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Economic Analysis of National Needs for Technology Infrastructure to Support the Materials Genome Initiative

Final Report

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The authors are responsible for all remaining mistakes and misunderstandings.

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Executive Summary

The aim of the Materials Genome Initiative is to enable U.S. industry to develop and deploy advanced materials more quickly and efficiently. NIST is a key player in supporting the MGI approach and the development of a national Materials Innovation Infrastructure. This report presents estimates of potential impacts attributable to improved infrastructure of between $123 billion and $270 billion per year.

The Materials Genome Initiative (MGI) is a strategic effort spanning multiple federal agencies to promote a globally competitive U.S. manufacturing sector by addressing important gaps in the Materials Innovation Infrastructure. Its aim is to enable U.S. companies to more rapidly and efficiently develop and deploy advanced materials, with applications ranging from consumer goods like the Apple Watch, to renewable energy generation and energy storage, to supercomputing and national defense.

The National Institute of Standards and Technology (NIST) is supporting the MGI through efforts to establish materials data-exchange and model-exchange protocols; the means to ensure the quality of materials data and models; and new methods, metrologies, and capabilities needed for accelerated materials development. Additionally, through its integration of these activities, NIST is working to test and disseminate elements of an improved Materials Innovation Infrastructure to stakeholders in other national laboratories, universities, and U.S. industry.

This report, commissioned by NIST, presents analysis of perspectives and opinions of U.S. manufacturers and other industry experts on their needs for new technological infrastructure supporting advanced materials innovation and the potential economic impacts of meeting those needs.

Estimated Value of Potential Impacts. The report presents estimates of the potential economic benefit of an improved Materials Innovation Infrastructure of between $123 billion and $270 billion per year, based on structured interviews with more than 100 industry experts.

Industry Needs Assessment. Six identified areas of industry need provided the common basis for the expert informant interviews (Table ES-1). All six areas of need were rated “very” or “critically” important by at least 60% of respondents. Five of the six needs were rated “very” or “prohibitively” difficult to address solely through private investment by at least 50% of respondents (Figures ES-1 and ES-2).

Table ES-1. Technology Infrastructure Needs for Advanced Materials Innovation

Industry Need	Examples of Infrastructure Technology to Address Need	Potential Impacts
Access to High-Quality Data Nonproprietary experimental data, computational data, metadata, and software code	▪ Fundamental materials data ▪ Data standardization and curation ▪ Models underpinning accurate and repeatable material measurement	▪ More easily leverage prior research with less duplication of effort ▪ Enable greater reliance on more efficient computational approaches ▪ Multiply the value of every other element of a Materials Innovation Infrastructure
Collaborative Networks Efficient means of sharing materials information (e.g., along a supply chain, among research collaborators)	▪ Methods for capturing, characterizing, and sharing materials data in structured formats ▪ Communication standards and translators ("MT Connect for material measurement equipment")	▪ Align academic and public-sector research to industry-relevant challenges ▪ Integrate experimental measurement and computational modeling to improve model fidelity and overall utility ▪ Realize network externalities
Material Design Methods Enabling application of a systems approach to materials development, from discovery and design all the way through to deployment	▪ Models, simulations, and metrologies for advanced materials design and means of integrating tools with one another. ▪ Machine learning tools	▪ Enable more targeted searches of design space for promising candidate materials ▪ Enable purposeful design of materials to meet specific performance requirements for targeted applications ▪ Target significant performance improvements with more-novel materials, as opposed to seeking smaller incremental improvements by refining known materials ▪ Enable co-design of new materials and new product applications
Production & Scale-Up Model-based alternatives to expensive physical testing, trial and error–based approaches Faster, cost-effective means of producing advanced materials at pilot and full scales	▪ Multiscale modeling frameworks (integrating macroscopic process models with microscopic materials simulation) ▪ Process technology platforms (e.g., cold sintering, additive manufacturing, roll-to-roll printing, directed self-assembly)	▪ Reduce trial and error when scaling up (from lab scale to pilot scale, from pilot scale to production scale) ▪ Allow consideration of production-scale processes to be integrated into the initial design process ▪ Overcome the "Valley of Death" between lab scale and production scale: pilot-scale manufacturing services and facilities are underprovided by the market

