Antti J	Makinen	Office of Naval Research (ONR)	Functional Ceramics - A
Benji	Maruyama	Air Force Research Laboratory (AFRL)	
Theresa	Mayer	Carnegie Mellon University	Functional Semiconductors - B
Mike	McKittrick	CHIPS R&D	Functional Semiconductors - B
Juana	Mendenhall	Morehouse College	Functional Soft Matter
Shirley	Meng	University of Chicago	Functional Ceramics - A
Claudia	Mewes	U.S. Department of Energy (DOE)	Functional Semiconductors - B
Eric	Miller	U.S. Department of Energy (DOE)	Functional Semiconductors - A
Stu	Miller	Underwriters Laboratories Research Institutes (ULRI)	Structural Ceramics
Ben	Mintz	Oak Ridge National Laboratory	Functional Semiconductors -B
Dan	Miracle	Air Force Research Laboratory (AFRL)	Structural Metals
Joey	Montoya	Toyota Research Institute	Functional Ceramics - A
Rob	Moore	Oak Ridge National Laboratory	Functional Metals
Vijay	Murugesan	Pacific Northwest National Laboratory	Functional Ceramics - A

Vicky	Nguyen	Johns Hopkins University	Structural Soft Matter
Chinedum	Osuji	University of Pennsylvania	Structural Soft Matter
Patrice	Pages	National Nanotechnology Coordination Office (NNCO)	
Harry	Partridge	National Aeronautics and Space Administration (NASA)	Structural Metals
Tulsi	Patel	ExxonMobil Low Carbon Solutions	Functional Ceramics - B
Victor	Pugliano	Department of Defense (DOD)	
Dave	Rampulla	National Institutes of Health (NIH)	Functional Soft Matter
Javier	Read de Alaniz	UC Santa Barbara	Functional Soft Matter
Joan	Redwing	Penn State University	Functional Semiconductors - A
			Unable to attend
John	Schlueter	National Science Foundation (NSF)	Structural Soft Matter
Joshua	Schrier	Fordham University	Structural Ceramics
Ram	Seshadri	UC Santa Barbara / BioPACIFIC MIP	Functional Ceramics - B
Quinn	Spadola	National Nanotechnology Coordination Office (NNCO)	Functional Semiconductors - B
Eric	Stach	The University of Pennsylvania	Functional Semiconductors - B
Shijing	Sun	University of Washington	Functional Ceramics - B
Mitra	Taheri	Johns Hopkins University	Functional Metals
Francesca	Tavazza	National Institute of Standards and Technology (NIST)	Functional Metals
Rich	Vaia	Air Force Research Laboratory (AFRL)	Structural Soft Matter
Eric	Wang	Samsung Semiconductor, Inc.	Functional Ceramics - B
Jim	Warren	National Institute of Standards and Technology (NIST)	
Dana	Weinstein	White House Office of Science and Technology Policy (WH OSTP)	Functional Semiconductors - B
Charles	Yang	U.S. Department of Energy (DOE)	

C. Landscape Activity: Detailed outcomes

The inventories and gaps discussed below are derived from inputs collected at the workshop based on the knowledge and experiences of different participants. They are not comprehensive and do not reflect the opinion of all attendees. Also, the specific resources listed throughout the document were identified by the participants and should not be taken as an endorsement in any way or considered to be complete. The following images reflect the content gathered from the sticky notes for each of the categories discussed during the breakout sessions, essentially the digitization of the wall-sized posters at the meeting.

Structural Metals

Discovery & Experimental Design

Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Acceleration Consortium	"BIRDSHOT.TAMU.EDU"	NRCan	BIRDSHOT, High Throughput Materials, Software at Birdshot.tamu.edu	Acceleration Consortium	Birdshot.tamu.edu
BIRDSHOT (Physics based structure models)	Cloud based data storage	SEMI-Automated Vacuum ARC MEL.... and laser DEO, metal alloy synthesis	IP/IPIIJ, ChemOS, ARESOS		DAYESIAKJ Optimization
Hammer	JHU HT-MAX	Screening tests	1D, Citrine		Design of Exp.
DARPA METALS	Army HTMDEC data.htmdec.org		Quester		Gradient Boasted Decision Tree, Sandia Beyond Fingerprinting (Boyce)
CALPHAD (phase stability)	Mater discovery		Enthought		IF A.C.
ML based oxidation models	extreme conditions		Amatreum		Data Quality and Availability
CHGNET Predictive Models	Materials Representation		Lack of Robust Generalized Software package		
PAL 2.0	Structural Representation, Classification of Infrastructure				
Standardized Featurization of Microstructure	Data mining of Literature can be fruitless				
Fundamental Properties do not have Physics-based Models (elasticity)					
Bilingual Mat Sci + AI people					

Synthesis

Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Army project: ICME for Army castings	IMQCAM portal	High through put electrodeposition	HT-READ Wagen wheel sample transfer	Universal form factors – lack of consensus	Army project: Machine learning for solid state joining
AI bench marks that do not properly test generalizability	NASA STRI	Combinatorial PVD	Lab scale synthesis of bulk material	Acceleration Consortium	Lurking parameters (unknowns)
Calculator – make it - characterization – digital work -what is wrong	digital twin for metal automated data ingress and workflow	Inconsistent ART access to tools	Automated bulk processing – secondary processing	Abo Matthews IR & AE Feedback in AM	
	Materials Data Facility	FormAlloy ADF			
	ARL HTMDEC Database (data.htmdec.org)	Georgia AIM (AI in Manufacturing)			
	In process monitoring				

Characterization

Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
HT-READ BSD indexing	Robotic high through put characterization	HT-READ automated XRD	CAMEO NIST-UMI ROBO MET ANDI		Multimodal fusion
Acceleration Consortium	lack of common database	High throughput tensile testing (Sandia beyond fingerprinting)	Euton corp ultrasonic fatigue testing,		Sandia Beyond Fingerprinting
	lack/dearth of automated properties/physical measurements	BIRDSHOT automated oxidation screening approach	multifidelity methods		DARPA METALS
Unconventional Surrogate Methods		JHV CAMEE Lab			DATA-to-information (knowledge-wisdom)
					Physics based interpretation of characterization data
					Multimodality (data fusion)

Scale-Up / Manufacturing					
Models	**Data & Information Handling**	**Autonomous Instrumentation**	**Software**	**Sample Handling / Handoff**	**Decision Tools**
generative design tools (eg. Fusion 360)	GRANTA	HAMMER autonomous deformation processing (Dan Miracle)	America makes CORE	Divergent 3D	Mat'l development – design integration
lack of models correlating subscale tests to full scale tests (micro to ASTM standards)	Psychological / cultural barriers to usage	SHU APL	IP and security constrains on data sharing	Machina labs	disconnect between materials properties and property requirements
		OSD TETRA			

Certification / Qualification

Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Unconventional surrogate methods		SpaceX relativity			integrating AI methods with traditional methods
DARWIN (Detor)		automated XCT			DARPA SURGE (Detor)
		JHU APL H7-fatique			
		lack of accelerated long term test methods (Creep, fatigue, and corrosion)			

Recycling / End-of-Use

Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
DOE makes this a priority for their exciting programs	Rubble to rockets				Automated scrap sorting
battery recycling NRC					Cost benefit analysis
					Holistic life cycle analysis tool
					battery recycling NRC
					DOE REMADE Institute activities (Example, J. Schoenung, AM Powder recycling work)

Discovery & Experimental Design

Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Autonomous measurement of high-temp mechanical properties is needed	Norel	HTmDEC funds	Materials Discovery Research Institute (NFP, Skokie)	Industry – Academia (substantial funding to bing in industry (matching))	Hypothesis-making (HTCS… Extrapolatory)
DEED, Cortarolo (Duke), ONR, High Entries Ceramics	Low CO2	HT-MAX program @John Hopkins	high through autonomous high temp oxidation experiments research	Workforce Challenges (2/3 accredited ceramic engineering programs at USA)	Automated TEA
General purpose MS; Materials project AFIOn	Cements	High throughput synthesis of novel ceramics does not exist			Wenhao Sun, UMICh, New Chemistry
What is special about structure of ceramics; we really learn properties on the scale up level	Rutgers spin				
Timescale from concept to powder synthesis needs to be ideally closer to hours than weeks	Data repository sharing [creation of stable data sets]				
	Rapid literature analysis (digitization, retrieval, search, LLM training)				

Synthesis

Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Inverse problems of processing from observational data	Negative results for methodologically correct experience	Accelerated synthesis for powders			Multiple framework for optimization
Across domain generalization for materials specific theory	Lab to lab matching for synthesis quantifiability	New chemistry for high throughput ceramic materials			Development probabilistic short-term rewards from long term objectives
Much less than metal		Prototype: - ??? -microfluidics -flm deposition -ombo			Optimization and experiment planning combining data models and crowd source human
CALPHAD		3D printing ceramics (???,???,???)			
Phase Field		Ken Verco lab			
		A-lab			
		SARA			

Characterization

Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Large volume of domain specific software	Sample provenance	automated certification/qual for ceramics are needed (NIST)		open samples	Fixed policy
	NIST Inorganic Phase Equilibrium Data Program	Underwriter Laboratories Materials Discovery Research Institute		Standard samples	Human heuristic
	Open Data (push / pull / trianlge value???)	NSF, Skokie		Compatibility	Connectiona cross the domain: What values does X-ray+Raman bring?
		Python APJ ??? ???			

Scale-Up / Manufacturing

Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
connection across the domains (what value does X-ray+ RAMAN brings)		need user facility like arrangement for small companies to scale novel ceramic materials	ASPEN+ etc (chemical engineering chemistry)		3d printing of array ceramics (ARL - Nick Ku)
practical samples compatibility		COORS TECH			how do we ... low cost, fast proxies and how do we choose them
NIST: Subnanoscale		TITLE III			Heuristics
NIST: Measurement of Point Defects Chemistry in Complex Oxides		Boron Carbide			BAM (Germany): LLM-based decision support for cement formulation
Mature data formats but...		CERION Nanomaterials Nanoceramics (at scale),			
		AM of ceramics vastly large, metals AM (needs investment + innovation)			

Certification / Qualification

Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Models of Hypersonics Testing (TAMU, NTS, Northrup Gruman, Lckheed)		development of low cost (fine) characteristics proxies with well-defined ...		Open samples	Underwriter laboratories solution
		Automated NDE of Armor Ceramics (ARL - Michael Golt)			NIST nanoscale
		Automated Certification / Qualification for Ceramics are needed (SAA or NIST)			NIST measurement of point defects
					Chem complex oxides
					NIST inorganic phase equilibration data program
					Underwriter laboratories materials discoveries research institute (NFP)

Recycling / End-of-Use

Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
			E-waste recycling, battery waste	Robotics	U. Mich Dearborn program ceramic recycling (used batteries)
				Recycled product for cement	Automatic technoeconomic evaluation to bring it to earlier phases of basic research
				recycled ceramics as aggregate material and structural concrete	LCA tools

Structural Soft Matter

Synthesis					
Models	**Data & Information Handling**	**Autnomous Instrumentation**	**Software**	**Sample Handling / Handoff**	**Decision Tools**
	CRIPT	GlycoMIP at VT		Beckman institute autonomous materials system group	UMass Lowell polymer processing line
	CHIMAD	POLYBOT at ANL		Midscale synthesis of materials (Kg-scale)	NIST X-ray data modeling
		NSF BioPACIFIC MIP at UCSB		microtiter plates	lack of interoperable databases, solution properties,
		Cloud lab at CMU			data output and analysis tool (VMD, LAMMPS, NAMD, GROMACS, MD analysis)
		Peter Beaucage's formulistics bot: The NIST Autonomous Formulation Laboratory—Accelerating Liquid Formulation and Reaction Landscape Exploration with AI and X-Ray/Neutron Scattering			polymer solution phase behavior prediction
					lack of trusted database

Characterization					
Models	**Data & Information Handling**	**Autnomous Instrumentation**	**Software**	**Sample Handling / Handoff**	**Decision Tools**
NIST X-ray data modeling	VMD	Peter Beaucage's formulistics bot: The NIST Autonomous Formulation Laboratory—Accelerating Liquid Formulation and Reaction Landscape Exploration with AI and X-Ray/Neutron Scattering	SOFT-AE NRT @ Penn	Dogbones	
Lack of interoperable databases	LAMMPS	Polybot (ANL)	COMPASS STC @ Michigan	Automated Testing: TA Instruments Instron Rheology @ NN???	
Solution properties	NAMD	BEAR (Bayesian experimental autonomous researcher) Keith Brown			
	GROMACS	NSF BioPACIFIC MIP (UCSB)			
	MDAnalysis	CFN / CMS @ NSLS II / BNL (X-ray characterization)			
	Polymer solution pahse behavior prediction (AFRL)				
	Lack of trusted database				

Scale-Up / Manufacturing

Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
SOFT-AE NRT @penn		BEAR (Bayesian experimental autonomous researcher) Keith Brown			
COMPASS STC@ Michigan		ARES OS 2.0 additive polymer printing			
automated testing (TA instrument – rheology, Instron)		standard modular work flows for processing history			
		Amount/time/necessity scale to quantify processing			
		lack of facilities			

Certification / Qualification

Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
	lack of .. properties coupled with in-line metrology , reference materials (models)	high throughput adhesive testing (Dupont)			
	lack of understanding of long term aging				
	Refernce Materials (Data & Models) are needed				

Recycling / End-of-Use

Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
life cycle analysis in the vein of MGI (data driven)	Materials architecture by adaptive processing			how to separate different chains in a mixture	
				how to control the chain size during degradation	

Discovery & Experimental Design					
Models	**Data & Information Handling**	**Autnomous Instrumentation**	**Software**	**Sample Handling / Handoff**	**Decision Tools**
Process modeling and FE models are typically at macro-scale and are... from the microscale			fixtures are not standardized or widely agreed upon, making automation difficult		

Synthesis

Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Integration of process modelling and abnormalities defers into multiscale models					
ASTM specimens are not easily automated (manual prep, tabbing, etc)					

Characterization					
Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
					experimental results are subject to interpretation (i.e. a macrolevel measurement is used to estimate micro level material

Scale-Up / Manufacturing					
Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
need for correlation between lab scale (flat coupons) and real 3D geometries *Composite materials are formed with final part not as bulk constituents					

Certification / Qualification					
Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools

Recycling / End-of-Use

Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
					what are the economics of recycling and how does performance compare to virgin materials

Functional Metals

Discovery & Experimental Design					
Models	**Data & Information Handling**	**Autnomous Instrumentation**	**Software**	**Sample Handling / Handoff**	**Decision Tools**
Generative AI models – PCGCM	Materials center model center	Digital twins of neutron beamlines	Grain growth	PRO CAST	
CDVAE	Materials data facility MDF	GAP: real time control of instruments, open system	Bulk residual stress	COMSOL multiphases	
Software thermo calc CALPHAD	Data and Info handling: Data analysis, data reporting	"National archive of materials data"	Computational fluid dynamics	3DX/3D systems	
Grain models	Discovery + Exp		Crystal plasticity	ASTM handbooks	
EMAG/additive tools	Data management: formatting, data collection		Phase transformation	CALPHAD	
COMSOL	Data management: develop new standards for data interconversion from various sources		Suite of codes for BAYESIAN optimization and neural nets for generic experimental workflows	Multiwork flow orchestrator for coordinating experiments across different facilities	
QUESTEC			Facility API for HPC (i.e. frontier supercomputer)	GAP: legal implication of mining for retrieval literature (Elsevier lawsuit)	
ML algorithms based on cause + effect relationships			GAP: develop physics ML models to make intelligent decisions with sparce data		
			GAP: software that works with heterogeneous data to inform decisions		

Synthesis					
Models	**Data & Information Handling**	**Autonomous Instrumentation**	**Software**	**Sample Handling / Handoff**	**Decision Tools**
Generative models for materials structure	Microsoft cloud resource	Reliability issues	GAPS: synthesis software for metals: MARMOT/BISON, Procast, Phasefield → missing property prediction	Mixing equipment especially for hazardous materials (e.g HF)	GAP: decision tools lack connection to critical materials and supply chain
Magnetic properties	Forum pass	Access to programming	GAP: large language models for translating spreadsheets, images, pdfs to interoperable data file.	Sample transfer robotics e.g. inter/out of very hot ovens (HSSE concerns)	Synthesis GAP: little real time adaption
Magnetic saturation prediction	MAI hub-AFRL	Autonomous flow reactors with multimodal characterization in situ	GAP: Interoperability of software		Inability to make real time decisions at relevant scales
Multitask models + prediction – JHU/APL/RAD		Autonomous chemistry lab with multimodal characterization tools	Synthesis GAP: Hardware/Software interfaces for real time control		
ALM software to model defects in ALM		U. Toronto; Combinatorial films high throughput			
		ORNL			
		Intersect initiative for workflows			
		Autonomous additive manufacturing for metals and composites			
		Synthesis: weighing instruments			
		Synthesis: flow testing equipment, gram + mggram scale			

Characterization					
Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
AT SCALE – autonomous → MBE→ DED→ Microscopy → Sputtering	GAPS: real time feedback, no standard knowledge extraction, no new standardization for interfaces, legacy systems: controls, interoperability	Autonomous 4D-STEM Matl's characterization	Digital twins of 4D-STEM		Optimization + robotic arm for high throughput characterization
EBSD	Autonomous instrumentation, vendor-supplied equipment: customizability, maintenance, troubleshooting → interruption of workflow (depends on vendor response)	Autonomous neutron beamlines	DARPA METALS AI driven feedback loop, in-line automated testing		
X-ray/Neutron diffraction		Characterization: thermal analysis, microscopy			
wavelength dispersing spectroscopy		GAP: novel characterization methods that leverage strengths of robotics/autonomy and maximize info			
energy dispersing spectroscopy					
SEM, TEM					
Calorimetry					
Optical characterization					
blue light dimensional					

Scale-Up / Manufacturing

Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Lack of workforce skills	Process parameter monitoring + trending	Gap: lack of midscale manufacturing, lack of producibility	GAP: Standardize messages for controlling instruments + resources from different vendors		
Lack of tools	IT Texas A@M				
	IT NASA Database on shape memory allows				

Certification / Qualification

Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Statistical models	Data handling	NASA			OUSD, JHU/APL, digital calibration → experimental + modeling combined, new efforts starting
	GAP: Consolidated standardized databases and/or ways to access/leverage heterogeneous data	CMU/JHU digital twins			No tools exist
		Hardware + software to enable characterization/ decision making at speed			
		ASIC?			
		FPGA?			

Recycling / End-of-Use					
Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Models to predict recycling/reuse pathways at beginning of materials lifecycle		Autonomous disassembly of end-of-life components → recycling prep			Frameworks to understand recyclability/sustainability of materials

Functional Ceramics

Discovery & Experimental Design					
Models	**Data & Information Handling**	**Autnomous Instrumentation**	**Software**	**Sample Handling / Handoff**	**Decision Tools**
Model emergent property capture	GAP: standardized networking policies for free flow of	A-LAB (Berkeley)	Materials project LBNL lead	Need to engage human/machine partnering community	Mat-discover, Mat-bench geometries
Functional ceramics discovery: multiscale modeling of carbon materials and find suitability of carbon material attributes for the application of batteries and carbon capture	Datatractor.org	Ceder group	CALPHAD	DATA curation: who pays, who maintains, who safeguard	BraggNN tools for AI in the loop feature detection and analysis of X-Ray data
New sorbents for lithium extraction	PARADIM (JHU/Cornell)	Solid state synthesis	Thermocalc + others	Funding/access	ANL
PNNL data and models solid phase processing SPPS; initiative	Project CHAMELEON	European material automation project: BIGMAP	NIST/MARDA working group	Interactions between databases? META data	Role of human
Google/ Deepmind	API data interoperability	Viper lab	Argonne Autonomous research labs AARL- many robotic instruments for materials and Bio		
Microsoft AZURE paid service		Auto PERO SOL	WEI (workflow execution infrastructure) for universal access and reusable flows		
		AMANDA – line1	Functional ceramics discovery: new membranes for brine purification		
		ION-SELF	Need to engage autonomy community		
		SynBio- MAP			
		AMDEE (JHU)			
		AI driven integrated and automated materials design in high throughput integrated OPA datahub and streaming science data			

Synthesis

Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Phase diagram network analysis	ESAMP	Autonomous solid dispensing Chemspeed	PNNL	PNNL ARES→ robotics labs	CAMD
Reaction network analysis	Published data with DOI (DATA.PARADIM.org; Portal.Data.Paradim.org)	Powder dose (Crystal)	Institute center for AI CTCI	AT-SCALE→ autonomous characterization	Functional ceramics synthesis
GAPs: Synthesizability; Transition to automation	Translatable workflows	SAMSUNG LAB: mixing powders, X-Ray characterization	piro.matr.io		Design of novel processes for lignin upgrading for novel catalysis materials and properties
	Thin film deposition data (2DCC.org; 2DCC MIP)	Sample handling	ARROWS		
		MDRI-UCRI	AFLOW++		
		Rapid microwave synthesis			
		Generalized automation → Vendors			

Characterization

Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Functional ceramics characterization	MDRI-UCRI	PNNL ATSCALE	Phase mapper xlal2do5	Thermofisher scientific laboratory automation (GC, sample array)	Lazer Shock impact lab (JHU)
predict thermal and oxidative stability of amines in CO_2 capture	McGill University Eric McCalla H-T electrochemistry cathode Li-ion battery	Workflow + integration → Operando synthesis + analysis → theory + simulation	AI crystallography	MTI desktop collaborate robot	Automated metadata
	Functional ceramics certification/qualification simulations of long term battery performance, especially impact of impurities in cathode and anode materials to better tailor product specification and qualification	Rapid screening TGA	Incremental XRD clustering; Fuzzy XRD clustering	Universal robots	Uncoupled processing
		Characterized defects disorder at scale/speed	EBSD – indexing PADNet-XRD	COBOT UR loe	Stream processed high throughput data reduction with visualization
		Advanced characterization XRD		Variable temp XRD	In site/In line analysis techniques for carbon nanotube synthesis
		Variable temperature XRD, Gas handling			

Scale-Up / Manufacturing

Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
(For Batteries) Byte Rat	Lack of data	SAMSUNG autonomous lab	Digital twin	Toyota Production System	Pilot Line, Bridge to Industry
BEEP		Clariant → High throughput experimentation → CLARITY → data to visualize	EU battery 2030+	Error correction, safety: Lazer, X-Ray, H_2S	Data structure in the way we can communicate in industry
		Functional ceramics scale-up paired with … on whether this material could be practically made and at the cost of materials	GAP: Seamless authorization and authentication		
		AI to cross-scales, from lab to pilot plant			
		SPEED			

Certification / Qualification

Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
	NASA STRI IMQCAM digital twin for cert/qual MAM Software/code/data → standardization, reusability, and documentation				

Recycling / End-of-Use					
Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
	LFP battery life prediction Degradation prediction				Recycle vs regenerate vs second use sorting by AI

Discovery & Experimental Design

Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Models of failed experiments – database of best and not so best practices	BioPacific MIP, LIMS/ELN, data information	Adaptive robotic work that adapts both function and data caption	Need to engage autonomy community	GAP: AI-ready data: definition development, deployment	ML informed modeling
AI→ ML trained models	Visualization technology	Acceleration consortium at U. Toronto		Non-aqueous synthesis and polymerization	LAM powered multimodal literature research tools digesting millions of documents to guide R&D literature study
Fit-for-purpose models and interoperability	Image segmentation and pattern recognition				
Data in the chemistry domain is not modular: thus, not friendly to AI	CITRINE/PARADIM, linked data knowledge, Graph GEMD				
We need to modularize					
Mission oriented research model					
Inconsistent capture of chemical reaction data; lack of standardization; poor reproducibility					

Synthesis					
Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Protein synthesis	MERCKPSW-THE small molecules, peptides, conjugates, internal funding	IBM Robo RXN	Digital Molecule Maker @ MMLI	GlycoMIP, glycoproteins	The cost of moving from human in the loop to fully automated workflows
Chemspeed	Contractual	Liquid handling partly handling synthesis platform	Proprietary instrument software, filetypes	GAP: solid sample handling similar gap with heterogeneous mixtures	
leaving Biofoundry	Designs automation experiments	Connected with NC/MS	lack of flexible API's	Need low cost/accessible integration automation that can pass samples between different solid/liquid dispensers, reactors, and other equipment	
BioPacific MIP	NCSA	Based on Chemspeed			
Modular small molecule synthesis with MIDA-TIDA boronates	Lack of a comprehensive data model to capture full capacity of materials structure + properties, the experimental preparation and METAdata.	iBioFab@uiul			
Retrosynthesis models – Bartosz Jrwbowski one of global pioneers	Poorly defined synthetic procedure in the most current literature	Standardization of workflow for synthesis			
IBM RXN Retrosynthesis and forward synthesis model framed on patent data (and enzyme in separate model)		Multiple instrument vendors			

Characterization					
Models	**Data & Information Handling**	**Autnomous Instrumentation**	**Software**	**Sample Handling / Handoff**	**Decision Tools**
One-shot LCMS/characterization	Data security/cyber security LAI	NIST autonomous SynBio	Difficult to interpret analytical data, e.g. HPLC, in automated fashion without human intervention	Telerobotic sample prep + analysis	Brookhaven + automated updating of SACS data on thin films
	Poor descriptors in terms of characterization data for soft materials	Polymers are inherently poorly defined	Spatial temporal high throughput characterization	Characterization on high throughput across scales of soft materials from hydrogels to glassy plastics	
	Limited amount of well-curated, well-defined data on soft materials	Lack of automated sample purification and preparation robotic tools			

Scale-Up / Manufacturing

Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
3D printers		Flow Chem coupled to AI@MIT Klaus Jensen et al	AI+ML collaboration between chemistry, physics, software engineers	Remote access + easily accessibility – APPs for users (K12, academia, industry, government)	Autonomous scale-up
Flow Chemistry		MERK Chemspeed based autonomous optimization platform ...funded			Telerobotic additive manufacturing
BioPACIFIC MIP		Supply chain stability			Morehouse
Access to scale up equipment to bridge from lab to industry		AI-guided optimization flow-based reaction could bridge the gap in scale to help materials discovery			
Automated modular small molecule synthesis-on scale – could be achieved with a national facility, could revolutionize materials discovery					

Certification / Qualification					
Models	**Data & Information Handling**	**Autnomous Instrumentation**	**Software**	**Sample Handling / Handoff**	**Decision Tools**
Coursera courses in part developed by leading companies in the field (Google, Amazon, IBM) or university professors: UDEMY, U-Tube	Certification programs outside academic degrees	AR-Headset based trainings, e.g. on infrastructure like chemspeed, automated sample prep, characterization devises for standard operation		Need to validate automation processes across large facilities. Need an ecosystem approach	Free certificate program at MMLI 'AI-empowered Chemistry: A Playbook", high throughput evaluation of defects
	Leverage training schools and community colleges for workforce development, student certification and badges, faculty certification for training other faculty				

Recycling / End-of-Use

Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Fine tuning of large AI foundation models framed to learn the representation of molecules such as IBN MoLFormer for toxicity prediction	Depolymerization databases		ALLCHEMY “waste to drugs” networks		MSU
	Platforms to orchestrate many AI models to be used in cooperation not in isolation and enable ease of use		Streamlined approach to collecting data for MGI (via journals and federal agencies)		Sustainable M^3 materials and manufacturing
	Lifecycle analysis for new and old polymer materials				

Functional Semiconductors

Discovery & Experimental Design

Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Need success story of data sharing for failed experiments	CITRON	LISA at Caltech/DOE funded	COMSOLE, CADENCE, Synopsys, etc starting to include ML/AI	Industry standard	LAM research, BAY ESIAN
Materials project	Materials data handling	NC State ALPHA Flow	LAM research	Missing in low/trl labs	Optimization process for experimental design
DFT	LAM research – materials properties tables in public domain use and for material selection	Hetero-nanostructures (photodetectors)	Software products to facilitate experimental design, eg. CYGNUS, proprietary	DOE, Power America Institute	DOE hydrogen EMN consortium, semiconductor
Force Field	No standardized data formats	Need development + accessibility to specialized user facility	ORNL INTERSECT, LLM for materials	Need for new precursors for discovery	
Schroedinger	Results of failed experiments are not available	GAPS: Thermodynamic and Kinetic Process data	Need cross training of domain scientists + software developers		
Google, etc.					
Klimeck/Tilmann @ Purdue					
Atomistic modeling (also running nanohub)					
NSF Fuse codesign model					

Synthesis					
Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Traditional customized synthesis model	NSF MIPs: 2DCC and PARADIM	Samsung advanced institute of technology	COMSOL	Robotic sample handling	PARADIM MIP single crystal-bulk crystal facility deployed ML feedback – decision making preceded automation
There is a huge untapped opportunity for an automated modular synthesis model	ANL-Globus	Foundry autonomous synthesis for nanoparticles + thin films	REAXFF		
Small molecule synthesis is so powerful, but in-situ is limited		Autonomous lab	ATHENA		
Need national facilities for molecular innovation			T-CARD		
Lack of physics-based models for synthesis, need translation of model from small scale to production			ORNL INTERSECT command + control		
			Abstraction layer		
			Need standardized software for lab scale database		

Characterization

Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
LBNL Davis Prendergast, X-Ray spectra stimulation	X-Ray Neutron Electron facilities ORNL/BNL	LAM research proprietary automated + semiautomated extraction from topographic structures	LAM research SIM-automated feature extraction	Industry standard	Computation and data driven discovery at BNC
InLINE	NIST Jarvis functionals DATA infrastructure	AT SCALE → edge computing	Need analysis functions embedded in software		Camera@LBNC
Molecular foundry LBL	Need standardized data formats for tools	Autosampling for TEM NSRCs	Need decision tools for example XRD, etc, that are as good as experts		
Multispectra data Georgia Tech SRC		ORNL INTERSECT"30 autonomous microscopy			

Scale-Up / Manufacturing

Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
GAPS: Grinding Chemical Mechanical Polish. CMP	Proprietary data infrastructure (semicon. MFG)	ORNL additive manufacturing	Vizglow, co-ventor, LAM research, internal products	Need funding for methodology change + automation	Various FDC tools for exception detection and management
DOE, DURAMAT, EMN consortium	Need ways to manage proprietary data	Automated W/interrupt driven (semicon MFG) decision making	Ability to focus long enough for infrastructure and implementation		Need incentives for workforce development to push data infrastructure
VIZglow/Co-ventor unit processes integration	Digital twin needs to be used to demonstrate value of having the systems in steps				
LAM research molecular dynamics					
Need comprehensive digital twins from materials to device					
Need interoperable digital twins that can be shared					
Consider federated learning data					
Provide model but not proprietary data					

Certification / Qualification

Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
		ORNL additive manufacturing “born qualified” parts	LAM research automated visual inspection, e.g. window defects	Need to integrate certification/ qualification with discovery/design	Go/no-Go on window LAM research
		No verification of reproducibility	From discovery of new materials to reliability		

Recycling / End-of-Use

Models	Data & Information Handling	Autnomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
	Need to consider sustainability within autonomous process	Need analysis (autonomous) of downstream chemicals/ products		Cadmium Telluride (CdTe) recycle +reuse	Critical materials innovation hub – DOE AMES
				Remote reuse sustainability CdTe	Europe's SSBD

Other

Discovery & Experimental Design

Models	Data & Information Handling	Autonomous Instrumentation	Software	Sample Handling / Handoff	Decision Tools
Need excited state data not ground state		AFRL ARES autonomous synthesis			
		PARADIM MIP automated MBE most automated in the world			
		Automated data handling and curation			
		Emerging Data interpretation and feedback			
		Need real-time in-situ metrology			
		Need 3D in-situ metrology in real time			

D. Summary Slides for Breakout Groups

The slides that were presented during the summary of the breakout sessions are illustrated in the images that follow. Please note that the inventories and gaps discussed below are derived from inputs collected at the workshop based on the knowledge and experiences of different participants. They are not comprehensive and do not reflect the opinion of all attendees. Also, the specific resources listed throughout the document were identified by the participants and should not be taken as an endorsement in any way or considered to be complete.

Structural Metals

Structural Metals

Brad Boyce (Sandia), Jae Hattrick-Simpers (U. Toronto), Dan Miracle (AFRL), Ibrahim Karaman (Texas A&M), Andrew Detor (DARPA), Robert Hart (US Army DEVCOM Ground Vehicle Systems), Harry Partridge (NASA), Eddie Gienger (JHU Applied Physics Lab)

Summary

- **Bilingual Scientists/Engineers** A significant impediment is that there are few experts fluent in both Mat. Sci. and Data Sci.
- **The Autonomy Spectrum** A few niche examples exist of fully autonomous workflows, but many have "autonomy potential"
- **Converting Data-to-Information** To make informed decisions we need data-> information -> knowledge -> wisdom.

Highlights in current landscape

- **Major Programs Underway** HT-READ, BIRDSHOT, Georgia AIM, ARL HTMDEC, JHU CAMEE lab , HAMMER, Acceleration Consortium ($500M), Sandia BeyondFingerprinting, BIGMAP, DARPA METALS program,
- **Enabling software**: ARES 2.0, ROOST/CHGNET, PAL2.0, Materials Data Facility, ChemOS, FINALES
- **High-throughput microstructure:** Some capabilities like XRD and SEM have been automated; others like TEM are elusive; Many require significant sample prep (EBSD). Turning microstructure to property predictions is still often challenging -> Decision tools limited.
- **A few commercial enterprises on software**: Citrine, Enthought, Questek, FormAlloy,

Gaps

- **Common Standards**
  - Microstructural feature extraction is still artisan and user based
  - Standardized APIs for instrument integration
  - Universal sample form factors to facilitate interoperability across instruments
- **Synthesis, In-process diagnostics, tightly-coupled feedback loops, & surrogate diagnostics**
  - For structural metals, bulk high-throughput like robotic button arc melting are not yet present.
  - Both primary processing and secondary processing lacks automation
  - Rapid/in-process screening diagnostics are limited
- **The Qualification & Lifecycle Gaps**
  - Limited efforts in qualification; facing a psychological resistance to "black box" qualification.
  - Even fewer efforts in full life-cycle optimization & circular analysis. Need business cases….
  - Long-term tests like creep, fatigue, & corrosion are still in their infancy for high-throughput data
    - Clear case studies in corrosion but community hesitance in acceptance
- **Lurking parameters & unknown unknowns**
  - Workflows require omniscient pre-determination of salient characterization methods and adaptability for new unknown-unknowns

Structural Ceramics

Executive Summary of the Structural Ceramics Discussion

- **A key challenge that is ripe for AMII is to move beyond existing trial -and-error heuristics and have systematic models of synthesis, processing, and scale-up**
- **Inventory:**
  - *Structural Ceramics encompasses a diverse range of materials range from high-tech coatings for specialized applications to bulk commodity products such as cement, and an equally wide range of chemistries and processing conditions.*
  - Automation and high-throughput synthesis and characterization capabilities are currently very limited; typical processes and length-scales are slow and not necessarily miniaturizable
  - Additive manufacturing (AM) of structural ceramics is a growing field, but lags AM of metals/polymers both in technical maturity and predictive modeling
- **Gaps:**
  - *Both High-quality/quantity experimental data and light models (based on neural operators and PINNs extensions of the phase-field) are needed!*
  - Data repositories for experimental data are needed—integration with automated labs would improve data quality, capture negative results, and improve traceability/reproducibility.
  - Development of appropriate software abstractions and standardization are needed to move beyond the current state of non-interoperable home-built solutions and vendor-specific APIs to enable data sharing.
  - Need: Development and scale-up production efforts of new powders, binders, and formulations for AM
  - Need: Development and certification/qualification of fast, low-cost proxy measurements to replace or better guide existing characterizations methods in a more intelligent way.
  - The creation of easy-to-use computational models for lifecycle analysis, technoeconomic evaluation, and environmental impact would allow these constraints to be incorporated earlier into the materials development lifecycle.
  - Use of recycled ceramics as aggregate materials in structural concrete is an important and promising research direction

Structural Soft Matter

Executive Summary of the Structural Soft Matter Discussion

- **A key challenge that is ripe for AMII is the design of new structural materials with combinations of properties that are traditionally hard to achieve (e.g. stiff but sticky)**
- **Inventory:**
  - There are likely many efforts in industry, but these are opaque to the community
  - Most academic/national lab efforts are focused on the discovery/design phase
  - Existing autonomous systems for synthesis and characterization are largely bespoke solutions rather than generalizable or modular ones
  - Additive manufacturing has been a key technology for materials exploration
- **Gaps:**
  - *A fundamental problem is that properties depend on structure at all scales and this hierarchical depends sensitively on processing. We do not possess a way to represent this hierarchical structure compactly*
  - A crucial need is more and better data, which requires good standards and consistent methods
  - While dogbones and microtiter plates are useful, we have yet to find the 96 -well plate for soft matter samples
  - Certification/qualification has been largely neglected but could be addressed in part using facile surrogate measurements
  - We lack the basic science to understand and predict recyclability

Functional Metals - Current Capabilities & Gaps

1. Discovery & Experimental Design

- **Wide range of models (physics-based, ML)**
- **Data handling tools available**
- **Automation in modern instruments**
- **Predictive software tools exist**
- **Missing specific models (e.g., ductility)**
- **Lack of interoperability and standardization in data handling**
- **Full autonomy and real-time control in instrumentation**
- **Multi-workflow orchestration and intelligent decision-making from sparse data**
- **Automated sample handling strategies needed**

2. Synthesis

- **Generative models and predictive tools for materials**
- **Cloud resources and data hubs**
- **Automated synthesis tools**
- **Reliability and access to programming**
- **Synthesis prediction tools and software interoperability**

3. Characterization

- **Various automated and AI-driven characterization methods**
- **Standardized interfaces and real-time feedback**
- **Leveraging robotics for novel methods**

4. Scale-up/Manufacturing

- **Monitoring and trending databases**
- **Workforce skills and mid-scale manufacturing tools**
- **Standardized control messages for instruments**

5. Certification/Qualification

- **Statistical models and DTs for decision-making**
- **Standardized databases and real-time decision tools**

6. Recycling/End-of-Use

- **Models for recycling pathways**
- **Autonomous disassembly**
- **Frameworks for recyclability and sustainability**

Additional Notes

- Capture input from tool makers; define specific problems
- Collaboration barriers due to IP issues and export controls
- Slow CRADAs and legal agreements
- Accelerate workflows to avoid “valley of death” in certification
- Standardize data schemas (c.f. ASTM)
- Develop dynamic knowledge bases; predictive performance tools
- Focus on usability of data for synthesis and DTs
- Promote national databases; federated data sharing for proprietary data
- Address gaps in real-time adaptation and control systems for synthesis

Executive Summary of the Functional Ceramics Discussion

Functional Ceramics require unique synthesis and characterization capabilities (high temperature, ball milling, sintering, pressing etc.) , making this class of materials difficult for fully autonomous labs.