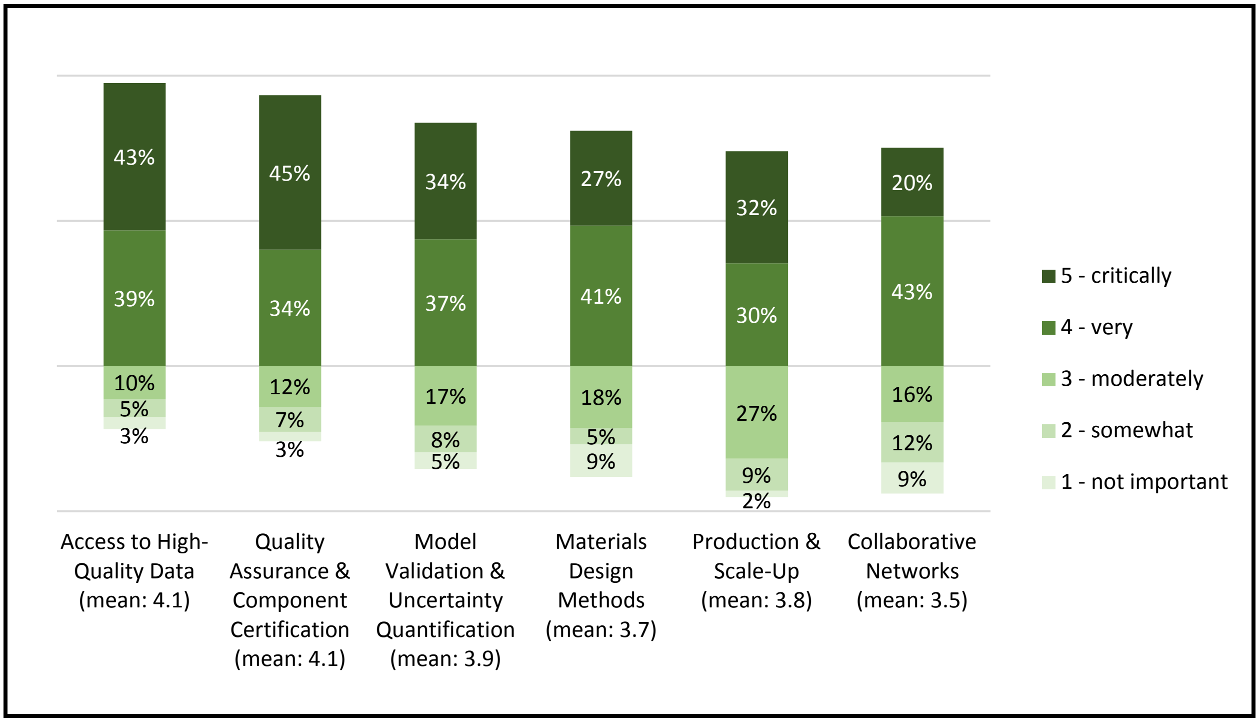
(continued)

Table ES-1. Technology Infrastructure Needs for Advanced Materials Innovation (continued)

Industry Need	Examples of Infrastructure Technology to Address Need	Potential Impacts
Quality Assurance, Quality Control & Component Certification Ability to model, predict, and control formation of defects Ability to forecast manufacturing variation	▪ Performance metrics (benchmarks, reference data, testbeds to characterize performance of systems and components) ▪ Process control tools (test protocols, objective scientific and engineering data, reference databases)	▪ Reduce the cost of controlling and verifying the performance attributes of materials—and components and products embodying those materials ▪ Reduce the risk of large costs incurred if defects are not detected and lead to product failures in use (e.g., lithium-ion battery fires)
Model Validation & Uncertainty Quantification Basis for trust and acceptance of computational models Basis for objective decision-making regarding reliance on computational analysis and simulation at a business level	▪ Generally accepted and easily applied methods for uncertainty quantification for both experimental and computational data ▪ Validation of analytical methods and procedures, emphasizing industrially relevant systems, comparing predicted and measured properties from multiple sources	▪ Enhance the utility of computational approaches from an engineering perspective ▪ Enable rational decision-making regarding computational approaches from a business perspective ▪ Advance industry's reliance on computational approaches in situations where they can save cost and add value

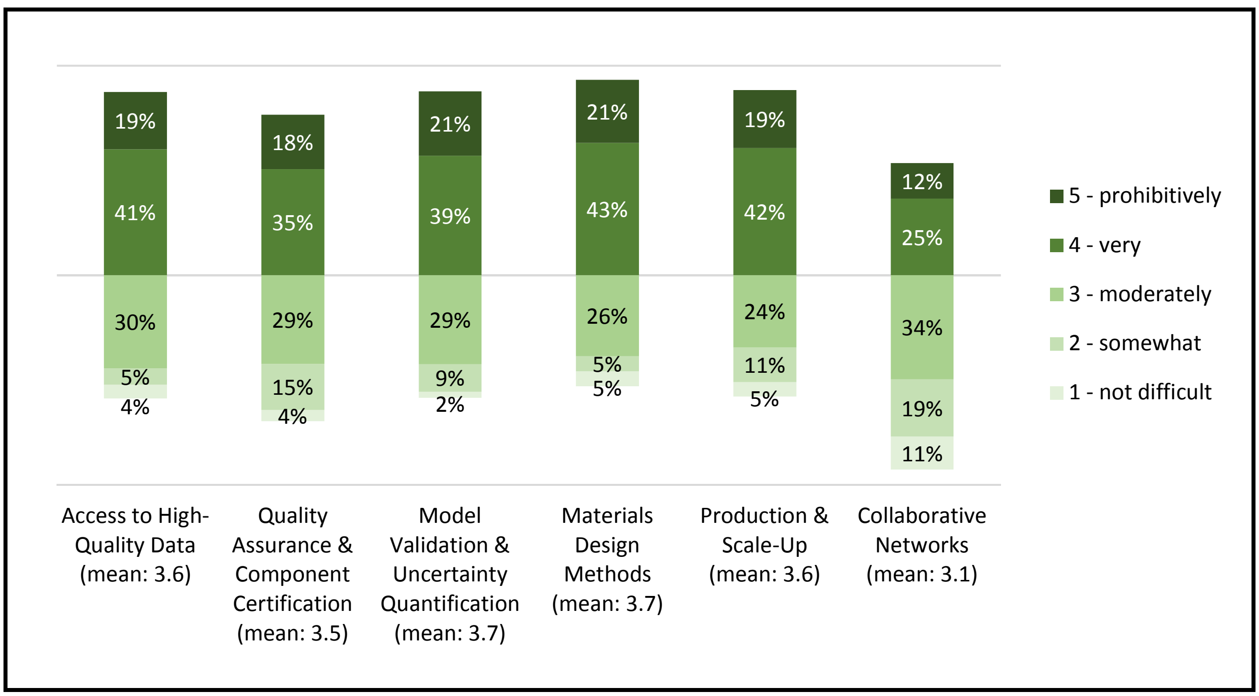
Access to high-quality data emerged as a linchpin of a Materials Innovation Infrastructure. Industry experts stressed the strong complementarity among the six areas of need and the consequent overlap among the types of infrastructure and potential impacts. But the complementarity was not completely symmetrical: access to high-quality data was perceived to play a pivotal role, being a prerequisite for model validation and uncertainty quantification and for the productive application of machine learning, modeling and simulation, and other elements of an envisioned Materials Innovation Infrastructure. The upshot is that addressing industry's need for high-quality, nonproprietary digital data can be expected to lower the barriers—faced by both the public and the private sectors—to addressing the other areas of need.