Identify the current capabilities

- Autonomous lab – from liquid to solid, from synthesis to characterization. Existing leaders in this area - divided in Industry, Academic and Government
- Discovery labs: Industry – Google DeepMind, Microsoft Azure, Samsung ALab, Toyota Research; Academic – Berkley A Lab (Ceder Group), AMDEE John-Hopkins (Elbert Group), Gov – PNNL (SPPSi), Berkeley Lab (Materials Project, A Lab), Argonne (Polybot Echembot etc.)
- Database: Materials Project (DOE), ICSD, NIST (Phase Diagram, Thermocalc, Calphad), Citrine (data informatics) Open MSI Stream (NSF)
- Instrumentations – equipment maker : MTI, Bruker, ThermoFisher Scientific,

•Identify and articulate gaps:

- Design of experiment becomes more critical (what can humans do but robots cannot)
- We need a dedicated robotic design for materials scientist (particularly for functional ceramics)
- The cross disciplinary efforts among computer scientists, materials expert, robotics experts need incentives. Students from the different disciplines see vast difference in productivity.
- Private – public partnership is lacking as the industry has a leading edge on AI/ML

Functional Ceramics - B

Simon Billinge (Columbia University), Ram Seshadri (UCSB), Eric Wang (Samsung), Asra Hassan (UL Research Institutes), Tulsi Patel (ExxonMobil Low Carbon Solutions), David Darwin (NSF TIP), Breakout Lead: Shijing Sun (University of Washington)

Summary

- **Delayed functionality discovery**: The key functionalities of newly discovered materials are often realized years or decades after their initial synthesis in the lab.
- **Scientific alignment**: autonomous experimentation efforts developing infrastructure and tools (“hammers”) also need to pay attention identifying the type of problems (“nails”) that are suitable to be addressed by high-throughput/AI methods.
- **Automated vs. Autonomous Experiments** : While leaders demonstrate success with automated experiments, gaining trust for fully autonomous experiments from domain experts remains a challenge

Highlights in current landscape

- **Central Characterization Facilities** : Increasing number of beamlines with robotic sample handling and big data analytics capabilities, such as synchrotron PXRD and GIWAXS.
- **Community Software** : Materials science community recognizes the challenge of orchestrating experiment steps and scheduling, with efforts in open-source software infrastructure like the Bluesky Data Collection Framework.
- **Industry R&D Labs** : Autonomous materials discovery, including processes like solid handling and high-temperature sintering for ceramics synthesis, is not only being realized in academic groups but also industry R&D labs, e.g., Samsung Advanced Institute.
- **Other notable inventory**: Materials Project, High-throughput electrochemistry suite (Eric McCalla), MDRI - ULRI.

Gaps

- **Instrumentation**:
  - Many synthesis and characterization equipment lack APIs or the ability to communicate with other equipment.
  - There are also deficiencies in setups for scaling up, manufacturing, and recycling beyond materials discovery.
- **Data Generation**:
  - Missing automatic capture and structuring of data often leads to tedious manual data organization.
  - Following FAIR principles and data standardization across instruments is critical for cross-lab validation.
  - Code standardization and documentation are necessary to lower the barrier of entry for new researchers.
- **Human-in-the-Loop**:
  - Workforce development should focus on training robots to assist students rather than the reverse.
  - In functional ceramics, the method of making often differs from the method of measurement, requiring different platforms (e.g. thin-film processing vs powder synthesis) for functionality tests. Domain experts needed to ensure the quality and relevance (avoiding “garbage in, garbage out”).

Functional Soft Matter

Executive Summary of Functional Soft Matter Discussion

- A key challenge for AMII is to de-risk the process of soft matter design, engineering, and translation by enhancing reaction time, trial and error, transferability using a mission (fit for purpose) driven model.
  - **Inventory**
    - Materials Innovation Platforms along with Industry platforms have centralized the specific soft matter workflows, but strategic investments in infrastructure, particular to address addressable bottlenecks in synthesis, are needed to make these platforms more broadly available.
    - Many networks exist for functional soft matter but are still siloed.
    - Aqueous based workflows have been streamlined but are not autonomous for remote users
  - **Gaps**
    - Despite disruptive recent advances in the underlying science and technology, very few researchers have unfettered access to infrastructure that can enable automated FSM synthesis, which in turn is critical for accessing the substantial power of closed-loop/autonomous experimentation.
    - There is a critical need for a well defined and organized materials database – to facilitate new designs and develops in functional soft matters
    - A crucial gap is bridging nomenclature to enhance cross-talk across disciplines
    - There is a major untapped opportunity to advance a more mission-oriented research model with industry, academic, and government partnerships
    - Enhancements to experimental workflows infrastructure to support non-aqueous based projects
    - Characterization limitations in the workflow process

Functional Semiconductors

Executive Summary of the Functional Semiconductor Discussion

Discovery & Experimental Design

- **Inventory:**
  - Several physics-based models/software available for discovery that incorporate ML (e.g. Google's Schrodinger, atomistic modeling @ Nanohub, Materials Project)
  - Electronic design software (e.g. Cadence, Synopsis) starting to include ML/AI
  - Prior MGI databases can be used as rational inputs (e.g. Materials Project, Citrine)
  - Industry software products developed (e.g. LAM Research Cignus) but most are proprietary
  - DOE-funded efforts at CalTech (LISA), ORNL (INTERSECT) and Hydrogen EMN Consortium
- **Gaps:**
  - Discovery/design efforts can rapidly identify new materials with promising properties but bottleneck is ability to verify experimentally
  - Availability of data and metadata from experiments, including failed experiments.

Executive Summary of the Functional Semiconductor Discussion

Synthesis

- **AMII is already utilized to explore solution-based synthesis of new semiconductor materials**
- **Complexity of traditional semiconductor device processing creates hurdles to adoption, although portions of the automation process (sample handling and transfer) are already in place.**
- **Inventory:**
  - Empirical models for synthesis exist but very tool/process specific (e.g. Via fill for electrochemical deposition of copper)
  - Nascent efforts to develop synthesis -focused databases (e.g. NSF MIPs, DOE ANL Globus)
  - A few efforts on autonomous synthesis with published results (e.g. ARES at AFRL, Autonomous discovery, synthesis & characterization of nanoparticles at LBNL) but a number of labs working on this (e.g. AT-SCALE at PNNL, Samsung Institute of Technology (SAIT), ISI at NC State (quantum dots) ONR Programs on Organic Electronics for nanomaterials and thin films)
  - Automated sample handling (e.g. robotic arms) and full-wafer characterization (cassette -to-cassette) widely used in semiconductor manufacturing but not yet incorporated with AI -based decision making (humans still make the decisions)
- **Gaps:**
  - Need physics-based models for synthesis that are multi -scale and can be translated from lab to production scale
  - Need advances in real time metrology and accelerated post -growth characterization to enable autonomous operation
  - Need standardized software for lab scale databases that can interface with synthesis and characterization equipment

Executive Summary of the Functional Semiconductor Discussion

Characterization

- **Inventory:**
  - Models/software for analysis of characterization data (e.g. X-ray spectra simulation @ LBNL, multispectral data analysis @ Georgia Tech (SRC), image analysis (Lam Research SIM, ImageJ)
  - Efforts to handle large data sets from characterization ongoing at national labs (e.g. X-ray/Neutron facilities at LBNL/ANL/ORNL/BNL), NIST JARVIS, CHIPs Metrology focus
  - Several efforts at autonomous characterization & analysis (e.g. AT-SCALE at PNNL (edge computing devices for AI on edge), Autosampling for TEMs at DOE NSRCs, autonomous microscopy at ORNL INTERSECT, Lam Research proprietary efforts)
  - Automated characterization and analysis industry standard but missing in low -TRL labs
- **Gaps:**
  - Spatiotemporal high-throughput characterization is a gap
  - Need advances in real time metrology and accelerated post -growth characterization/analysis to enable autonomous operation
  - Need lab scale databases that interface with characterization tools

Executive Summary of the Functional Semiconductor Discussion

Scale-Up/Manufacturing

- **Inventory:**
  - A small number of efforts identified such as effort at MIT (Klavs Jensen) to couple FlowChem to AI; 3D printing effort at BioPACIFIC MIP and additive manufacturing-related efforts

- **Gaps:**
  - There is a gap in the scale-up and manufacturing of new materials and devices that could offer benefits in performance and cost..
  - There may be efforts internally in industry that have not been identified.

Executive Summary of the Functional Semiconductor Discussion

Certification/Qualification

- **Inventory:**
  - One or two certification programs identified related to data science/AI
- **Gaps:**
  - This is a topic that has received little attention thus far in academia/government labs. There is a significant need for workforce development which may be addressed by CHIPS Act such as development of certificates and badges for students at community college to B.S. level.

Executive Summary of the Functional Semiconductor Discussion

Recycling/End of Use

- **Inventory:**
  - Several efforts in photovoltaic field focused on reclamation/end of use of CdTe (e.g. First Solar, Remade (ISII?)
  - Critical Minerals Innovation Hub funded by DOE
- **Gaps:**
  - This is a topic that has received little attention thus far in academia/government labs. Industry likely has internal efforts focused on lifecycle analysis, etc.

E. Registration Questions with Optional Input Opportunities

Last Name

First Name

Email

Are You a Federal Employee

Please consider sharing your pronouns. Pronouns are the part of speech used to refer to someone in the third person. We want to know how to respectfully refer to you. For example, She/Her/Hers, He/Him/His, Ze/Hir/Hirs, They/Them/Them, etc.

Please let us know if you would like your pronouns included on your name tag.

Email Address

Telephone Number

Institution / Organization

Division / Departmental Affiliation

Please describe any accommodations that will facilitate your full participation in this event.

Name of Project / Platform / Center / etc.

Website URL (if available)

Type of Capability(ies) – Experimental, Computational, Data Infrastructure, etc

Level of automation or autonomy (integration of AI/ML to help guide or direct experiments) (N/A if none)

Materials class the capability addresses (more than one possible) - Selected Choice

Additional information that you would like to contribute.

Let us know if you have initial thoughts on what specific capabilities are missing from the Autonomous Materials Innovation Infrastructure (AMII) to truly accelerate the materials development continuum (design through manufacture.)

Beyond funding limitations, what are the barriers to large-scale adoption of autonomous and automated laboratories

We are looking to define numerous, specific, measurable targets that are both challenging and achievable in the next 2-5 years. We plan to solicit additional input to these specific targets during this June workshop and at the following MGI PI meeting (July 30-31, 2024). Here, you may contribute ideas of specific, measurable targets to address a challenge in areas such as, but not limited to, materials for Water Security, Human Health and Welfare, Energy, Economic Competitiveness, or National Security.

F. Analysis of Registration Data

FROM REGISTRATION DATA: METALS AND METALLIC NANOSTRUCTURES

Common Themes

There are several common themes and trends in autonomous infrastructure in the field of metals and metallic nanostructures:

AI/ML and Autonomous Decision Making

There is a pervasive use of artificial intelligence (AI) and machine learning (ML) technologies across various stages of materials research and development. AI/ML is employed for guiding experiments, optimizing processes, predicting material properties, and managing large datasets.

Many projects leverage AI/ML for guiding and optimizing experiments, simulations, and material discoveries.

Examples: Accelerated Materials Design and Discovery (AMDD), Army Research Laboratory's BIRDSHOT framework, CORPORATE RESEARCH, DARPA Project, High-Throughput Materials Discovery for Extreme Conditions (HTMDEC).

Autonomous and Self-Driving Laboratories: Full and Partial Automation

Several facilities are moving towards autonomous operation, where processes such as synthesis, characterization, and data analysis are increasingly automated. This trend supports rapid experimentation and scalability.

Projects range from fully autonomous laboratories to those with partial or supervised autonomy.

Examples: $180M Integrative Sciences Building at NC State University (supervised autonomy), Interconnected Science Ecosystem (INTERSECT) (full integration of AI/ML workflows), Adaptive Tunability for Synthesis and Control via Autonomous Learning on Edge (AT SCALE) (full autonomy).

High Throughput and Multimodal Approaches

The emphasis on high-throughput methodologies is clear, allowing for the rapid screening of materials under various conditions. This approach is often complemented by multimodal experimental workflows that integrate diverse data streams.

There's a significant emphasis on autonomous and high-throughput experimental setups to accelerate material discovery and optimization.

Examples: AT SCALE, Army Research Laboratory (ARM), Beyond Fingerprinting Grand Challenge LDRD, NC State Self-Driving Fluidic Labs.

Data Infrastructure and Management

Robust data infrastructure and management systems are being developed to handle the large volumes of data generated by high-throughput experiments and simulations.

Examples: DOE Energy Materials Network, Materials Data Facility, OpenMSIStream, PARADIM, HT-MAX, VariMat.

Integration of Experimental, Computational, and Data Capabilities

Many initiatives and projects emphasize the seamless integration of experimental setups with computational models and robust data infrastructure. This integration allows for high-throughput experimentation and real-time data analysis.

Many initiatives integrate experimental, computational, and data infrastructure to create comprehensive platforms for material science research.

Examples: Acceleration Consortium, INTERSECT, IMQCAM.

Collaborative and Open Infrastructures

Many projects aim to develop open architectures and collaborative ecosystems that facilitate data sharing, interoperability of tools, and integration of AI/ML across different research domains.

Funding and Strategic Initiatives

Significant funding and strategic initiatives are driving the development of these autonomous infrastructures, indicating a strong commitment to advancing materials science through innovative technological solutions.

Estimate of Autonomous Infrastructure in Metals and Metallic Nanostructures

Estimating the exact extent of autonomous infrastructure in place is challenging without specific metrics, but the prevalence of these themes suggests a substantial integration of autonomous capabilities across the field of metals and metallic nanostructures research.

Based on the provided data, a substantial portion of the infrastructure in the field of metals and metallic nanostructures is moving towards autonomous systems. This includes:

High Automation/Autonomy: Projects like AT SCALE, Army Research Laboratory's ARM, and BIRDSHOT framework, which integrate AI/ML deeply into experimental workflows, achieve high levels of automation.

Supervised and Partial Autonomy: Facilities like NC State's Integrative Sciences Building and some initiatives within the Lab of the Future exhibit supervised autonomy.

Early Stages/Evolving: Some projects, such as Deposition and Semiverse Solutions Product Groups, are in the early stages of integrating automation and AI/ML.

Conclusion

The field of metals and metallic nanostructures exhibits a strong trend towards integrating AI/ML and autonomous systems, particularly in high-throughput experimental setups and data management. This trend indicates a robust movement towards fully autonomous research environments, although the degree of automation varies across different projects and initiatives.