Figure ES-1. Interviewees' Rating of Importance of Technology Infrastructure Needs



Note: Percentages shown reflect the distribution of ratings. Average ratings are given in parentheses below each area of industry need.

Figure ES-2. Interviewees' Rating of Difficulty of Meeting Needs through Private Investment



Note: Percentages shown reflect the distribution of ratings. Average ratings are given in parentheses below each area of industry need.

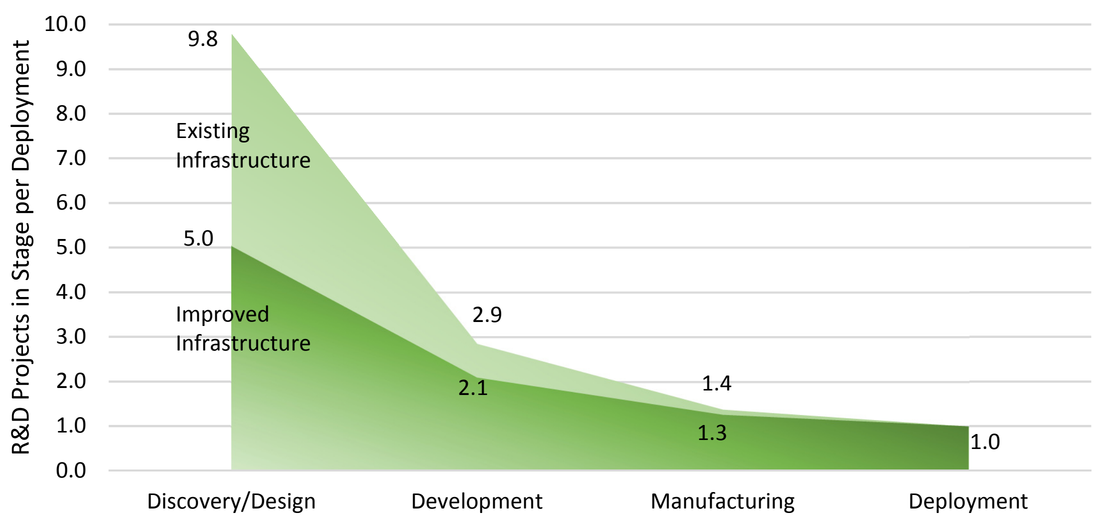
Estimated potential impacts include the elimination of almost half of R&D project attrition and a 35% acceleration of R&D projects to market. Overall, potential impacts achieve a 71% improvement in R&D efficiency, worth an estimated $39 billion to $69 billion per year to U.S. companies.

Potential Impact on Risk. Companies developing new materials face the risk that a research and development (R&D) project will fail to reach deployment and generate investment returns. We estimate that the total risk could be reduced by almost half with improved infrastructure: for each new material deployed, only 5 R&D projects would need to enter the R&D pipeline at the discovery/design stage, down from an estimated 9.8 in the current environment (Figure ES-3).

Potential Impact on Time to Market. We estimate that development of a new material takes on average more than 10 years and that an average acceleration of 3.5 years could be possible with improved infrastructure (Figure ES-4).