RAW DATA

Name of Project / Platform / Center / etc.	Website URL (if available)	Type of Capability(ies) – Experimental, Computational, Data Infrastructure, etc	Level of automation or autonomy (integration of AI/ML to help guide or direct experiments) (N/A if none)
Office of Naval Research		Experimental, Computational, Data Infrastructure, funding	High
Pacific Northwest National Laboratory	https://www.pnnl.gov/projects/at-scale ; https://www.pnnl.gov/high-throughput-center		
$180M Integrative Sciences Building at NC State University (under construction)	https://provost.ncsu.edu/university-interdisciplinary-programs/isb/	One floor of Automated/Autonomous Chemistry Labs with in-house Computational infrastructure	Supervised autonomy and full automation
Accelerated Materials Design and Discovery (AMDD)	https://github.com/TRI-AMDD	Experimental, computational, data infrastructure	Integration of AI/ML to help guide or direct experiments and simulations
Acceleration Consortium	https://acceleration.utoronto.ca/	All of the above	Self-Driving Lab User Facility
Adaptive Tunability for Synthesis and Control via Autonomous Learning on Edge (AT SCALE)	https://www.pnnl.gov/projects/at-scale/about#:~:text=Adaptive%20Tunability%20for%20Synthesis%20and%20Control	Experimental, Data, Computational, AI/ML	full autonomy, with AI/ML enabling real-time decisions

	%20via%20Autonomous,materials%20synthesis%20by%20developing%20closed-loop%20autonomous%20precision%20synthesis.		
AI-enabled materials discovery	https://www.jhuapl.edu/news/news-releases/230503-ai-discovers-novel-superconductor	Experimental (synthesis, characterization), Computational (structure prediction, AI models, frameworks for discovery)	AI-enabled framework with SME in the loop, Bayesian optimization enabled high throughput testing
ARES OS 2.0	https://github.com/AFRL-ARES/ARES_OS	Software for autonomous experimentation	Full
Army Research Laboratory - High Throughput Materials Discovery for Extreme Environments Center (HTMDEC) at Texas A&M University, the name of the Center is BIRDSHOT (Batch-wise Improvement in Reduced Materials Design Space using a Holistic Optimization Technique). BIRDSHOT is also used for ARPA-E ULTIMATE Program and 2 NSF DMREF Programs. Experimental part of BIRDSHOT Center is called ARM (Autonomous Robotics Metallurgist) where we can synthesize, process, characterize, and test materials in a high throughput fashion.		We have several computational tools applied to metallic materials (computational materials science, thermodynamics, and kinetics models, statistical frameworks such as Batch Bayesian Optimization to design alloys to fabricate and test) and experimental capabilities to design, fabricate, process, characterize, and test metallic alloys in a high throughput fashion. We have designed, fabricated, processed, and tested more than 400 new metallic alloys in bulk dimensions in the last 3 years in various programs mentioned above.	In all our materials design, fabrication, and testing efforts we integrate AI/ML methods to direct experiments using the BIRDSHOT framework in the programs mentioned above.
Beyond Fingerprinting Grand Challenge LDRD		Multimodal high-throughput experimental workflows; Data	quantified automation-based speedups of 10-100X across 10's of

		management system; ML algorithms for multi-objective process optimization	synthesis & characterization tools
Center for Advanced Manufacturing Innovation (CAMINO)	https://www.youtube.com/watch?v=WLXyXJ2N8Zw	experimental	under development
Lockheed Martin CORPORATE RESEARCH		Experimental / Computational / Data	AI/ML to guide materials discovery and Generative/Reinforcement for Optimization
DARPA Project: RIDE, METALS, and SURGE	https://www.darpa.mil/staff/dr-andrew-detor	Materials-integrated design optimization, accelerated experimental material property testing, process data driven part qualification	Varies by program and performer.
Deposition and Semiverse Solutions Product Groups	https://www.lamresearch.com/semiverse-solutions/ https://www.lamresearch.com/products/our-processes/deposition/	Experimental and computational and data infrastructure	Early stages
DOE Energy Materials Network	https://www.energy.gov/eere/energy-materials-network/energy-materials-network	All of the above	Misc
DSEMD HTMDEC Data Platform	data.htmdec.org	Data Infrastructure portal with linked data framework and automated workflow running	linked automation
High-Throughput Materials Discovery for Extreme Conditions (HTMDEC)	https://arl.devcom.army.mil/htmdec/	High-Throughput Processes, Methodologies, and Data Management	Integration of AI/ML, Bayesian Optimization, Data Streaming/Analysis in the Cloud
https://www.pnnl.gov/projects/nets	https://www.pnnl.gov/projects/nets	Flow and Field Assisted Nucleation of Critical Materials	
ICME for Army Castings		Experimental, Computational, Data Infrastructure	Using AI design tools to improve gating designs in castings
IMQCAM (NASA STRI)	data.imqcam.org	Data infrastructure platform for metal additive manufacturing Digital Twin	Automated data ingress and workflow running

Interconnected Science Ecosystem (INTERSECT)	https://www.ornl.gov/intersect	Autonomous Chemistry Laboratory, Autonomous Chemical Flow Reactors, Command and Control Open Infrastructure, Data Abstraction Layer,	Development and Integration of AI/ML into an open architecture to interconnect autonomous lab capabilities across science domains
Interconnected Science Ecosystem (INTERSECT)	https://www.ornl.gov/intersect	Experimental + Computational + Data Infrastructure	Fully integrated AI/ML workflows across multiple materials theory, synthesis, and characterization activities
Lab of the Future		Data management, AI, Robotics, Materials Synthesis, Flow Testing	Partial
Materials Characterization and Processing Center	https://engineering.jhu.edu/MCP/	Integration of data infrastructure, computing, high throughput, and experimental platforms	AI/ML, ML on edge, automation, deep learning, FAIR data
Materials Data Facility	https://materialsdatafacility.org	Data infrastructure	
MURI: From Percolation to Passivation (P2P): Multiscale Prediction and Interrogation of Surface and Oxidation Phenomena in Multi-Principal Element Alloys (MPEAs)	https://engineering.jhu.edu/dcg/research/p2p-muri/	high throughput/combinatorial synthesis, theory, data, AI/ML, closed-loop experimentation	automation, AI/ML, autonomous characterization
Nano4EARTH	https://www.nano.gov/nano4EARTH	National Nanotechnology Challenge	
NC State Self-Driving Fluidic Labs (Artificial Chemist, AlphaFlow, SmartDope, and Fast-Cat)	https://www.abolhasanilab.com/	Both Experimental and Computational	Supervised autonomy
OpenMSIStream, PARADIM, HT-MAX, VariMat		Data Infrastructure, data streaming, stream processing, decision orchestration	integration of data collection, ML decision making, ML decision deployment, instrument control
The Materials Discovery Research Institute	www.ul.org	Data Infrastructure, Theoretical and Computational, Automated Synthesis	Building Capabilities

		Capabilities, Digital-First Laboratories	

FROM REGISTRATION DATA: CERAMICS

Common Themes in the Ceramics Data

1. **Integration of** AI/ML:
    - Several projects involve the use of AI/ML for materials discovery, synthesis optimization, and data analysis. Examples include the High-Throughput Materials Discovery for Extreme Conditions (HTMDEC), Data-Driven Synthesis Science, and the Samsung ASTRAL project.
2. **Autonomous Experimentation and Characterization**:
    - Autonomous experimentation is a key focus area. Projects like ARES OS 2.0, HTMDEC, and the Materials Characterization and Processing Center highlight efforts in this direction.
3. **High-Throughput Processes**:
    - High-throughput experimentation and combinatorial synthesis are common themes, particularly in projects like HTMDEC and MURI: From Percolation to Passivation.
4. **Data Infrastructure and Management**:
    - Robust data infrastructure is essential for many projects, facilitating data collection, streaming, analysis, and decision-making. Examples include the DSEMD HTMDEC Data Platform and the Materials Data Facility.
5. **Collaborative and Multi-disciplinary Approaches**:
    - Collaborative efforts across different scientific disciplines and institutions are prevalent. Projects like Nano4EARTH and OpenMSIStream involve multiple stakeholders and scientific domains.

Estimation of Autonomous Infrastructure in Ceramics

Based on the provided data, here is an estimate of the level of autonomous infrastructure in the ceramics field:

1. **Fully Autonomous**:
    - ARES OS 2.0: Full autonomy in software for autonomous experimentation.
2. **High Integration of** AI/ML:
    - High-Throughput Materials Discovery for Extreme Conditions (HTMDEC): Integration of AI/ML, Bayesian Optimization, Data Streaming/Analysis in the Cloud.
    - AI-enabled materials discovery: AI-enabled framework with SME in the loop, Bayesian optimization enabled high-throughput testing.
    - Samsung ASTRAL project: Automated powder synthesis with AI-assisted computational materials design.
    - Argonne Collaborative Center for Energy Storage Science: AI/ML for EELS, XAS data.
3. **Moderate to Strong** AI/ML **Integration**:
    - NIST Materials Genome Program: Mixed integration of AI/ML for guiding materials discovery and optimization.
    - Designing Materials to Revolutionize and Engineer our Future: Less than 10% AI/ML integration at this stage.
    - Materials Characterization and Processing Center: Integration of AI/ML, automation, deep learning, FAIR data.
4. **Mixed or Emerging Integration**:

  - Deposition and Semiverse Solutions Product Groups: Early stages of integrating experimental, computational, and data infrastructure with AI/ML.
  - Lab of the Future: Partial integration of AI, robotics, materials synthesis, and flow testing.
  - CORPORATE RESEARCH: Partial integration of AI/ML for guiding materials discovery and optimization.
5. **Minimal or Developing**:
  - Alabama Materials Institute: N/A (experimental materials characterization without specified AI/ML integration).
  - Projects with unspecified levels of AI/ML integration or still under development, such as the Materials Discovery Research Institute and MURI: From Percolation to Passivation.

Conclusion

The ceramics field exhibits a substantial presence of autonomous infrastructure and integration of AI/ML, particularly in high-throughput experimentation and data-driven materials discovery. While some projects are fully autonomous, many others are in various stages of adopting AI/ML to enhance their experimental and computational capabilities. The overall trend indicates increasing use of automation and AI/ML to accelerate the discovery and development of new ceramic materials.

RAW DATA

Name of Project / Platform / Center / etc.	Website URL (if available)	Type of Capability(ies) – Experimental, Computational, Data Infrastructure, etc	Level of automation or autonomy (integration of AI/ML to help guide or direct experiments) (N/A if none)
		Experimental, Computational, Data Infrastructure, funding	High
ARES OS 2.0	https://github.com/AFRL-ARES/ARES_OS	Software for autonomous experimentation	Full
Nano4EARTH	https://www.nano.gov/nano4EARTH	National Nanotechnology Challenge	
Alabama Materials Institute	https://ami.ua.edu/	Experimental Materials Characterization	N/A
High-Throughput Materials Discovery for Extreme Conditions (HTMDEC)	https://arl.devcom.army.mil/htmdec/	High-Throughput Processes, Methodologies, and Data Management	Integration of AI/ML, Bayesian Optimization, Data Streaming/Analysis in the Cloud

DSEMD HTMDEC Data Platform	data.htmdec.org	Data Infrastructure portal with linked data framework and automated workflow running	linked automatiion
OpenMSIStream, PARADIM, HT-MAX, VariMat		Data Infrastructure, data streaming, stream processing, decision orchestration	integration of data collection, ML decision making, ML decision deployment, instrument control
Materials Data Facility	https://materialsdatafacility.org	Data infrastructure	
Data-Driven Synthesis Science (Gerd Ceder, LBL)		Experimental, computational, data infrastructure	AI/ML materials discovery
NIST Materials Genome Program	www.nist.gov/mgi	Experimental, Computational, Data Infrastructure	Mixed
CORPORATE RESEARCH		Experimental / Computational / Data	AI/ML to guide materials discovery and Generative/Reinforcement for Optimization
Lab of the Future		Data management, AI, Robotics, Materials Synthesis, Flow Testing	Partial
Designing Materials to Revolutionize and Engineer our Future	DMREF.org	Experimental, Computational, Data Infrastructure	Less than 10% at this stage
Accelerated Materials Design and Discovery (AMDD)	https://github.com/TRI-AMDD	Experimental, computational, data infrastructure	Integration of AI/ML to help guide or direct experiments and simulations
AI-enabled materials discovery	https://www.jhuapl.edu/news/news-releases/230503-ai-discovers-novel-superconductor	Experimental (synthesis, characterization), Computational (structure prediction, AI models, frameworks for discovery)	AI-enabled framework with SME in the loop, bayesian optimization enabled high throughput testing

Materials Characterization and Processing Center	https://engineering.jhu.edu/MCP/	Integration of data infrastructure, computing, high throughput, and experimental platforms	AI/ML, ML on edge, automation, deep learning, FAIR data
MURI: From Percolation to Passivation (P2P): Multiscale Prediction and Interrogation of Surface and Oxidation Phenomena in Multi-Principal Element Alloys (MPEAs)	https://engineering.jhu.edu/dcg/research/p2p-muri/	high throughput/combinatorial synthesis, theory, data, AI/ML, closed-loop experimentation	automation, AI/ML, autonomous characterization
Deposition and Semiverse Solutions Product Groups	https://www.lamresearch.com/semiverse-solutions/ https://www.lamresearch.com/products/our-processes/deposition/	Experimental and computational and data infrastructure	Early stages
The Materials Discovery Research Institute	www.ul.org	Data Infrastructure, Theoretical and Computational, Automated Synthesis Capabilities, Digital-First Laboratories	Building Capabilities
		Developing an MGI relevant Strategy and Roadmap for the DoD	N/A
	https://www.pnnl.gov/projects/at-scale ; https://www.pnnl.gov/high-throughput-center		
Samsung ASTRAL project at Advanced Materials Lab	https://www.nature.com/articles/s44160-024-00502-y	Experimental, Computational, Data Infrastructure	Automated powder synthesis with AI-assisted computational materials design
Argonne Collaborative Center for Energy Storage Science		Cryo EM, Advanced Photon Source	AI/ML for EELS , XAS data

From Registration Data: Soft Materials - Polymers and Biomaterials

The common themes, as well as estimate the level of autonomous infrastructure in the field of soft materials, were analyzed:

Common Themes in the Data

Integration of AI/ML**:** Many projects and platforms are incorporating AI/ML to enhance materials discovery and experimentation. This includes:

- AI/ML to guide and direct experiments.
- Autonomous chemistry labs.
- AI-guided synthesis and discovery.

Autonomous Experimentation: Several initiatives focus on fully autonomous or semi-autonomous experimentation. This is evident in projects like ARES OS 2.0, Brown research group, and Interconnected Science Ecosystem.

Data Infrastructure: Emphasis on data infrastructure to support experimental and computational research. Platforms like the Materials Data Facility and BioPACIFIC MIP highlight the need for robust data handling and integration.

Collaborative and Multi-disciplinary Approaches: Many projects involve collaborations across different scientific disciplines and institutions. Examples include the DREAM platform and the NSF 24-567 initiative.

High-throughput Experimentation: There is a trend towards high-throughput experimentation enabled by AI/ML and automation. This allows for rapid screening and discovery of new materials.

Estimation of Autonomous Infrastructure in Soft Materials

Based on the information in the table, here's an estimate of the level of autonomous infrastructure in the field of soft materials:

Fully Autonomous:

- ARES OS 2.0: Software for autonomous experimentation.
- Brown research group: Fully autonomous systems for studying polymers.
- AI-enabled materials discovery: AI-enabled framework with SME in the loop for high-throughput testing.

High Integration of AI/ML:

- Materials Discovery Research Institute (MDRI): Integration of AI/ML to guide experiments.
- Interconnected Science Ecosystem: Development and integration of AI/ML into an open architecture.
- BioPACIFIC MIP: Integration of AI/ML to guide experiments and develop high-throughput robotic experimentation.

Moderate to Strong AI/ML **Integration**:

- NRT on Soft Autonomous Experimentation: Moderate to strong AI/ML integration.
- NSF 24-567: AI/ML required for polymer design and synthesis, with autonomous lab manipulations allowed.
- Molecule Maker Lab and Molecule Maker Lab Institute: Automated modular synthesis integrated with AI.

Mixed or Emerging Integration:

- NIST Materials Genome Program: Mixed level of AI/ML integration.
- Materials Characterization and Processing Center: AI/ML, ML on edge, automation, and deep learning.
- NSF MRSEC at UC Santa Barbara: Small but growing integration of AI/ML.

Minimal or Developing:

- Designing Materials to Revolutionize and Engineer our Future: Less than 10% integration at this stage.
- Projects with unspecified levels of AI/ML integration or still under development, such as thermal protection systems/Ames.

Conclusion

Overall, the field of soft materials research is witnessing significant advancements in the integration of autonomous infrastructure. While some projects are fully autonomous, many are at various stages of integrating AI/ML to enhance experimental and computational capabilities. The trend indicates a growing emphasis on automation and AI/ML to accelerate materials discovery and development.

RAW DATA

Name of Project / Platform / Center / etc.	Website URL (if available)	Type of Capability(ies) – Experimental, Computational, Data Infrastructure, etc	Level of automation or autonomy (integration of AI/ML to help guide or direct experiments) (N/A if none)
Materials Discovery Research Institute (MDRI)	https://ul.org/research/materials-discovery	All the above, experimental,	integration of AI/ML to help guide

		computational and data Infrastructure	
Interconnected Science Ecosystem	https://www.ornl.gov/intersect	Autonomous Chemistry Laboratory, Autonomous Chemical Flow Reactors, Command and Control Open Infrastructure, Data Abstraction Layer,	Development and Integration of AI/ML into an open architecture to interconnect autonomous lab capabilities across science domains
ARES OS 2.0	https://github.com/AFRL-ARES/ARES_OS	Software for autonomous experimentation	Full
Nano4EARTH	https://www.nano.gov/nano4EARTH	National Nanotechnology Challenge	
Workshops on Self-Driving Labs	https://events.mcs.cmu.edu/ac-sdl_workshop/ and https://research.ncsu.edu/futurelabsworkshop/	Eventually will be experimental and data infrastructure, combined.	Human intervention as well as AI-driven
NRT on Soft Autonomous Experimentation	https://soft-ae.seas.upenn.edu/	Experimental; Curricular	Moderate to Strong
NSF 24-567: Molecular Foundations for Sustainability: Sustainable Polymers Enabled by Emerging Data Analytics (MFS-SPEED)	https://new.nsf.gov/funding/opportunities/molecular-foundations-sustainability-sustainable/nsf24-567/solicitation	Current Solicitation accepting proposals	AI/ML is required for polymer design and synthesis; autonomous lab manipulations are not required, but are allowed
Laboratory for Research on the Structure of Matter / Singh Center for Nanotechnology / Interdisciplinary Training in Data Driven Soft Materials Research and Science Policy	lrsm.seas.upenn.edu ; nano.upenn.edu ; soft-ae.seas.upenn.edu	Microfabrication, Materials Characterization, Computational facilities	N/A

thermal protection systems/Ames		experimental, computational, data	
Materials Data Facility	https://materialsdatafacility.org	Data infrastructure	
DREAM: Data-driven Reinvigorated Advanced Membrane Discovery Platform (Xiaodan Gu, U. So. Miss)		Experimental	AI/ML for synthetic discovery of polymers
NIST Materials Genome Program	www.nist.gov/mgi	Experimental, Computational, Data Infrastructure	Mixed
Acceleration Consortium	https://acceleration.utoronto.ca/	All of the above	Self Driving Lab User Facility
BioPACIFIC MIP	https://biopacificmip.org/	Experimental, Data Infrastructure	Integration of AI/ML to help guide experiments, develop high-throughput robotic experimentation and develop data infrastructure
Designing Materials to Revolutionize and Engineer our Future	DMREF.org	Experimental, Computational, Data Infrastructure	Less than 10% at this stage
Accelerated Materials Design and Discovery (AMDD)	https://github.com/TRI-AMDD	Experimental, computational, data infrastructure	Integration of AI/ML to help guide or direct experiments and simulations
Brown research group	kablab.org	Experimental	Fully autonomy. We have one one self-driving lab since 2018 to study 3D printing polymers with a second new fully-autonomous system now coming online to study electrodeposited polymers.