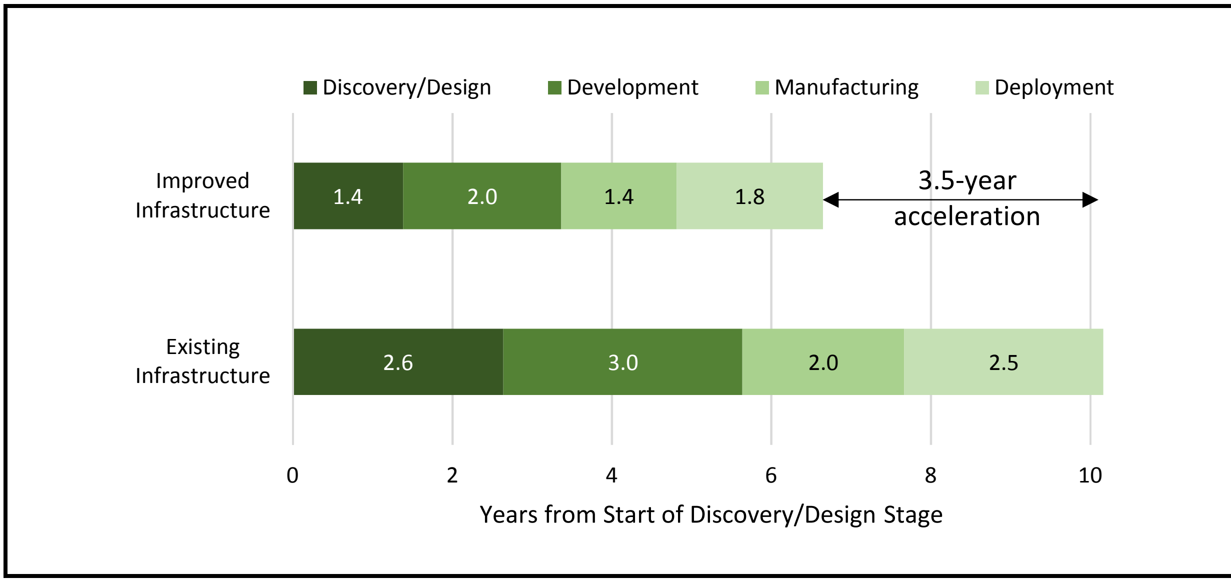
Potential Impact on Relative Costs per Project per Year. We estimate that improved infrastructure has the potential to reduce relative costs by an average of 25% in the discovery/design stage, 45% in the development stage, 48% in the manufacturing stage, and 28% in the deployment stage (Figure ES-5).

Figure ES-3. Potential Impact on Risk



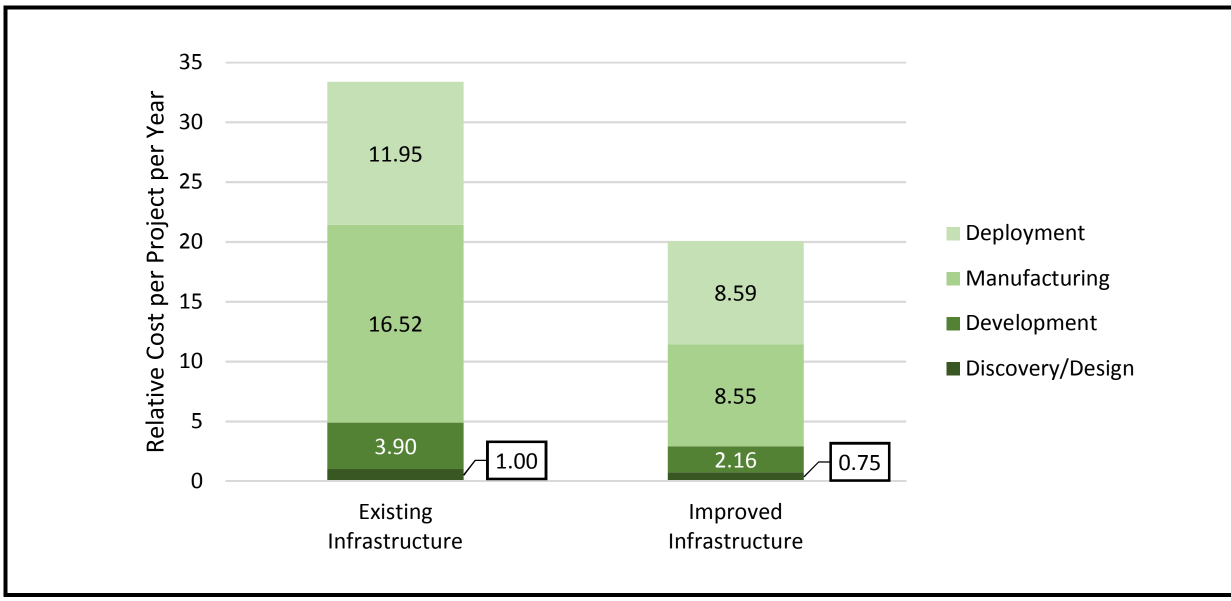
Note: With improved infrastructure, materials R&D projects are more likely to transition to successive stages. The number of projects that must enter the R&D pipeline at the discovery/design stage for each one that successfully reaches the final deployment stage improves from 9.8 to 5.0 (a 20% chance of deployment with improved infrastructure versus a 10% chance currently). The number of projects that must enter the development stage for every one that reaches the deployment stage improves from 2.9 to 2.1 (a 48% chance of deployment, conditional on reaching the development stage, with improved infrastructure versus a 35% chance currently).

Figure ES-4. Potential Impact on Time to Market



Note: U.S. manufacturers would be able to bring new materials to market faster with the benefit of improved infrastructure. Average time to market is estimated to be 6.6 years with improved infrastructure compared with 10.2 years in the current environment.

Figure ES-5. Potential Impact on Relative R&D Cost per Project per Year



Note: Cost per project, per year, in the discovery/design stage in the current environment was normalized at 1.0. In the current environment, manufacturing and deployment stages are estimated to be, respectively, roughly four times and three times more cost-intensive than the development stage, which is, in turn, roughly four times more cost-intensive than the discovery/design stage. Improved infrastructure is estimated to reduce relative costs by an average of 25% in the discovery/design stage, 45% in the development stage, 48% in the manufacturing stage, and 28% in the deployment stage.

Overall, estimated potential impacts of an improved Materials Innovation Infrastructure achieve a 71% improvement in R&D

efficiency, worth an estimated $39 billion to $69 billion per year to U.S. companies that comprise the new materials supply chain (Table ES-2).[1]

Beyond increasing R&D efficiency, improved infrastructure could also create new opportunities for companies to improve product quality and performance, expand product offerings, and enter new markets.

Potential Impacts on Product Quality and Performance. The potential benefits of an improved Materials Innovation Infrastructure do not stop at raising R&D efficiency. The improved infrastructure could also enable companies to undertake R&D projects they would not otherwise have done, leverage that R&D to commercialize improved products and new product lines, and expand into new markets. Not only would the expected R&D cost be lower for a given R&D result, the anticipated R&D result would also be superior.

One way in which this could happen is by enabling companies to incorporate new materials into the product design process earlier, so that new product applications take full advantage of new materials' capabilities. Going even further, computational materials design methods, fed with high-quality, nonproprietary digital data, could enable co-design of new materials and new product applications.

Table ES-2. Potential Economic Impact Estimates (Millions of 2013 U.S. Dollars Per Year)

Type of Potential Impact	Point Estimate	95% Confidence Interval
R&D Efficiency	56,421	(38,846, 68,836)
Improved R&D Outcomes	151,447	(82,515, 203,036)
Total	**207,869**	**(123,229, 270,047)**

Note: Potential R&D efficiency impact estimates are based on interview-based estimated impacts to the R&D process, summarized in Figures ES-3, ES-4, and ES-5, combined with industry R&D expenditure data (National Science Foundation, 2016) and interview-based estimates of the fraction of that expenditure related to developing new materials. Estimates of the value of improved R&D outcomes were also interview-based. Confidence intervals were calculated based on the variability of industry experts' responses to interview questions, using a bootstrap approach described in the report. The larger confidence interval for improved R&D outcomes (80% of the point estimate compared with 53% for R&D efficiency) reflects greater variability among experts' opinions and therefore greater uncertainty in the estimate. Point estimates of R&D efficiency and improved R&D outcomes impacts add to the total (the difference of 1 is due to rounding error). Confidence intervals cannot be added because the sources of uncertainty for the two types of potential impact are different and not perfectly correlated; the probability that both estimates (R&D efficiency and improved R&D outcomes) fall outside their respective confidence intervals is lower than the probability that either one does so.

[1] The estimated 71% improvement in R&D efficiency is the percentage reduction in average R&D investment cost per new material deployed. The range of $39 billion to $69 billion per year in potential impacts represents between 15% and 25% of R&D investment in the industries considered.

We estimate the value of these additional benefits to be roughly 2 to 3 times the value of potential R&D efficiency impacts, or between 4% and 9% of the annual value added for the industries considered (i.e., 4% to 9% of these industries' contribution to U.S. gross domestic product). Altogether, the potential economic benefits of an improved Materials Innovation Infrastructure are estimated to be worth between $123 billion and $270 billion per year (Table ES-2).

Public investment is needed to create the infrastructure, thereby spurring the private-sector investments that will realize the benefits.

Public investment is needed to create a Materials Innovation Infrastructure. To explain the difficulty of addressing infrastructure needs solely through private investment and so justify the need for public investment in Materials Innovation Infrastructure, industry experts emphasized the public-good content of this infrastructure and the multidisciplinarity required to develop it.

Nonproprietary data is an example of a public good. A repository of measured basic properties of nonproprietary materials from different materials classes would be valuable to industry, providing an essential step to trusting computational models. Yet companies have weak incentives to direct their experimental groups to generate this kind of basic data.

Another example: developing a general architecture and tools for model validation and uncertainty quantification requires a combination of statistical analytic and materials engineering expertise surpassing what is typically required by the business model of any one company. Even when the multidisciplinary expertise does reside within a company, companies have weak incentives to develop and disseminate general-purpose tools and methods because they are public goods with value that is difficult to capture in the market.

Although it is ultimately through private-sector R&D investments that the potential economic benefits of an improved Materials Innovation Infrastructure will be realized, public investment is needed to create the infrastructure, thereby creating opportunities for productive private-sector investment.

1 Introduction

The Materials Genome Initiative aims to promote U.S. global competitiveness in manufacturing by enabling U.S. companies to develop and deploy advanced materials more quickly and efficiently. This report presents an industry needs assessment and potential economic impact estimates, based on interviews with more than 100 industry experts.

Material properties determine the form and function of all manufactured products. Superior materials therefore expand the frontier of possibility for new technologies, with applications ranging from consumer goods like the Apple Watch, to renewable energy generation and energy storage, to supercomputing and national defense. The industrial capability to most quickly and efficiently develop and deploy advanced materials is therefore critical to a globally competitive manufacturing sector.

Launched in 2011 with the vision of enabling "the United States to discover, develop, manufacture, and deploy advanced materials at least twice as fast as possible today, at a fraction of the cost" (National Science and Technology Council, 2011, p. 5), the Materials Genome Initiative (MGI) is major effort spanning multiple U.S. government agencies to secure this critical capability for U.S. industry.

The National Institute of Standards and Technology (NIST) is supporting the MGI through efforts to establish materials data-exchange and model-exchange protocols; the means to ensure the quality of materials data and models; and new methods, metrologies, and capabilities needed for accelerated materials development. Additionally, through its integration of these activities, NIST is working to test and disseminate elements of an improved Materials Innovation Infrastructure to stakeholders in other national laboratories, universities, and U.S. industry.