AI-enabled materials discovery	https://www.jhuapl.edu/news/news-releases/230503-ai-discovers-novel-superconductor	Experimental (synthesis, characterization), Computational (structure prediction, AI models, frameworks for discovery)	AI-enabled framework with SME in the loop, bayesian optimization enabled high throughput testing
Molecule Maker Lab and Molecule Maker Lab Institute	moleculemaker.org	Automated Modular Synthesis, AI-Guided Closed-Loop Discovery, Functional Experimentation and Materials Characterization, Data Infrastructure (NCSA)	Automated Modular Synthesis integrated with AI
$180M Integrative Sciences Building at NC State University (under construction)	https://provost.ncsu.edu/university-interdisciplinary-programs/isb/	One floor of Automated/Autonomous Chemistry Labs with in-house Computational infrastructure	Supervised autonomy and full automation
Materials Characterization and Processing Center	https://engineering.jhu.edu/MCP/	Integration of data infrastructure, computing, high throughput, and experimental platforms	AI/ML, ML on edge, automation, deep learning, FAIR data
NSF BIOPacific Materials Innovation Platform	https://biopacificmip.org/	Experimental, computational, and data infrastructure	Central to the platform
NSF MRSEC at UC Santa Barbara	https://www.mrl.ucsb.edu/	Experimental and computaional	Small but growing
Tri-Service Biotechnology for a Resilient Supply Chain (T-BRSC) program		Experimental	
Enhanced Performance Composite Vehicle Structures		Experimental, Computational	N/A
Interconnected Science Ecosystem (INTERSECT)	https://www.ornl.gov/intersect	Experimental + Computational + Data Infrastructure	Fully integrated AI/ML workflows across multiple materials theory, synthesis, and characterization activities
DMREF:Materials Architected by Adapted Processing		Experimental, Computational, Data Infrastructure	Data driven control of materials processing.

CMU Cloud Lab, Pittsburgh Supercomputing Center, others	https://cloudlab.cmu.edu/, https://www.psc.edu/	Experimental, Computation, Data	high
		Developing an MGI relevant Strategy and Roadmap for the DoD	N/A
	https://www.pnnl.gov/projects/at-scale ; https://www.pnnl.gov/high-throughput-center		

From Registration Data: Solid State and Materials Chemistry

Based on the data provided, here are some common themes and an estimate of the extent of autonomous infrastructure in the field of solid-state and materials chemistry:

Common Themes:

Integration of AI/ML:

- Many initiatives are incorporating AI and machine learning to guide and optimize experiments and simulations.
- Examples include the Accelerated Materials Design and Discovery (AMDD), CORPORATE RESEARCH, and the Samsung ASTRAL project.

High-Throughput and Autonomous Experimentation:

- A significant focus on developing fully or partially autonomous laboratories.
- Notable examples include the Brown research group, CMU Cloud Lab, and the Interconnected Science Ecosystem (INTERSECT).

Data Infrastructure:

- Emphasis on creating robust data infrastructures to support experimental and computational workflows.
- Initiatives like the Materials Characterization and Processing Center and the OpenMSIStream project are focused on data integration and management.

Experimental and Computational Synergy:

- Combining experimental setups with computational models to accelerate materials discovery and characterization.
- Projects such as the Alabama Materials Institute and AI-enabled materials discovery at JHUAPL exemplify this integration.

Collaborative and Interconnected Systems:

- Several programs aim to develop interconnected lab environments that allow for seamless data and process integration.
- The Interconnected Science Ecosystem and the NSF Q-Amase-i Quantum Foundry are key examples.

Automated Synthesis and Discovery:

- Automated modular synthesis and AI-guided closed-loop discovery are central themes.
- The Molecule Maker Lab and the Materials Discovery Research Institute highlight these capabilities.

Estimate of Autonomous Infrastructure:

High-Level Autonomous Infrastructure:

- Initiatives such as the Brown research group and the Self Driving Lab User Facility demonstrate fully autonomous capabilities, where AI/ML systems run experiments with minimal human intervention.
- The Samsung ASTRAL project and the INTERSECT program also showcase significant autonomous features.

Partial or Supervised Autonomy:

- Several projects exhibit supervised autonomy, where human oversight is still required to some extent.
- Examples include the NC State Self-Driving Fluidic Labs and the NIST Materials Genome Program.

Developing or Experimental Stages:

- Some programs are in the early stages of developing autonomous capabilities or are currently integrating AI/ML into their workflows.
- The Designing Materials to Revolutionize and Engineer our Future and the OpenMSIStream project fall into this category.

Conclusion

From the data, it appears that the field of solid-state and materials chemistry is progressively incorporating autonomous infrastructure. About 30-40% of the initiatives have high levels of autonomous infrastructure, with fully operational AI/ML-guided systems. Another 30% exhibit partial or supervised autonomy, while the remaining initiatives are in developmental stages, building towards more autonomous capabilities. Overall, the integration of AI/ML, data infrastructure, and high-throughput experimentation are central to advancing autonomy in this field.

RAW DATA

Name of Project / Platform / Center / etc.	Website URL (if available)	Type of Capability(ies) – Experimental, Computational, Data Infrastructure, etc	Level of automation or autonomy (integration of AI/ML to help guide or

			direct experiments) (N/A if none)
CORPORATE RESEARCH		Experimental / Computational / Data	AI/ML to guide materials discovery and Generative/Reinforcement for Optimization
Designing Materials to Revolutionize and Engineer our Future	DMREF.org	Experimental, Computational, Data Infrastructure	Less than 10% at this stage
https://www.pnnl.gov/projects/nets	https://www.pnnl.gov/projects/nets	Flow and Field Assisted Nucleation of Critical Materials	
Interconnected Science Ecosystem	https://www.ornl.gov/intersect	Autonomous Chemistry Laboratory, Autonomous Chemical Flow Reactors, Command and Control Open Infrastructure, Data Abstraction Layer,	Development and Integration of AI/ML into an open architecture to interconnect autonomous lab capabilities across science domains
Interconnected Science Ecosystem (INTERSECT)	https://www.ornl.gov/intersect	Experimental + Computational + Data Infrastructure	Fully integrated AI/ML workflows across multiple materials theory, synthesis, and characterization activities
Lab of the Future		Data management, AI, Robotics, Materials Synthesis, Flow Testing	Partial
Laboratory for Research on the Structure of Matter / Singh Center for Nanotechnology / Interdisciplinary Training in Data Driven Soft Materials Research and Science Policy	lrsm.seas.upenn.edu ; nano.upenn.edu ; soft-ae.seas.upenn.edu	Microfabrication, Materials Characterization, Computational facilities	N/A
Materials Characterization and Processing Center	https://engineering.jhu.edu/MCP/	Integration of data infrastructure, computing, high throughput, and experimental platforms	AI/ML, ML on edge, automation, deep learning, FAIR data

Materials Discovery Research Institute (MDRI)	https://ul.org/research/materials-discovery	All the above, experimental, computational and data Infrastructure	integration of AI/ML to help guide
Molecule Maker Lab and Molecule Maker Lab Institute	moleculemaker.org	Automated Modular Synthesis, AI-Guided Closed-Loop Discovery, Functional Experimentation and Materials Characterization, Data Infrastructure (NCSA)	Automated Modular Synthesis integrated with AI
Nano4EARTH	https://www.nano.gov/nano4EARTH	National Nanotechnology Challenge	
NC State Self-Driving Fluidic Labs (Artificial Chemist, AlphaFlow, SmartDope, and Fast-Cat)	https://www.abolhasanilab.com/	Both Experimental and Computational	Supervised autonomy
NIST Materials Genome Program	www.nist.gov/mgi	Experimental, Computational, Data Infrastructure	Mixed
NSF Q-Amase-i Quantum Foundry	https://quantumfoundry.ucsb.edu/	Experimental, computational, and data infrastructure	Small but growing
OpenMSIStream, PARADIM, HT-MAX, VariMat		Data Infrastructure, data streaming, stream processing, decision orchestration	integration of data collection, ML decision making, ML decision deployment, instrument control
Samsung ASTRAL project at Advanced Materials Lab	https://www.nature.com/articles/s44160-024-00502-y	Experimental, Computational, Data Infrastructure	Automated powder synthesis with AI-assisted computational materials design
SD2: RAPID		Distributed high-throughput experiment + data effort	"islands of automation" with AI/ML directed experiments.
The Materials Discovery Research Institute	www.ul.org	Data Infrastructure, Theoretical and Computational,	Building Capabilities

		Automated Synthesis Capabilities, Digital-First Laboratories	
Workshops on Self-Driving Labs	https://events.mcs.cmu.edu/ac-sdl_workshop/ and https://research.ncsu.edu/futurelabsworkshop/	Eventually will be experimental and data infrastructure, combined.	Human intervention as well as AI-driven

FROM REGISTRATION DATA: CONDENSED MATTER PHYSICS

Common Themes in Condensed Matter Physics Data:

Integration of AI/ML:

- Like in the previous data, the integration of AI and machine learning is a recurring theme, aimed at guiding and optimizing experiments.
- Examples include the Adaptive Tunability for Synthesis and Control via Autonomous Learning on Edge (AT SCALE), Army Research Laboratory, and CORPORATE RESEARCH.

High-Throughput and Autonomous Experimentation:

- There is a focus on developing systems that can perform high-throughput and autonomous experiments.
- The Army Research Laboratory's BIRDSHOT Center and the ARES OS 2.0 software are notable examples.

Data Infrastructure:

- Emphasis on establishing robust data infrastructures to support experimental and computational processes.
- Projects like the Materials Data Facility and the Materials Characterization and Processing Center highlight this focus.

Experimental and Computational Synergy:

- Combining experimental setups with computational models to accelerate the discovery and characterization of materials.
- Examples include the INTERSECT program and the MURI: From Percolation to Passivation project.

Collaborative and Interconnected Systems:

- Initiatives aimed at creating interconnected lab environments to facilitate seamless data and process integration.
- The Interconnected Science Ecosystem and the Laboratory for Research on the Structure of Matter exemplify these efforts.

Automated Synthesis and Discovery:

- Automated synthesis and AI-guided closed-loop discovery are key focuses.
- The Army Research Laboratory's ARM system and the Materials Discovery Research Institute are notable initiatives.

Estimate of Autonomous Infrastructure in Condensed Matter Physics:

High-Level Autonomous Infrastructure:

- Initiatives such as the Army Research Laboratory's BIRDSHOT Center and the AT SCALE project exhibit full autonomy, with AI/ML systems making real-time decisions.
- The ARES OS 2.0 software also supports full autonomous experimentation.

Partial or Supervised Autonomy:

- Some projects show partial autonomy, where human oversight is still necessary to some extent.
- Examples include the INTERSECT program and the Designing Materials to Revolutionize and Engineer our Future initiative.

Developing or Experimental Stages:

- Several programs are in the early stages of developing autonomous capabilities or are currently integrating AI/ML into their workflows.
- The NSF Q-Amase-i Quantum Foundry and the Laboratory for Research on the Structure of Matter are working towards more autonomous systems.

Conclusion

In the field of condensed matter physics, the integration of autonomous infrastructure is progressing, with about 30-40% of the initiatives demonstrating high levels of autonomous capabilities. These projects are incorporating AI/ML for real-time decision-making and optimization. Another 30% exhibit partial autonomy, requiring some level of human supervision, while the remaining initiatives are in the developmental stages. The common themes include AI/ML integration, high-throughput experimentation, robust data infrastructures, and the synergy between experimental and computational approaches.

RAW DATA

Name of Project / Platform / Center / etc.	Website URL (if available)	Type of Capability(ies) – Experimental, Computational, Data Infrastructure, etc	Level of automation or autonomy (integration of AI/ML to help guide or direct experiments) (N/A if none)
		Experimental, Computational, Data Infrastructure, funding	High
		Developing an MGI relevant Strategy and Roadmap for the DoD	N/A
	https://www.pnnl.gov/projects/at-scale ;		

	https://www.pnnl.gov/high-throughput-center		
Adaptive Tunability for Synthesis and Control via Autonomous Learning on Edge (AT SCALE)	https://www.pnnl.gov/projects/at-scale/about#:~:text=Adaptive%20Tunability%20for%20Synthesis%20and%20Control%20via%20Autonomous,materials%20synthesis%20by%20developing%20closed-loop%20autonomous%20precision%20synthesis.	Experimental, Data, Computational, AI/ML	full autonomy, with AI/ML enabling real-time decisions
Alabama Materials Institute	https://ami.ua.edu/	Experimental Materials Characterization	N/A
ARES OS 2.0	https://github.com/AFRL-ARES/ARES_OS	Software for autonomous experimentation	Full
Army Research Laboratory - High Throughput Materials Discovery for Extreme Environments Center (HTMDEC) at Texas A&M University, the name of the Center is BIRDSHOT (Batch-wise Improvement in Reduced Materials Design Space using a Holistic Optimization Technique). BIRDSHOT is also used for ARPA-E ULTIMATE Program and 2 NSF DMREF Programs. Experimental part of BIRDSHOT Center is called ARM (Autonomous Robotics Metallurgist) where we can synthesize, process, characterize, and test		We have several computational tools applied to metallic materials (computational materials science, thermodynamics, and kinetics models, statistical frameworks such as Batch Bayesian Optimization to design alloys to fabricate and test) and experimental capabilities to design, fabricate, process, characterize, and test metallic alloys in a high throughput fashion. We have designed, fabricated, processed, and tested more than 400 new metallic alloys in bulk dimensions in the last 3 years in various programs mentioned above.	In all our materials design, fabrication, and testing efforts we integrate AI/ML methods to direct experiments using the BIRDSHOT framework in the programs mentioned above.

materials in a high throughput fashion.			
CORPORATE RESEARCH		Experimental / Computational / Data	AI/ML to guide materials discovery and Generative/Reinforcement for Optimization
Designing Materials to Revolutionize and Engineer our Future	DMREF.org	Experimental, Computational, Data Infrastructure	Less than 10% at this stage
Interconnected Science Ecosystem (INTERSECT)	https://www.ornl.gov/intersect	Experimental + Computational + Data Infrastructure	Fully integrated AI/ML workflows across multiple materials theory, synthesis, and characterization activities
Laboratory for Research on the Structure of Matter / Singh Center for Nanotechnology / Interdisciplinary Training in Data Driven Soft Materials Research and Science Policy	lrsm.seas.upenn.edu ; nano.upenn.edu ; soft-ae.seas.upenn.edu	Microfabrication, Materials Characterization, Computational facilities	N/A
Materials Characterization and Processing Center	https://engineering.jhu.edu/MCP/	Integration of data infrastructure, computing, high throughput, and experimental platforms	AI/ML, ML on edge, automation, deep learning, FAIR data
Materials Data Facility	https://materialsdatafacility.org	Data infrastructure	
Materials Discovery Research Institute (MDRI)	https://ul.org/research/materials-discovery	All the above, experimental, computational and data Infrastructure	integration of AI/ML to help guide
MURI: From Percolation to Passivation (P2P): Multiscale Prediction and Interrogation of	https://engineering.jhu.edu/dcg/research/p2p-muri/	high throughput/combinatorial synthesis, theory, data, AI/ML, closed-loop experimentation	automation, AI/ML, autonomous characterization

Surface and Oxidation Phenomena in Multi-Principal Element Alloys (MPEAs)			
Nano4EARTH	https://www.nano.gov/nano4EARTH	National Nanotechnology Challenge	
NSF Q-Amase-i Quantum Foundry	https://quantumfoundry.ucsb.edu/	Experimental, computational, and data infrastructure	Small but growing

From Registration Data: Electronic and Photonic Materials

Common Themes in Electronic and Photonic Materials Projects

Integration of AI/ML:

- A significant number of projects emphasize the integration of artificial intelligence and machine learning (AI/ML) to guide and optimize experiments, synthesize materials, and manage data. This is seen across multiple initiatives such as ARES OS 2.0, the Adaptive Tunability for Synthesis and Control via Autonomous Learning on Edge (AT SCALE), and the Interconnected Science Ecosystem (INTERSECT).

Focus on Automation:

- Full or partial automation is a recurring theme, with projects like ARES OS 2.0 and NC State Self-Driving Fluidic Labs showcasing autonomous or semi-autonomous lab environments. This reduces human intervention and increases efficiency in material discovery and characterization processes.

High-Throughput and High Efficiency:

- High-throughput experimental setups and automated workflows are commonly highlighted to speed up the discovery and optimization of materials. Projects like AI-enabled materials discovery and the Molecule Maker Lab illustrate this theme well.

Data Infrastructure and Management:

- Robust data infrastructure and management systems are crucial components, ensuring the effective collection, storage, and analysis of large datasets. The Materials Data Facility and projects like OpenMSIStream emphasize this aspect, integrating data streaming and decision orchestration.

Collaborative and Interconnected Research:

- Many initiatives focus on creating interconnected ecosystems and collaborative platforms that allow for the sharing of data, resources, and findings. Examples include the Interconnected Science Ecosystem (INTERSECT) and the DOE Energy Materials Network.

Experimental and Computational Integration:

- Projects often combine experimental capabilities with computational models and simulations to enhance the discovery process. This is evident in initiatives like the Materials Discovery Research Institute (MDRI) and the NSF Q-Amase-i Quantum Foundry.

Modular and Scalable Systems:

- The development of modular, scalable systems that can be easily adapted or expanded is a common theme. For instance, the Molecule Maker Lab features automated modular synthesis capabilities.

Funding and Infrastructure Development:

- Significant investment in new facilities and infrastructure, such as the $180M Integrative Sciences Building at NC State University, underscores the commitment to advancing materials science research.

National and Institutional Support:

- Many projects receive support from national programs and major research institutions, reflecting the strategic importance of materials science. Initiatives like Nano4EARTH and the NIST Materials Genome Program illustrate this support.

Emerging Technologies and Frontier Research:

- The focus on cutting-edge technologies and frontier research areas, such as quantum materials and AI-guided material synthesis, highlights the forward-looking nature of these projects. Examples include the NSF Q-Amase-i Quantum Foundry and AI-enabled materials discovery projects.

The common themes across electronic and photonic materials projects highlight a concerted effort to integrate AI/ML, automate processes, and build robust data infrastructures. There is a clear emphasis on high-throughput and efficient research methodologies, collaborative ecosystems, and the development of modular, scalable systems. The significant investment in infrastructure and national support further underscores the strategic importance of these research initiatives in advancing materials science.

Analysis of Autonomous Infrastructure in Electronic and Photonic Materials Projects

Fully Autonomous:

- ARES OS **2.0**: Full autonomy in software for autonomous experimentation.
- **Adaptive Tunability for Synthesis and Control via Autonomous Learning on Edge (**AT SCALE**)**: Full autonomy with AI/ML enabling real-time decisions.
- **Interconnected Science Ecosystem (**INTERSECT**)**: Fully integrated AI/ML workflows across multiple materials theory, synthesis, and characterization activities.

High Integration of AI/ML:

- **Materials Discovery Research Institute (**MDRI**)**: Integration of AI/ML to help guide experimental, computational, and data infrastructure efforts.
- **Molecule Maker Lab and Molecule Maker Lab Institute**: Automated Modular Synthesis integrated with AI for discovery and materials characterization.

- **Materials Characterization and Processing Center**: Integration of data infrastructure, computing, high throughput, and experimental platforms with AI/ML, ML on edge, automation, and deep learning.
- CMU **Cloud Lab, Pittsburgh Supercomputing Center, others**: High levels of automation in experimental, computational, and data capabilities.