This report, commissioned by NIST, presents analysis of the perspectives and opinions of U.S. manufacturers and other industry experts on their needs for new technological infrastructure supporting advanced materials innovation and the potential impacts of meeting those needs. It presents an assessment of industry needs for technology infrastructure—

including standards, measurement technology, and general-purpose technology—and provides estimates of the potential impacts of an improved Materials Innovation Infrastructure aligned with the MGI. The report also discusses the economic rationale for public investment toward this goal, integrating economic principles with illustrative examples provided by industry experts. The report is organized as follows:

Section 2 provides an overview of the MGI and the economic policy rationale for the public investment that supports it, particularly public investment in the technical elements of an improved Materials Innovation Infrastructure.

Section 3 provides an overview of the analytic approach to the industry needs assessment and economic impact assessment. The section presents the six areas of industry need on which the assessment focuses and describes the process by which they were identified, based in part on preliminary scoping interviews with industry experts. It presents and explains the quantitative materials research and development (R&D) process model and describes how it was used in structured interviews to collect the data that supported estimation of the potential impacts of improved infrastructure. It describes the composition of the group of 121 industry experts interviewed.

Section 4 describes the qualitative results of the industry needs assessment, summarizing relative importance ratings and difficulty ratings for each of the six identified needs and presenting commonly heard themes, insights, and examples that explain each need, its importance to industry, and the reasons public investment is required to address the need.

Section 5 presents the quantitative results of the economic impact assessment, developed using the materials R&D process model described in Section 3, calibrated based on the perceptions and opinions of industry experts. Potential impact estimates are based on a comparison of two calibrations of the model: first reflecting the current environment, then reflecting an environment with an improved Materials Innovation Infrastructure. Therefore, we are able to offer, in addition to potential impact estimates, current benchmark estimates of the risks, time to market, and costs of developing new materials.

Section 6 concludes the report with a summary of important results and policy implications.

2 Materials Genome Initiative: Overview

The MGI "offers a unique opportunity for the United States to discover, develop, manufacture, and deploy advanced materials at least twice as fast as possible today, at a fraction of the cost" (National Science and Technology Council, 2011, p. 5).

Advanced materials are an increasingly essential—and increasingly complex—component of the manufacturing environment, forming the first tier of advanced manufacturing supply chains (Moskowitz, 2014). This complexity demands larger, more diversified, and integrated R&D resources, which are not easily defined and implemented (Tassey, 2013, 2016). Recognizing this challenge, more industrialized nations are making larger and more sophisticated investments in new materials and their product applications, especially in materials R&D infrastructure.

Examples include the Industrial Technology Research Institute (ITRI) of Taiwan, the Electronics and Telecommunications Research Institute (ETRI) of South Korea, the Fraunhofer applied research institutes in Germany, and, in the United States, the National Network for Manufacturing Innovation (Manufacturing USA), Advanced Manufacturing Technology Consortia (AMTech), National Nanotechnology Initiative, the MGI, and other initiatives.[2]

2.1 VISION AND GOALS

Launched in 2011 as a key enabling element of an administration-wide effort to spark domestic competitiveness in manufacturing in high-demand and emerging technology markets, the MGI is a "multi-stakeholder effort to develop infrastructure to accelerate advanced materials discovery and development in the United States . . . [and] leverage existing Federal investments through the use of computational capabilities, data management, and an integrated approach to

[2] See www.manufacturing.gov/programs.

materials science and engineering" (National Science and Technology Council, 2011, p. 4).

Goals and efforts of the MGI overlap with and complement those of other U.S. manufacturing initiatives. Advanced materials design is central to the activities of the Manufacturing USA institutes, including among others LIFT, focused on lightweight materials manufacturing; PowerAmerica, focused on wide-bandgap power electronics manufacturing; IACMI, focused on fiber-reinforced polymer composites manufacturing; and NextFlex, manufacturing thin, flexible electronic devices and sensors. The MGI is also linked to the National Nanotechnology Initiative by the Nanotechnology Knowledge Infrastructure Signature Initiative to develop "models, simulation tools, and databases that enable predictions of nanoscale material properties [and] implement predictive tools for materials production and manufacturing" (National Science and Technology Council, 2014, p. 51).

The MGI envisions an integrated, systems approach to materials innovation, achieved through investment in a new Materials Innovation Infrastructure.

Motivating the initiative are the ideas that "development of advanced materials will fuel many of the emerging industries that will address challenges in energy, national security, healthcare" and that accelerating the process of moving an advanced material from laboratory to market "could significantly improve U.S. global competitiveness and ensure that the Nation remains at the forefront of the advanced materials marketplace" (National Science and Technology Council, 2011, p. 3).

Released in 2014, the MGI strategic plan sets out four defining goals for the initiative:

Culture change: MGI-aligned efforts will aim to improve knowledge flows and break down traditional silos in materials science and engineering, integrating the efforts of theorists and experimentalists and promoting collaboration "among academia, National and Federal laboratories, and industry" (National Science and Technology Council, 2014, p. 5).

Integration of experiments, computation, and theory: A defining feature of MGI-aligned efforts is "an integrated, collaborative workflow that draws simultaneously from experiments, computation, and theory" (National Science and Technology Council, 2014, p. 5). The Materials Innovation Infrastructure envisioned by the MGI includes "advanced simulation tools validated through experimental data, networks to share useful modeling and analysis code, and access to quantitative synthesis and characterization tools" (National Science and Technology Council, 2014, p. 5).

Access to digital data: MGI-aligned efforts will expand "access to validated data and tools generated by the materials community across the materials development continuum" (National Science and Technology Council, 2014, p. 6).

Workforce Development: To prepare the next generation of materials scientists and engineers to leverage a new Materials Innovation Infrastructure and apply the integrated, systems approach to materials innovation it enables, MGI-aligned efforts will support undergraduate- and graduate-level curriculum development together with workforce development and training for professionals in the workplace.

2.2 FEDERAL AGENCY PARTNERS

The efforts of multiple federal agencies are coordinated by the Subcommittee on the Materials Genome Initiative (SMGI), established in 2012 under the National Science and Technology Council's (NSTC) Committee on Technology. Each agency participating in the MGI is represented on SMGI.

Leading the MGI are the Department of Defense, Department of Energy, National Science Foundation, and NIST. Others agency partners in the MGI include the National Aeronautics and Space Administration; National Institutes of Health; and U.S. Geological Survey, Department of the Interior, among others (see https://www.mgi.gov/partners).[3]

2.2.1 Department of Defense

The Department of Defense (DOD) is a major consumer of advanced materials through its procurement of warfighting systems and invests in "multidisciplinary R&D efforts integrated along the full materials continuum from discovery through

[3] These agencies are identified in the MGI Strategic Plan (National Science and Technology Council, 2014) as having a leading role in several milestone tasks. Comparison of agencies' effort levels in terms of MGI-related expenditure is outside the scope of this report and would not be straightforward: "Like the President's FY2015 and FY2016 budgets, the FY2017 budget does not include a table of agency funding for the MGI" (Sargent et al., 2017).

development, deployment, sustainment, and retirement of assets" (National Science and Technology Council, 2014, p. 42).

Illustrative of MGI-aligned efforts by the DOD, the Air Force Research Laboratory Materials and Manufacturing Directorate's Composites Performance team is developing tools to predict behavior and life of ceramic and polymer matrix composite materials with less reliance on experimentation:

MGI-aligned efforts at DOD include physics-based modeling to predict the behavior and life of ceramic and polymer matrix composite materials.

"Through in-house developed, physics-based modeling techniques, the team determines how materials will behave under specific application environments—including extreme environments—that are relevant to current and emerging Air Force platforms. These models also aid in predicting material degradation and consequent damage initiation and growth over time. This predictive ability helps designers and maintainers develop better materials for highly demanding applications, define maintenance cycles more accurately, and evaluate effects of processing or in-service induced damage on system performance. As a result, aircraft designers will be able to avoid over-conservative or inefficient design, more accurately predict component life, and more effectively evaluate in-service issues that arise during system life" (Jordan, 2017, p. 1).

The U.S. Naval Research Laboratory (NRL) Center for Computational Materials Science recently announced the discovery of a candidate material for solid-state lasers and light emitting diodes (LEDs). The work, a collaboration between NRL researchers and an international team of physicists, identified nanocrystals made of cesium lead halide perovskites as having a unique property: rapid light emission in its lowest-energy state—i.e., a ground exciton state that is bright instead of dark. Applications include "more efficient lasers and LEDs with larger emission power at lower energy use, as well as faster switching for communication and sensors" (Parry, 2018, p. 1).

For more on DOD efforts aligned with the MGI, see www.mgi.gov/partners-involved/department-defense-dod.

2.2.2 Department of Energy

MGI-aligned efforts by the Department of Energy (DOE) run the gamut from basic research to applied R&D. The Office of Basic Energy Sciences "supports fundamental research in materials sciences and engineering, chemistry, geosciences, and physical biosciences to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels, including research to provide the foundations for new technologies relevant to DOE's missions in energy, environment, and national security" (National Science and Technology Council, 2014, p. 43). Other DOE offices, like the Office of Energy Efficiency and Renewable Energy and Office of Fossil Energy, are bringing MGI approaches to their mission-specific R&D efforts, for example seeking lightweight structural materials to save energy by reducing the weight of vehicles and aircraft and high-performance functional materials to improve solar panel efficiency and battery energy density.

MGI-aligned efforts at DOE include the application of supercomputing to develop powerful modeling and simulation tools to predict material properties and guide the design of next-generation functional materials.

In 2016, DOE launched two 4-year projects to leverage supercomputing capabilities at Oak Ridge National Laboratory (ORNL) and Lawrence Berkeley National Laboratory (LBNL) to develop software for the design of functional materials with applications in alternative and renewable energy. The two projects will "combine theory and software development with experimental validation, drawing on the resources of multiple DOE Office of Science User Facilities, including the Advanced Light Source at LBNL, the Advanced Photon Source at Argonne National Laboratory (ANL), the Spallation Neutron Source at ORNL and several of the five Nanoscience Research Centers across the DOE national laboratory complex" (Stark, 2016, p. 1).

Another DOE-led MGI showcase, the Energy Materials Network (EMN) "is taking a different approach to materials research and development (R&D) that aims to solve industry's toughest clean energy materials challenges." EMN is network of consortia, each convening "national labs, industry, and academia to focus on specific classes of materials aligned with industry's most pressing challenges related to materials for clean energy technologies."[4]

For more on DOE efforts aligned with the MGI, see www.mgi.gov/partners-involved/department-energy-doe.