Moderate to Strong AI/ML Integration:

- AI**-enabled materials discovery**: AI-enabled framework with SME in the loop and Bayesian optimization for high throughput testing.
- 2D **Crystal Consortium Materials Innovation Platform**: Thin film synthesis tools operate via computer control without feedback currently from AI/ML.
- NC **State Self-Driving Fluidic Labs**: Supervised autonomy in experimental and computational aspects.
- NSF **Q-Amase-i Quantum Foundry**: Small but growing integration of experimental, computational, and data infrastructure.

Mixed or Emerging Integration:

- NIST **Materials Genome Program**: Mixed integration of experimental, computational, and data infrastructure with some AI/ML capabilities.
- CORPORATE RESEARCH**- Lockheed Martin**: Partial integration of AI/ML to guide materials discovery and optimization.
- **Deposition and Semiverse Solutions Product Groups**: Early stages of integrating experimental, computational, and data infrastructure with AI/ML.

Minimal or Developing:

- **Alabama Materials Institute**: Experimental materials characterization without specified AI/ML integration.
- **Designing Materials to Revolutionize and Engineer our Future**: Less than 10% AI/ML integration at this stage.
- **Workshops on Self-Driving Labs**: Combines human intervention with AI-driven experimental and data infrastructure efforts.
- **$**180M **Integrative Sciences Building at** NC **State University**: Supervised autonomy and full automation in development.

No AI/ML Integration Specified:

- **Nano**4EARTH: National Nanotechnology Challenge without specified AI/ML integration.
- DOE **Energy Materials Network**: Miscellaneous integration of experimental, computational, and data infrastructure capabilities.
- **Materials Data Facility**: Data infrastructure without specified AI/ML integration.
- **Developing an** MGI **relevant Strategy and Roadmap for the DoD**: N/A (integration not specified).

Conclusion

The analysis of electronic and photonic materials projects shows a significant focus on integrating AI/ML for automation, especially in high-throughput experimentation, synthesis optimization, and data management. While some projects have achieved full autonomy, others are in various stages of adopting AI/ML technologies. The overall trend indicates a growing emphasis on using AI/ML to accelerate discovery and innovation in the field of electronic and photonic materials.

Semiconductor Related Efforts

Based on the provided data, the following efforts have a focus on semiconductors:

Semiconductor, advanced packaging and assembly

- Type of Capability: Experimental, future data infrastructure
- Level of Automation: AI/ML manufacturing with new materials

CHIPS Manufacturing USA Institute - Digital Twins for Semiconductor Manufacturing

- Type of Capability: Unspecified in provided data

NC State Self-Driving Fluidic Labs (Artificial Chemist, AlphaFlow, SmartDope, and Fast-Cat)

- Website URL: https://www.abolhasanilab.com/
- Type of Capability: Both Experimental and Computational
- Level of Automation: Supervised autonomy

Deposition and Semiverse Solutions Product Groups

- Website URL: https://www.lamresearch.com/semiverse-solutions/ and https://www.lamresearch.com/products/our-processes/deposition/
- Type of Capability: Experimental and computational and data infrastructure
- Level of Automation: Early stages

These efforts specifically mention semiconductors or related technologies in their focus.

RAW DATA

Name of Project / Platform / Center / etc.	Website URL (if available)	Type of Capability(ies) – Experimental, Computational, Data Infrastructure, etc	Level of automation or autonomy (integration of AI/ML to help guide or direct experiments) (N/A if none)

		Experimental, Computational, Data Infrastructure, funding	High
Materials Discovery Research Institute (MDRI)	https://ul.org/research/materials-discovery	All the above, experimental, computational and data Infrastructure	integration of AI/ML to help guide
Interconnected Science Ecosystem	https://www.ornl.gov/intersect	Autonomous Chemistry Laboratory, Autonomous Chemical Flow Reactors, Command and Control Open Infrastructure, Data Abstraction Layer,	Development and Integration of AI/ML into an open architecture to interconnect autonomous lab capabilities across science domains
ARES OS 2.0	https://github.com/AFRL-ARES/ARES_OS	Software for autonomous experimentation	Full
Nano4EARTH	https://www.nano.gov/nano4EARTH	National Nanotechnology Challenge	
Alabama Materials Institute	https://ami.ua.edu/	Experimental Materials Characterization	N/A
Workshops on Self-Driving Labs	https://events.mcs.cmu.edu/ac-sdl_workshop/ and https://research.ncsu.edu/futurelabsworkshop/	Eventually will be experimental and data infrastructure, combined.	Human intervention as well as AI-driven
OpenMSIStream, PARADIM, HT-MAX, VariMat		Data Infrastructure, data streaming, stream processing, decision orchestration	integration of data collection, ML decision making, ML decision deployment, instrument control
semiconductor, advanced packaging and assembly		experimental, future data infrastructure	AI/ML manufacturing with new materials
DOE Energy Materials Network	https://www.energy.gov/eere/energy-materials-	All of the above	Misc

	network/energy-materials-network		
Materials Data Facility	https://materialsdatafacility.org	Data infrastructure	
NIST Materials Genome Program	www.nist.gov/mgi	Experimental, Computational, Data Infrastructure	Mixed
CORPORATE RESEARCH- Lockheed Martin		Experimental / Computational / Data	AI/ML to guide materials discovery and Generative/Reinforcement for Optimization
2D Crystal Consortium Materials Innovation Platform	2dccmip.org	Experimental, Computational, Data Infrastructure related to Synthesis of 2D Materials	Thin film synthesis tools operate via computer control but without feedback currently from AI/ML.
Designing Materials to Revolutionize and Engineer our Future	DMREF.org	Experimental, Computational, Data Infrastructure	Less than 10% at this stage
AI-enabled materials discovery	https://www.jhuapl.edu/news/news-releases/230503-ai-discovers-novel-superconductor	Experimental (synthesis, characterization), Computational (structure prediction, AI models, frameworks for discovery)	AI-enabled framework with SME in the loop, bayesian optimization enabled high throughput testing
Molecule Maker Lab and Molecule Maker Lab Institute	moleculemaker.org	Automated Modular Synthesis, AI-Guided Closed-Loop Discovery, Functional Experimentation and Materials Characterization, Data Infrastructure (NCSA)	Automated Modular Synthesis integrated with AI
CHIPS Manufacturing USA Institute - Digital Twins for Semiconductor Manufacturing	https://www.nist.gov/chips/research-development-programs/chips-manufacturing-usa-institute		
$180M Integrative Sciences Building at NC State University (under construction)	https://provost.ncsu.edu/university-interdisciplinary-programs/isb/	One floor of Automated/Autonomous Chemistry Labs with in-house Computational infrastructure	Supervised autonomy and full automation
NC State Self-Driving Fluidic Labs (Artificial	https://www.abolhasanilab.com/	Both Experimental and Computational	Supervised autonomy

Chemist, AlphaFlow, SmartDope, and Fast-Cat)			
Materials Characterization and Processing Center	https://engineering.jhu.edu/MCP/	Integration of data infrastructure, computing, high throughput, and experimental platforms	AI/ML, ML on edge, automation, deep learning, FAIR data
Adaptive Tunability for Synthesis and Control via Autonomous Learning on Edge (AT SCALE)	https://www.pnnl.gov/projects/at-scale/about#:~:text=Adaptive%20Tunability%20for%20Synthesis%20and%20Control%20via%20Autonomous,materials%20synthesis%20by%20developing%20closed-loop%20autonomous%20precision%20synthesis.	Experimental, Data, Computational, AI/ML	full autonomy, with AI/ML enabling real-time decisions
NSF Q-Amase-i Quantum Foundry	https://quantumfoundry.ucsb.edu/	Experimental, computational, and data infrastructure	Small but growing
Deposition and Semiverse Solutions Product Groups	https://www.lamresearch.com/semiverse-solutions/ https://www.lamresearch.com/products/our-processes/deposition/	Experimental and computational and data infrastructure	Early stages
Interconnected Science Ecosystem (INTERSECT)	https://www.ornl.gov/intersect	Experimental + Computational + Data Infrastructure	Fully integrated AI/ML workflows across multiple materials theory, synthesis, and characterization activities
The Materials Discovery Research Institute	www.ul.org	Data Infrastructure, Theoretical and Computational, Automated Synthesis Capabilities, Digital-First Laboratories	Building Capabilities
CMU Cloud Lab, Pittsburgh Supercomputing Center, others	https://cloudlab.cmu.edu/, https://www.psc.edu/	Experimental, Computation, Data	high
		Developing an MGI relevant Strategy and Roadmap for the DoD	N/A

FROM REGISTRATION DATA: BARRIERS TO ADOPTION OF AUTONOMOUS AND AUTOMATED LABORATORIES

Addressing these barriers will require concerted efforts in **standardization, education, interdisciplinary collaboration, and technological innovation** to advance the adoption of autonomous and automated laboratories across scientific disciplines:

Vendor Fragmentation and Support:

- Robotic equipment often comes from various vendors, leading to integration challenges.
- Maintenance and troubleshooting may require vendor-specific expertise, causing dependency.
- A single malfunction can halt entire workflows, highlighting the fragility of integrated systems.

Complexity and Interdisciplinary Expertise:

- Developing autonomous systems requires expertise across AI/ML, robotics, data science, and domain-specific knowledge.
- Limited commercial availability necessitates research groups to develop systems internally, which is resource-intensive and requires diverse skills.

Technical Standards and Integration:

- Lack of standardized APIs and interfaces across equipment hinders seamless integration and automation.
- Inconsistent hardware standards prevent plug-and-play integration of new instruments, complicating system scalability and adaptability.

Infrastructure and Resource Constraints:

- Existing computing and storage infrastructures may not be optimized for handling large volumes of experimental data generated by automated systems.
- Physical lab spaces and power requirements may not support the demands of automated workflows, especially in older facilities.

Data Management and Sharing:

- Challenges in managing, sharing, and standardizing data formats across different laboratories and institutions.
- Issues with data security, access controls, and the interoperability needed for collaborative research efforts.

Validation and Certification:

- Establishing trust in automated systems requires rigorous validation of results and certification processes.
- Ensuring that autonomous systems produce reliable and reproducible data that meet industry and regulatory standards.

Skills Gap and Workforce Training:

- Shortage of professionals with combined expertise in experimental science, AI/ML, and automation technologies.
- Need for comprehensive training programs to bridge the gap between traditional experimental techniques and autonomous methodologies.

Cultural and Educational Challenges:

- Academic and industry cultures still favor traditional methods over autonomous systems, affecting adoption rates.
- Educational curricula often do not adequately prepare students and researchers in the necessary interdisciplinary skills for autonomous laboratories.
- Incentive structures in academia may prioritize short-term gains over long-term infrastructure development.

Resistance to Change and Cultural Mindset:

- Inertia in adopting new technologies and methodologies within academic and industrial research communities.
- Resistance to moving away from traditional Edisonian approaches to more automated, data-driven methodologies.

RAW DATA

Beyond funding limitations, what are the barriers to large-scale adoption of autonomous and automated laboratories	Materials class the capability addresses (more than one possible) - Selected Choice
1) Robotic equipment necessary is typically from a variety of vendors. Often troubleshooting and maintenance can be done only by the vendor. A single flaw in the chain of robotics can paralyze the entire sequence. Thus the strength of the automation sequence is also subject to the individual parts.	

1. Autonomous and automated laboratories currently have to be designed and developed by research groups; there are few examples where these systems are commercially available from vendors. As a result, research teams developing AMII must have broad expertise in data science, AI/ML, robotics, equipment design and construction as well as the relevant materials domain knowledge. This can be difficult to achieve outside national labs. 2. Most of the current research in AMII is being done by theory/computational groups who are broadening out to include ML/AI to accelerate simulations and make predictions based off of limited training data. Experimental groups need to be more involved both to generate larger data sets for training and to develop feedback systems needed for autonomous operation. 3. Development of AMII requires significant time/effort which may not be rewarded in the current tenure track system. It is easier to get high impact publications by having an army of graduate students working manually on a problem than spending time to develop AMII. What can be done to incentivize faculty to think long term about advancements in research infrastructure?	Electronic Materials
A collective efforts to integrate extendable software/codes that are developed for automated labs	Ceramics Solid State and Materials Chemistry
A principle challenge in developing autonomous laboratories is vendor buy-in. To create autonomous workflows, we must be able to autonomously control instrumentation within the workflow. This requires vendors to create APIs that allow remote control of instruments and remote access to instrument data. Developing such APIs that do not reveal proprietary information is possible, but requires vendor effort. A principle barrier is creating workarounds for vendors who are not yet engaged or supportive of developing such autonomous laboratories.	Electronic Materials Materials in/for Condensed Matter Physics Metallic Nanostructures Metals Polymers Solid State and Materials Chemistry
Access to automated laboratories, universal standards across automated labs and infrastructure to collect and share data.	Biomaterials Polymers
Buy-in and training of faculty at smaller colleges.	
Change in culture; need for education and training; concerns related to safety and safe use.	Biomaterials Electronic Materials Solid State and Materials Chemistry
Coordinated efforts to establish interfaces that work for lab and industrial scale R&D	Biomaterials Ceramics Electronic Materials Materials in/for Condensed Matter Physics Metallic Nanostructures Metals Photonic Materials Polymers

	Solid State and Materials Chemistry
Data management policies including sharing between organizations, access controls, retention and security. Propriety data formats (instruments), network speed (for very large files).	Polymers
Design of discovery workflows that balance complex observables and distant rewards	
equipment, methodology, and infrastructure for autonomous polymer synthesis and materials and mechanical characterization	Polymers
Flexibility of autonomous laboratories -- approaches must be capable of covering a wide range of materials and applications. Niche autonomous platforms will rapidly become obsolete. Physical lab space, infrastructure, and workforce training are additional barriers.	Metallic Nanostructures Metals Other - Energetic Materials
Flexible, low-cost, reproducible, and accessible automation tools for all. Identifying the biggest challenge of different testbed materials and focusing on developing a low-cost and accessible automation tool to address it. Digitalization of existing tools in chemistry and materials science labs.	Electronic Materials Metallic Nanostructures Metals Other - Fine Chemicals Photonic Materials Solid State and Materials Chemistry
Fully autonomous laboratories can only be developed for very targeted niche solutions, and in those niche applications they are very impressive. But a more holistic, generalizable approach to accelerated, multiobjective materials & process optimization can be achieved without full autonomy, by taking advantage of keeping an expert in the loop.	Metallic Nanostructures Metals
I haven't seen a lot in the automated handling of dry powdered materials, moving to say a sintering state to create a ceramic type material - trickier than liquids handling. Then, I've heard reports that when synthesis is AI/ML automated driven, the characterization techniques might not be sufficient enough to prove the newness or value of the material. Just thoughts.	Polymers
I understand that there are challenges in lacks of standards, APIs, and other interfaces for equipment that hampers automation, plus improvements needed in AI-driven and modeling-driven control, calibration, characterization, and analysis.	
i. Computing Infrastructure: Existing High-Performance Computing (HPC) architectures are suboptimal for experimental data analytics, necessitating high-availability, deterministic networking, and computing resources. The prevalent centralized, scheduler-based model impinges upon automated workflows due to network congestion and resource availability. A bespoke computational infrastructure, tailored for scientific workloads, should be developed, incorporating high-availability, self-healing, and load-balancing functionalities via Kubernetes or similar orchestrators, thereby facilitating continuous deployment and AI/ML-based	Ceramics Solid State and Materials Chemistry

control over data flows. ii. Storage Infrastructure: Achieving Findable, Accessible, Interoperable, and Reusable (FAIR) scientific data is a pressing issue. Developing open-source, rigorously documented file formats and metadata schemas is crucial.30 Community-wide standardization, or at least interoperability standards, are essential, along with platforms for secure data sharing and hosting. iii. Skill Development and Science Education: The skill set of the contemporary experimental scientist is increasingly computation-centric. Thus, curricula must be restructured to include core computational tools like data analytics and AI/ML techniques pertinent to data collection and analysis across scientific disciplines.11,16 iv. Interdisciplinary Collaboration: The facile adaptability of AI methods to scientific questions raises concerns, especially given the propensity for overfitting in machine learning models that can masquerade as genuine understanding. A concerted effort to break disciplinary silos is imperative for the co-design of machine learning techniques and validation methodologies that respect both the foundational principles of ML and parsimony required for materials science. v. Open Science and Hardware: The proprietary nature of scientific instrumentation hinders technique innovation. A shift towards an open-source community development model, compliant with standards like IEEE and ISO for data transfer and curation as well as experimental protocols (i.e. ASTM-like), is necessary. Purchasing power should be leveraged to demand Software Development Kits (SDKs) and Application Programming Interfaces (APIs) from manufacturers, thereby lowering barriers to automation and interoperability. Moreover, codebases should be well-documented and architecturally sound to be accessible to scientists with limited coding expertise.	
If large-scale adoption means wide-spread across the community, then barriers are IP, tool sets that address a wide array of material synthesis/metrology needs, and accessible curriculum/training. If large-scale adoption means extension to high-volume manufacturing from outcomes of autonomous labs, then validation/verification and integration concepts are most critical to fold in to the materials search and co-optimization. Training/curriculum are critical here too.	
Inadequate support for team science approaches to challenging materials problems via the use of autonomous laboratories	
Inertia in the academic and corporate materials communities	Ceramics Electronic Materials Materials in/for Condensed Matter Physics Metallic Nanostructures Metals

	Photonic Materials
	Solid State and Materials Chemistry
infrastructure gaps, knowledge gaps, interoperability, governance and safety aspects.	Metallic Nanostructures
	Metals
Infrastructure. From a defense perspective many of our buildings and labs need upgrades to support the power and potential space needs of automation.	
-It is challenging for independent groups to develop autonomous research systems, so it is necessary to determine processes and standards for collaborating and sharing existing autonomous systems. -A lack of consistent hardware standards that allow the addition of new instruments in a plug-and-play fashion is a key challenge. -Coherent pedagogical materials that the community can share and build upon would aid in workforce and autonomous system development.	Polymers
	Solid State and Materials Chemistry
Lack of training. Lack of commercial autonomous laboratory equipment.	
legacy platforms, integration of AI/ML into existing platforms, communication between instrumentation	Electronic Materials
	Materials in/for Condensed Matter Physics
	Metallic Nanostructures
	Metals
	Photonic Materials
Mindset is a big one, many university researchers, national laboratories, and industry still rely on Edisonian research. We must break out of this archaic mindset. Equipment/technology - while things like combinatorial chemistry has been utilized by Pharma for decades, it is not amenable to materials like metals and/or ceramics. Workforce - One of the reasons guys like Alan Gaspuru has been so successful at Univ of Toronto is because he recruited much of the top talent in AE out of the U.S.. We must not only train this next generation of autonomous materials scientists, but also retain them. Not easy.	Ceramics
	Metallic Nanostructures
	Metals
Policy and acquisition changes to promote data sharing and protection	Biomaterials
	Ceramics
	Electronic Materials
	Materials in/for Condensed Matter Physics
	Metallic Nanostructures
	Metals
	Other

	Photonic Materials Polymers Solid State and Materials Chemistry
Protocols for round-robin experiments, automated thin film synthesis, automated integration into microsystems and automated analysis of integrated systems	Ceramics Electronic Materials Metallic Nanostructures Metals
Some method, such as catalyst testing are quite difficult to fully automate. Serial operation of individual components of an entire workstream can create weakness in productivity. Some components are vendor maintained and troubleshooting can depend entirely on vendor availability or parts availability.	Ceramics Metallic Nanostructures Metals Other Solid State and Materials Chemistry
Standardization of data format, democratized data sharing platform, striking a balance between open source and monetization of information and data from autonomous laboratories. Instrument companies must participate and be incentivized.	
testing in relevant manufacturing device structures	Electronic Materials
The ability to synthesize (primary and secondary) bulk (≥100 gms) metallic and ceramic candidate alloys 'on-demand' (≤1 hr after composition and/or microstructure specification) is essential for automated laboratories but is not currently possible with the current state-of-the-art.	
The diversity of materials research.	Biomaterials Polymers
The two major barriers, beyond funding, are: 1) physics based models that can guide the AI/ML for materials discovery 2) scientists lacking coding and data-analysis capabilities to make autonomous/automated labs viable.	Ceramics
There is a need for relatively large multidisciplinary teams with a proven track record of working together to make autonomous and automated laboratories in an institution a reality. Often, the efforts and resources are distributed to places without these large teams.	Materials in/for Condensed Matter Physics Metallic Nanostructures Metals
There is still a lack of knowledge of physics of materials under extremely high strain rate conditions (ballistic, blast, other), so until we can better understand the fundamental physics of how materials respond under these extreme conditions, we cannot expect to automate the development of materials to suit these applications.	Metallic Nanostructures Metals
Training efficiency	Ceramics Metallic Nanostructures Metals Polymers

	Solid State and Materials Chemistry
Training: The requisite skills in both instrument use and development, and machine learning itself, represent non-trivial barriers Instruments: There is a lack of readily available platforms that can enable the specific types of experiments that are of interest to the soft materials community Surrogate properties: Accelerating research relies on having surrogate properties that can more readily be measured. Identification of robust surrogate properties for research questions of interest represents a limitation.	Biomaterials
	Polymers
Trust and Certification on material properties were performed with the rigor and fidelity required for traceability.	Ceramics
	Electronic Materials
	Materials in/for Condensed Matter Physics
	Metallic Nanostructures
	Metals
	Photonic Materials
	Solid State and Materials Chemistry
Workforce (or lack thereof)	Other - soft matter
Workforce education.	Materials in/for Condensed Matter Physics
	Polymers
	Solid State and Materials Chemistry
Workforce.	Biomaterials
	Ceramics
	Electronic Materials
	Materials in/for Condensed Matter Physics
	Metallic Nanostructures
	Metals
	Photonic Materials
	Polymers
	Solid State and Materials Chemistry

From Registration Data: Missing Capabilities

Several common themes emerge regarding the development and challenges associated with Autonomous Materials Innovation Infrastructure (AMII). These themes underscore the multifaceted approach required for advancing AMII, involving technological, infrastructural, educational, and collaborative efforts. The integration of automation, data management, high-throughput capabilities, and interdisciplinary collaboration is crucial for overcoming existing gaps and accelerating the deployment of new materials and technologies:

Automation and Robotics:

- Essential for synthesis, data-driven frameworks, and closed-loop feedback systems.
- Challenges in automating synthesis procedures where unexpected phenomena occur.
- Need for reproducible automation technologies for accelerated synthesis.

Data Infrastructure and Management:

- Requirement for a centralized data repository, FAIR data principles, and interoperability.
- Importance of AI-ready data infrastructure and shareable data infrastructure.
- Automated data extraction and handling of multi-modal data.

High-Throughput Experimentation:

- Automated labs with high-throughput characterization.
- Lack of infrastructure for autonomous synthesis and characterization.
- Coordinated network of synthetic capabilities for rapid production and testing.

Integration and Interoperability:

- Need for hardware/software and hardware/hardware interfaces.
- Co-design of hardware and software to ensure microstructurally sensitive autonomous platforms.
- Standards for hardware integration and common digital infrastructure.

Collaboration and Democratization:

- Close collaboration with tool vendors for system design and manufacturing.
- Democratizing access to resources, data, AI infrastructure, and education.
- Establishing connections between education (especially at smaller colleges) and research.

Challenges in Material Translation:

- Translating material properties into device functionality.
- Addressing the "Valley of Death" between materials discovery and deployment.
- Emphasis on finding synthetic routes alongside new materials discovery.

Educational and Workforce Development:

- Expanding efforts in education and workforce development to support AMII.
- Intellectual awareness and training in emerging toolsets for materials scientists.

Performance and Testing:

- Proper interpretation of materials performance data and filtering good versus bad data.
- Extended testing of catalytic materials and performance testing setup.

Societal and Structural Issues:

- Need for systems interoperability and addressing societal-level grand challenges.
- Interoperable decision deployment infrastructure and community integration.

Gaps and Recommendations:

- Explicit connections between new materials development and design integration.
- Growing library of open access databases for AI models in self-driving labs.
- Deployment of modules for adapting existing infrastructure to automated tool suites.

RAW DATA

Let us know if you have initial thoughts on what specific capabilities are missing from the Autonomous Materials Innovation Infrastructure (AMII) to truly accelerate the materials development continuum (design through manufacture.)	Materials class the capability addresses (more than one possible) - Selected Choice
Automated data-driven frameworks are essential for development of AMII.	
Extraction and processing of critical minerals (e.g., lithium, graphite, etc.)	
1) Automation of synthesis procedures where unexpected phenomena occur requires attention (e.g unexpected precipitation or other phase separation events) 2) transfer and setup of materials for analysis and performance testing is sometimes not trivial - especially for extended testing of catalytic materials 3) Proper interpretation of materials performance data and filtering for good versus bad data is difficult to automate	

The development of AMII will require close collaboration with tool vendors to design and manufacture systems that incorporate robotics and enable closed loop feedback from AI/ML algorithms. For processing tools, in situ characterization techniques are needed for timely closed loop feedback.	Electronic Materials
There are numerous use inspired materials research activities where there is a desire to advance future technologies based on fundamental materials science. While these activities yield many exotic materials, there is a grand challenging in translating material property into device functionality. There needs to be an expanded effort in understanding how to fabricate devices out of contemporary materials without disrupting desired material properties to accelerate technological advancements.	Electronic Materials Materials in/for Condensed Matter Physics Metallic Nanostructures Metals Polymers Solid State and Materials Chemistry
Automated labs coupled with high-throughput characterization.	Biomaterials Polymers
Establishing a sustained connection between undergraduate education (at small colleges) with low overhead.	
Need for democratizing access to resources, common data and AI infrastructure, education and workforce development.	Biomaterials Electronic Materials Solid State and Materials Chemistry
Hardware/Software interfaces, hardware/hardware interfaces	Biomaterials Ceramics Electronic Materials Materials in/for Condensed Matter Physics Metallic Nanostructures Metals Photonic Materials Polymers Solid State and Materials Chemistry
Advances in physics based ML.	Polymers
We lack the infrastructure for autonomous synthesis and characterization of polymer materials.	Polymers
Explicit connection between new materials development and design integration/optimization is a major gap preventing rapid deployment. Legacy part/process qualification procedures are also a significant bottleneck.	Metallic Nanostructures Metals Other - Energetic Materials
Reproducible automation technologies for accelerated and miniaturized synthesis of emerging advanced functional materials.	Electronic Materials Metallic Nanostructures Metals Other - Fine Chemicals Photonic Materials

	Solid State and Materials Chemistry
As we outline in our article on "Machine Learning for material science: barriers to adoption" [Matter, 2023], there are four broad categories of gaps: (a) intellectual awareness on the part of materials scientists regarding the emerging toolsets, (b) infrastructural resources both in terms of automated high-throughput experimentation and automated data management, (c) algorithms with embedded physical guard rails, and (d) psychological trust in the novel approaches.	Metallic Nanostructures
	Metals
I am one of the co-host for a workshop conducted at U Chicago - we have a manuscript regarding "Materials Laboratories of the Future for Alloys, Amorphous, and Composite Materials" - the major gas are identified there.	Ceramics
	Solid State and Materials Chemistry
- more extensive training datasets including bad/failed material synthesis - deployable modules for adapting existing infrastructure to automated tool suites - shared central physical facilities to pilot autonomous materials experiments. These may best be housed at one or more national labs or a new national institute. - growing library of open access database for AI models for self-driving labs	
Substantial autonomous and automated laboratories	
A centralized data repository that has both FAIR data and siloed data.	Ceramics
	Electronic Materials
	Materials in/for Condensed Matter Physics
	Metallic Nanostructures
	Metals
	Photonic Materials
	Solid State and Materials Chemistry
Through going semantics; systems interoperability; appropriate societal-level Grand Challenges; interoperable decision deployment infrastructure; community integration	Metallic Nanostructures
	Metals
The ability to optimize for affordable manufacturability is as important as process and structure. Process does not equate to manufacturable.	
-Coordinated network of synthetic capabilities to allow materials to be rapidly produced and tested by several independent systems. -Common digital infrastructure to coordinate data sharing and instrument control. -Standards for hardware integration that industry can follow.	Polymers
	Solid State and Materials Chemistry
co-design of hardware and software is a huge gap, as well as microstructurally sensitive autonomous platforms	Electronic Materials
	Materials in/for Condensed Matter Physics
	Metallic Nanostructures
	Metals

	Photonic Materials
With apologies for being vague: Equipment, Software, and Workforce	Ceramics
	Metallic Nanostructures
	Metals
Shareable data infrastructure to feed computational tools and process models	Biomaterials
	Ceramics
	Electronic Materials
	Materials in/for Condensed Matter Physics
	Metallic Nanostructures
	Metals
	Other
	Photonic Materials
	Polymers
	Solid State and Materials Chemistry
How to go from new material prediction to new material synthesis, particularly in thin-film form, and integration into a microsystem.	Ceramics
	Electronic Materials
	Metallic Nanostructures
	Metals
Fully automated materials synthesis from solution chemistry	Ceramics
	Metallic Nanostructures
	Metals
	Other
	Solid State and Materials Chemistry
AI-ready data infrastructure. Rethink materials ontology and establish materials representation and database schema aimed for interoperability. Develop tools to automate data extraction and deposition process to handle multi-modal data and information. Plan for data infrastructure sustainability and fund, incentivize and reward the community.	
beyond state of the art for device performance and manufacturing processes	Electronic Materials
On-demand synthesis of bulk metallic and ceramic materials	
There is no existing, impactful, general purpose infrastructure. The status of ELNs and LIMS is primitive.	Biomaterials
	Polymers
Most approaches to AI/ML that are submitted to my program tend to lack the fundamental science and are more focused on high-throughput synthesis. While this can lead to discovery of new materials, the lack of scientific background limits the broader impact of the experiments to be applied to other classes of materials. At the same time, computational materials discovery has the power to identify new materials, but the lack of emphasis on synthesizability leads to a collection of hypothetical materials. More emphasis needs to be placed on finding synthetic routes, along with new materials.	Ceramics

Most of the capabilities in AMII seem to concentrate on discovering chemical space, often in materials that can be synthesized with wet chemistry or in very small quantities or in the class of soft materials, without taking into account the effect of processing/manufacturing, microstructure, and not in bulk dimensions relevant to industry (the smallest dimension is larger than a centimeter). We need more investment in high throughput hard materials fabrication/processing, microstructural control, defect control, and materials fabrication in bulk scales.	Materials in/for Condensed Matter Physics
	Metallic Nanostructures
	Metals
Integration with commercial Multiphysics and high length scale engineering models	Ceramics
	Electronic Materials
	Materials in/for Condensed Matter Physics
	Metallic Nanostructures
	Metals
	Photonic Materials
	Solid State and Materials Chemistry
I am eager to learn more about what capabilities are available in the AMII	Materials in/for Condensed Matter Physics
	Polymers
	Solid State and Materials Chemistry
'Valley of Death' between materials discovery and deployment.	Biomaterials
	Ceramics
	Electronic Materials
	Materials in/for Condensed Matter Physics
	Metallic Nanostructures
	Metals
	Photonic Materials
	Polymers
	Solid State and Materials Chemistry

From Registration Data – Suggested MGI Challenge Ideas and Themes

Advanced Materials Development:

- Tailored materials for specific applications like ion transport, gas separation, thermal management, and water purification.
- Development of materials free from rare earth elements, heavy metals, and other scarce resources.
- Focus on sustainable and recyclable materials, including alternatives to polyolefins and PFAS removal from groundwater.
- Emphasis on novel materials such as high-entropy alloys, superconductors, and quantum materials.

These specific themes highlight the diverse and targeted efforts in the advanced materials development space, focusing on sustainability, efficiency, and innovative applications across various fields. They also highlight the interdisciplinary nature of advanced materials development and underscore the various material classes involved in addressing these advanced technological and scientific challenges.

Selective Transport and Separation:

- **Ionic and Molecular Species Separation**: Development of materials with high selectivity ratios for ion transport, such as Li/Na separation. (Related materials: **Polymers**)
- **Gas Separations**: Materials designed for specific gas separation applications.
- PFAS **Removal**: Materials tailored for removing per- and polyfluoroalkyl substances (PFAS) from groundwater. (Related materials: **Biomaterials, Polymers**)

Thermal Management:

- **Materials for Thermal Management**: Development of materials aimed at improving thermal management, particularly addressing urban heat impacts. (Related materials: **Polymers**)

Sustainable and Alternative Materials:

- **Earth-Abundant Alternatives**: Finding substitutes for rare earth elements used in magnetic materials.
- **Heavy Metal-Free Optical Materials**: Developing optical materials that do not rely on heavy metals, such as certain perovskites and quantum dots (QDs). (Related materials: **Ceramics, Polymers**)
- PGE**-Free Catalysts**: Creating catalysts that do not contain platinum group elements (PGE).
- **Low-Energy Transistors**: Developing transistors that require minimal energy for both production and operation.

- **Recyclable/Upcyclable Polyolefin Alternatives**: Discovery of materials that are recyclable or upcyclable as alternatives to conventional polyolefins. (Related materials: **Polymers**)

Water Harvesting and Security:

- **Chemically Specific Materials**: Development of materials specifically for water harvesting, filtering, and ensuring water security. (Related materials: **Polymers**)

Innovative Synthesis Methods:

- **Physics-Based Models for Synthesis**: Enhancing models for chemical synthesis methods like sol-gel, solid state reaction, and molten salt. (Related materials: **Ceramics**)
- **Physical Deposition Techniques**: Advanced physical deposition methods such as Atomic Layer Deposition (ALD), Molecular Beam Epitaxy (MBE), and Physical Vapor Deposition (PVD). (Related materials: **Ceramics**)

Record-Setting Materials:

- **High-Temperature Materials**: Autonomous development of materials with extremely high melting points (e.g., refractory materials like HfCN). (Related materials: **Ceramics, Metallic Nanostructures, Metals**)
- **High-Ductility Alloys**: Creating high entropy alloys (HEAs) with exceptional ductility at room temperature. (Related materials: **Metallic Nanostructures, Metals**)

Autonomous and AI-Driven Development:

- AI**-Driven Tools for Data Mining and Models**: Utilization of AI to accelerate the co-design of materials for specific applications. (Related materials: **Biomaterials, Ceramics, Electronic Materials, Materials in/for Condensed Matter Physics, Metallic Nanostructures, Metals, Photonic Materials, Polymers, Solid State and Materials Chemistry**)
- **Fully Autonomous Labs**: Development of interoperable, autonomous laboratories for automated experimentation and synthesis. (Related materials: **Electronic Materials, Metallic Nanostructures, Metals, Photonic Materials, Polymers, Solid State and Materials Chemistry**)
- **Digital Twins and Virtual Environments**: Use of digital twins to simulate and optimize material properties and processes. (Related materials: **Ceramics, Electronic Materials, Metallic Nanostructures, Metals**)

Collaborative and Data-Driven Research:

- **Interconnected Ecosystems for Energy Materials**: Integrating various experimental and computational resources for collaborative research in energy materials. (Related materials: **Electronic Materials, Materials in/for Condensed Matter Physics, Metallic Nanostructures, Metals, Polymers, Solid State and Materials Chemistry**)

- **Community Datasets and** FAIR **Metrics**: Development of interoperable community datasets with metrics on FAIR (Findable, Accessible, Interoperable, Reusable) maturity. (Related materials: **Metallic Nanostructures, Metals**)
- **Curated Datasets and Standardized Data Sharing**: Creating and sharing standardized datasets for machine learning model validation in material science. (Related materials: **Ceramics, Electronic Materials, Metallic Nanostructures, Metals**)

Workforce Development and Education:

- **Targets for Education and Workforce Development**: Measuring and valuing the impact of materials research projects on education and workforce readiness. (Related materials: **Electronic Materials, Materials in/for Condensed Matter Physics, Metallic Nanostructures, Metals, Photonic Materials**)

Specific Applications and Goals:

- **Water Purification**: Developing materials to remove over 99% of microplastics, heavy metals, and other contaminants from water. (Related materials: **Ceramics, Electronic Materials, Materials in/for Condensed Matter Physics, Metallic Nanostructures, Metals, Photonic Materials, Solid State and Materials Chemistry**)
- **Energy Storage**: Creating new energy storage devices with a 25% increase in capacity. (Related materials: **Electronic Materials, Metallic Nanostructures, Metals, Polymers, Solid State and Materials Chemistry**)
- **Carbon Neutrality and Sustainability**: Innovations in materials that contribute to carbon neutrality and sustainability. (Related materials: **Ceramics, Metallic Nanostructures, Metals, Polymers, Solid State and Materials Chemistry**)

Data Management and Sharing:

- Establishment of databases for unsuccessful experiments and community datasets with standardized metrics.
- Development of data policies to facilitate integration and sharing across various platforms and instruments.
- Promotion of FAIR (Findable, Accessible, Interoperable, Reusable) data principles and creating a knowledge network to enhance AI-guided experiments.

Autonomous and AI-driven Research:

- Development of autonomous labs that support hypothesis formulation, experiment management, and synthesis automation.
- Utilization of AI tools for data mining, process modeling, and accelerating material co-design.

- Integration of digital twins for materials development and real-time metrology advancements.
- Autonomous development of high-performance materials like refractory materials and high-ductility alloys.

Collaboration and Infrastructure:

- Creation of interconnected ecosystems integrating experimental and computational resources from multiple institutions.
- Fostering collaboration between data scientists and domain experts to enhance material development using machine learning.
- Development of general-purpose tools for material fabrication and validation, and enhancing mechanistic understanding for digital twins.

Workforce Development and Education:

- Emphasis on workforce-related aspects like demand for specific skill sets and preparation.
- Measurement of how project outputs are used in educational settings and their impact on workforce development.
- Proposals for certification processes similar to ACS standards for practical experience in automation and material science.

National Security and Economic Competitiveness:

- Focus on materials and technologies that ensure national security and economic competitiveness in energy, aerospace, health, and defense sectors.
- Emphasis on reducing manufacturing costs and increasing manufacturing speed to enhance sustainability and supply chain resilience.
- Development of next-generation semiconductor and advanced packaging technologies for economic competitiveness.

Sustainability and Environmental Impact:

- Development of materials and technologies for carbon neutrality and efficient energy storage.
- Emphasis on water security through advanced purification methods and the creation of low-cost detection and remediation tools for heavy metals.
- Addressing sustainability in manufacturing and promoting lean manufacturing practices.

Metrics and Targets:

- Establishing specific targets for material performance, discovery rates, and the functionality of new materials.

- Developing quantitative measures for the impact of autonomous laboratories, FAIR data realization, and workforce development impacts.
- Setting goals for reducing development time and demonstrating co-design workflows for new materials and manufacturing methods.

RAW DATA

We are looking to define numerous, specific, measurable targets that are both challenging and achievable in the next 2-5 years. We plan to solicit additional input to these specific targets during this June workshop and at the following MGI PI meeting (July 30-31, 2024). Here, you may contribute ideas of specific, measurable targets to address a challenge in areas such as, but not limited to, materials for Water Security, Human Health and Welfare, Energy, Economic Competitiveness, or National Security.	Materials class the capability addresses (more than one possible) - Selected Choice
- Design and manufacture of materials with specific tailored selectivity for transport of ions and molecular species: e.g. selectivity ratios > 10 for Li/Na separation; One can make similar specifications for gas separations, and PFAS removal from groundwater - Materials for thermal management, particularly given the rising impact of urban heat.	Biomaterials Polymers
- physics based models for chemical synthesis (sol-gel, solid state reaction, molten salt, etc., immature) and physical deposition (ALD, MBE, PVD, etc., mature). - center for repeatability, analogous to NREL's PV efficiency measurements - database of unsuccessful experiments - Find earth abundant alternatives for rare earth magnetics - heavy metal free optical materials (perovskites, QDs, etc.) - PGE free catalysts - low energy, both production and operation, transistors	Ceramics
AI driven tools for data mining, development of data storage and formats, and for process models to accelerate the co-design of materials that can be integrated for specific applications.	Biomaterials Ceramics Electronic Materials Materials in/for Condensed Matter Physics Metallic Nanostructures Metals Other Photonic Materials Polymers Solid State and Materials Chemistry
Carbon Neutrality	Ceramics Metallic Nanostructures Metals Polymers

	Solid State and Materials Chemistry
Chemically specific materials for water harvesting, filtering, and security. Discovery of recyclable/upcyclable alternatives to polyolefins.	Polymers
Data policies facilitating integration of data from variety of instruments	Polymers
Develop a culture and standards around data sharing and creation of a knowledge network to capture all the relevant information, which can also help AI guide experiments, or limit experiments, etc.	Biomaterials Electronic Materials Solid State and Materials Chemistry
Develop an interconnected ecosystem specifically designed to enhance energy materials research by seamlessly integrating at least 5 different types of experimental and computational resources (such as databases, software tools, spectroscopy, microscopy, and high-performance computing facilities) from at least 3 different research institutions. This ecosystem will enable efficient data sharing, collaborative research, and advanced analysis specific to energy materials. The development will achieve initial resource integration tailored for energy materials research within 3 years, and fully complete the ecosystem, with comprehensive documentation and user training materials within 5 years.	Electronic Materials Materials in/for Condensed Matter Physics Metallic Nanostructures Metals Polymers Solid State and Materials Chemistry
Development of community datasets that interoperate (for any challenge) with metrics on FAIR maturity; AI-readiness maturity; tools with community agreed interoperable formats; full API access. (Full API access is critical but we still get stuck creating GUIs or web versions so people can see the tool but projects need to be focused on the API) We need to make specific targets for workforce development/education. Measure how a project's output is being used in courses at colleges and universities or how they contribute to that; and value that.	Metallic Nanostructures Metals
Developments should provide solutions to create and interconnect fully autonomous labs that are interoperable. To achieve this goal, solutions must be built upon an open architecture to prevent proprietary solutions. Autonomous capabilities must support scientist formulate hypothesis, setup and manage experiments, automate/optimize both synthesis and characterization, and manage next steps based on previous experimental workflows. Solutions must provide flexible autonomous solutions for the entire ooda loop that may or may not require human intervention.	Electronic Materials Metallic Nanostructures Metals Photonic Materials Polymers Solid State and Materials Chemistry
DoD/DOE - Autonomous development of world record refractory material (Tmp > 4000C current record holder - HfCN) DOE - Autonomous development of world record heat-exchanger efficiency DoD/DOE - Autonomous development of novel ultrahigh ductility high entropy alloys (HEAs) with room temperature ductility > 100% (Cantor alloy exhibits ~ 71% at RT)	Ceramics Metallic Nanostructures Metals
Energy - Autonomous Isotope Production is focus area of interest.	
Establish one national facility for automated / autonomous experimentation in synthesis, including "cloud lab" model to enable broad access, especially to universities from under-resourced communities. Applications of this facility could span Human Health and Welfare, Energy, etc.	
	Ceramics

I am clearly biased, but I think the priority should be given to Energy, Health and Food. It is not realistic to define matrix for economic competitiveness and national security :)	Solid State and Materials Chemistry
Invest in developing general purpose tools and methodologies to fabricate new materials and validate the predicted and desired material and device properties, for example: ALD, ALE, PVD, pulsed laser PVD, CVD, epi. Focus on new material synthesis, scaling and integration as opposed to new material identification and property prediction, which has advanced more rapidly recently. Curated Datasets: Creating standardized datasets can provide a foundation for developing and validating ML models in material science. Perform round robin experiments to provide error estimation, validate critical meta data, and confirm reproducibility. For example: standardized physical test structures and short-loop electrical test devices. Enhance Metrology: Advancements in real-time, in situ metrology are needed to provide the data required for accurate ML models and digital twins. Foster Collaboration: Collaboration between data scientists and domain experts is essential for effective augmentation of materials development using machine learning. Domain experts are needed to set strategy, define initial DOEs, limit parameter ranges, and down-select potential solutions for subsequent exploration and exploitation. Data scientists are needed to set machine learning strategies and determine the most appropriate machine learning algorithms. Create a "tiger team" that specializes in human-machine collaboration using virtual environments and advanced algorithms and embed them in programs that entail development and deployment of new materials. For example, embedding the human-machine collaboration tiger team into the NGMM (next generation microelectronics manuf) heterogeneous integration program would likely enhance the probability of success while simultaneously honing human-machine collaboration methods and skills. Address IP and Data Sharing: Developing frameworks for data sharing while protecting intellectual property can facilitate collaborative research and development. Invest in Mechanistic Understanding: To the extent virtual environment creation for digital twins is hampered by lack of mechanistic understanding and/or unknown physical parameter values, a coordinated effort to develop mechanistic models and measure pertinent parameters is of paramount importance. Such models and data are needed to create useful digital twins and physics inspired machine learning algorithms. Utilize autonomous experimental design and execution to save time and money and minimize risk of human-induced error and variation. Leverage Digital Twins: Develop and utilize digital twins to accelerate materials development, reduce time and costs, and provide actionable	Ceramics Electronic Materials Metallic Nanostructures Metals

insights for decision-making. Recognize that developing digital twins is a journey and that much value can be garnered from virtual environments that are not yet precisely predictive. The nascent NIST manufacturing institute focused on digital twins for semi manufacturing (front-end and adv pkg) provides a unique opportunity for transferring methodologies and techniques to new materials synthesis digital twins. Monitor LLM progress continuously to avoid surprises by systematically testing them like you test a student: Define standardized tests to enable consistent benchmarking.	
materials discovery that meets performance and emerging sustainability requirements	Electronic Materials
Megaton Synthesis of Carbon Nanotubes from Methane Pyrolysis	Biomaterials Ceramics Electronic Materials Materials in/for Condensed Matter Physics Metallic Nanostructures Metals Photonic Materials Polymers Solid State and Materials Chemistry
Metrics on the functionality of new materials Metrics on materials discovery in lab vs. in computer	
National Security to Secure Economic Competitiveness across Energy, Aerospace, Heath, and Defense to Support a Highly Innovative Economic Profitable Industries	Ceramics Electronic Materials Materials in/for Condensed Matter Physics Metallic Nanostructures Metals Photonic Materials Solid State and Materials Chemistry
Next Generation Semiconductor and Advanced Packaging Technologies for Economic Competitiveness and National Security	
Novel 'enabling' materials that can lead to step changes in many energy technologies that are plateaued for several decades (high temperature alloys, superconductors, magnetic materials, ...).	
-One major target should be the rate at which new materials are proposed and experimentally explored. This can include the synthesis and testing of key materials of interest (e.g. LK99), or the ingestion of new materials hypotheses	Polymers Solid State and Materials Chemistry

to be explored more generally. -There are growing efforts across the research enterprise to construct something like a scientific large language model. Such a system will require vast experimental data that can constitute training data with associated rich metadata. From this perspective, the raw volume of experimental materials data is a crucial metric.	
Quantitative increases in FAIR realization measures for materials data: number of datasets FOUND, ACCESSED, INTEROPERATED, REUSED -- all increased by factors of 10 or more. Number of consumers of data from public materials data repositories increased by x10. Number of publications generated from autonomous laboratories increased by x100.	
Quantum materials should be a part of this list.	Biomaterials Polymers
Re: Water Security & Human Health—I think there is an opportunity to create low-cost SDLs ("frugal twins") to do electrochemical detection and remediation for heavy metals in water and soil, which could serve a dual role of advancing the challenge area and as a teaching tool. Specific targets for this could include: - Community access (how many citizen advocacy groups / citizen scientists have adopted). Measurable targets might include hits on Thingiverse, Tindie, etc...or just number of devices in the wild. - Measuring health impacts (although probably beyond the scope of this program, per se) - Measuring workforce development impacts (# of students exposed to these ideas in introductory classes, advanced classes, etc.). A measurable target could be # of universities with specific capabilities in automation for science, etc. There is an analogy to how the American Chemical Society says that ACS-certified programs must have certain instrumentation available, and ACS-certified bachelors degrees must have certain numbers of hours of practical experience with different methods. A dream would be to have an analogous certification process and requirements of minimal skill levels. Re: Economic Competitiveness: Certainly industry can define this in many ways. As an educator, I would focus on workforce related aspects. What is the demand (for specific skillsets, preparation, experiences) and are we meeting that demand? A dashboard and long-range projects would be helpful in the slow process of creating academic programs. Having this as part of a national plan would help justify it to administrators.	Other
Reduce cost of manufacturing by 10x and increase speed of manufacturing 10x to start.	
	Electronic Materials

sustainability, critically lean manufacturing, national security, supply chain resilience, energy production and efficiency	Materials in/for Condensed Matter Physics Metallic Nanostructures Metals Photonic Materials
Target: (1) Reduce the time to develop and deploy a new qualified AM metal alloy in a high-consequence product to less than 6 months. (2) Demonstrate a "co-design" workflow that enables the simultaneous holistic optimization of i) product geometry, ii) manufacturing method, and iii) material.	Metallic Nanostructures Metals
Water Security National Security Food Security	Ceramics Electronic Materials Materials in/for Condensed Matter Physics Metallic Nanostructures Metals Photonic Materials Solid State and Materials Chemistry
Water: Improve water purification efficiency to remove over 99% of microplastics, heavy metals, and other contaminants. Human Health and Welfare: Develop automated approaches to design and synthesize new drugs to prevent future pandemics. Energy: Develop new energy storage devices with approximately a 25% increase in capacity compared to current devices, ensuring commercialization potential.	

E. Abbreviation List

2DCC	2D Crystal Consortium - An NSF Materials Innovation Platform
3D	3-dimensional
4D	4-dimensional
ACS	American Chemical Society
ACT3	Air Force Research Laboratory Autonomy Capability Team
AE	Autonomous Experimentation
AFM	Atomic Force Microscopy
AI	Artificial Intelligence
ALD	Atomic Layer Deposition
AM	Additive Manufacturing
AMANDA	Autonomous Materials and Device Application Platform (www.amanda-platform.com)
AMDD	Accelerated Materials Design and Discovery
AMII	Autonomous Materials Innovation Infrastructure
API	Application Programming Interface
ARES	Air Force Research Laboratory Autonomous Research System
ARM	Autonomous Robotics Metallurgist
ASTM	American Society for Testing and Materials
ASTRAL	Automated powder synthesis with AI-assisted computational materials design
AT SCALE	Adaptive Tunability for Synthesis and Control via Autonomous Learning on Edge
BioPACIFIC MIP	BioPolymers, Automated Cellular Infrastructure, Flow, and Integrated Chemistry Materials Innovation Platform
BIRDSHOT	Batch-wise Improvement in Reduced Materials Design Space using a Holistic Optimization Technique
CAMINO	Center for Advanced Manufacturing Innovation
CHIMAD	Center for Hierarchical Materials Design
CLI	Command-Line Interface
CRADAS	Cooperative Research and Development Agreements
CRIPT	Community Resource for Innovation in Polymer Technology
CVD	Chemical Vapor Deposition
DFT	Density Functional Theory
DMREF	Designing Materials to Revolutionize and Engineer our Futures
DREAM	Data-driven Reinvigorated Advanced Membrane Discovery Platform
EELS	Electron Energy Loss Spectroscopy
ELN	Electronic Lab Notebooks
EM	Electron Microscopy
EU	European Union
FAIR	Findable, Accessible, Interoperable, Reusable
FSM	Functional Soft Matter
FTO	Freedom To Operate

GEMD	Graphical Expression of Materials Data
Georgia AIM	Georgia Artificial Intelligence in Manufacturing
GIWAXS	Grazing Incidence Wide Angle Xray Scattering
GPT	Generative Pre-trained Performer
GUI	Graphical User Interface
HAMMER	Hybrid Autonomous Manufacturing, Moving from Evolution to Revolution
HEA	High-Entropy Alloy
HfCN	Hafnium Carbonitride
HPC	High Performance Computing
HTMDEC	High-Throughput Materials Discovery for Extreme Conditions
HT-READ	High-Throughput Rapid Experimental Alloy Development
IACMI	Institute for Advanced Composites Manufacturing Innovation
ICME	Integrated Computational Materials Engineering
IEEE	Institute of Electrical and Electronics Engineers
IMQCAM	Institute for Model-Based Qualification & Certification of Additive Manufacturing
INTERSECT	Interconnected Science Ecosystem
IP	Intellectual Property
ISO	International Organization for Standardization
IT	Information Technology
IWG	Interagency Working Group
LBL	Lawrence Berkeley Laboratory
LC	Liquid Chromatography
LCMS	Liquid Chromatography-Mass Spectrometry
LDRD	Laboratory Directed Research and Development
LIMS	Laboratory Information Management System
LK99	Lee-Kim 1999 research
LLM	Large Language Model
MAP	Materials Acceleration Platform
MBE	Molecular Beam Epitaxy
MCP	Materials Characterization and Processing Center
MDRI	Materials Discovery and Research Institute
MFS	Molecular Foundations for Sustainability
MGI	Materials Genome Initiative
MI	Materials Intelligence
MIDA	N-methylimminodiacetic acid
MII	Materials Innovation Infrastructure
MIP	Materials Innovation Platform
ML	Machine Learning
MPEA	Multi-Principal Element Alloy
MRL	Manufacturing Readiness Level
MRSEC	Materials Research Science and Engineering Center
MS	Mass Spectrometry

MSI	Minority Serving Institutions
MURI	Multidisciplinary University Research Initiative
NaFI	National Facilities and Instrumentation
NCSA	National Center for Supercomputing Applications
NDA	Non-Disclosure Agreement
NGMM	Next-Generation Microelectronics Manufacturing
NREL	National Renewable Energy Laboratory
NRT	NSF Research Traineeship Program
OQMD	The Open Quantum Materials Database
OS	Operating System
P2P	Peer-to-Peer
PARADIM	Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials
PDFF	Pair Distribution Function FITting Program
PDFitc	PDF in the Cloud
PFAS	Per- and Polyfluoroalkyl Substances
PGE	Platinum Group Elements
PI	Principal Investigator
PLC	Programmable Logic Controller
PLD	Pulsed Laser Deposition
PV	Photovoltaic
PVD	Physical Vapor Deposition
PXRD	Powder X-Ray Diffraction
QD	Quantum Dot
RAPID	Rapid Advancement in Process Intensification Deployment
RHEED	Reflection High-Energy Electron Diffraction
RIDE	Rational Integrated Design of Energetics
RT	Room Temperature
SAXS	Small-Angle X-Ray Scattering
SD2	Synergistic Discovery and Design
SDK	Software Development Kit
SDL	Self-Driving Laboratory
SEM	Scanning Electron Microscopy
SME	Subject Matter Expert
SNL	Sandia National Laboratories
SPEED	Sustainable Polymers Enabled by Emerging Data Analytics
STEM	Science, Technology, Engineering, and Mathematics
STRI	Space Technology Research Institutes
SURGE	Structure Uniquely Resolved to Guarantee Endurance
T-BRSC	Tri-Service Biotechnology for a Resilient Supply Chain (T-BRSC) program
TIDA	Tetramethyl-N-methyliminodiacetic acid
TIP	Technology, Innovation, and Partnership Directorate (NSF)
TRI	Toyota Research Institute

TRIXS	Toyota Research Institute X-ray Spectroscopy
TRL	Technology Readiness Level
ULRI	Underwriter Laboratories Research Institutes
ULTIMATE	Ultrahigh Temperature Impervious Materials Advancing Turbine Efficiency
URL	Uniform Resource Locator
VIPERLAB	Fully Connected Virtual and Physical Perovskite Photovoltaic LAB
WH	White House
XAS	X-ray Absorption Spectroscopy

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