2.2.3 National Science Foundation

Through its program Designing Materials to Revolutionize and Engineer our Future (DMREF), the National Science Foundation (NSF) is supporting the MGI with extramural research funding.

[4] See https://www.energy.gov/eere/energy-materials-network/energy-materials-network.

DMREF grants fund research that "seeks to advance fundamental understanding of materials across length and timescales, thereby elucidating the effects of microstructure, surfaces, and coatings on the properties and performance of engineering materials" (National Science and Technology Council, 2014, p. 48).

Examples of recent DMREF-funded research results include a fundamental discovery that provides a technology platform for next-generation communications and computing applications of oxide electronics materials (Meiller, 2018) and the discovery, based on predictive atomistic calculations performed at the National Energy Research Scientific Computing Center, that incorporating boron into the indium-gallium nitride material commonly used for solid-state lighting can improve energy efficiency (McAllister and Kioupakis, 2017).

For more on NSF efforts aligned with the MGI, including information on recent DMREF awards, see www.nsf.gov/funding/pgm_summ.jsp?pims_id=505073.

2.2.4 National Institute of Standards and Technology

NIST is supporting the MGI through efforts to establish materials data-exchange and model-exchange protocols; the means to ensure the quality of materials data and models; and new methods, metrologies, and capabilities necessary for accelerated materials development. Additionally, through its integration of these activities, NIST is working to test and disseminate elements of an improved Materials Innovation Infrastructure to stakeholders in other national laboratories, universities, and industry.

NIST is leveraging its expertise in generating, integrating, and curating critically evaluated data and models to establish essential materials data exchange protocols and the means to ensure the quality of materials data and models.

NIST is host to numerous projects focusing on materials research, including material-, process-, and application-specific efforts and cross-cutting initiatives. The NIST Material Measurement Laboratory is coordinating these activities in partnership with the NIST Information Technology Laboratory and with broad participation across the Institute.

NIST's support for MGI is consistent with its mission to promote U.S. innovation and industrial competitiveness. Through its established role in meeting U.S. industry's needs for measurement and related infrastructure technologies and standards, NIST supports both conventional materials innovation and computational materials science and engineering. NIST, first as its predecessor agency the National Bureau of Standards, has been involved in leveraging high-quality materials data for new material design since this aim first drew the combined attention of industry and federal agencies (Rumble and Westbrook, 1985).

Prominent among NIST's MGI-aligned efforts is its support for the Center for Hierarchical Materials Design, a consortium of university and national laboratories and industry partners focused on "developing the next generation of computational tools, databases and experimental techniques in order to enable the accelerated design of novel materials and their integration to industry" (http://chimad.northwestern.edu/about/).

Complete details of NIST's MGI-related efforts can be found on NIST's website, http://mgi.nist.gov.

2.3 MGI IN ACTION

Three short vignettes illustrate how the types of potential impacts discussed in this report are already happening in a limited way, as opportunities are realized by pioneers working in especially fruitful niches of industry, leveraging the Materials Innovation Infrastructure that exists today. The potential impacts presented in this report could be realized by improving and extending this infrastructure so that more companies can follow these examples.

Virtual Aluminum Casting

MGI-aligned approaches enabled Ford Motor Company to accelerate the development of engine components by 15% to 25%, saving millions of dollars over just a few years.

Ford Motor Company developed the Virtual Aluminum Castings (VAC) software, enabling its engineers to design engine components and simulate their production and testing on a computer over many iterations before touching any raw materials. Integrating commercial software packages and data with Ford's proprietary data and original code, VAC tools "bridge the many key dimensional scales from the atomistic level to the component level" (Allison, Li, Wolverton, and Su, 2006, p. 28).

In 2006, when VAC was relatively new, Ford credited the software with a "15-25% reduction in the time it takes to develop a new cylinder head or block [and] millions of dollars in direct cost savings or cost avoidance" (Allison, Li, Wolverton, and Su, 2006, p. 35).

The development of VAC involved collaboration between Ford engineers and researchers at the University of Michigan, University of Illinois, Imperial College, Pennsylvania State University, and the University of Southern California and was "accomplished by a combination of theoretical, experimental, and computational technologies and . . . the development of a deep, fundamental understanding of dozens of separate phenomena" (Allison, Li, Wolverton, and Su, 2006, p. 28).

Rapid Qualification of New Structural Alloys in Aerospace

MGI-aligned approaches enabled QuesTek to accelerate the development of a new steel for Navy aircraft.

QuesTek Innovations LLC has applied a collection of computational models to the design, development, and aerospace certification and flight qualification of advanced metal alloys, integrating different models and data sources into a suite of tools it has trademarked *Materials by Design*. QuesTek credits its use of these computational modeling tools with accelerating the development of several advanced alloys. (Sebastian and Olson, 2014).

Ferrium M54 steel progressed from clean-sheet design to flight-qualified, production hook shank parts for the U.S. Navy's T-45 aircraft in 9 years, compared with a 10- to 20-year timeframe typical for flight-critical components (Materials Innovation Case Study, 2016a).

Directed Self-Assembly of Block Copolymers

Exponential growth in computing power and data storage capacity over several decades has been driven by the increasing resolution of optical lithography, enabling the number of integrated circuits that fit on a microchip to roughly double every two years, following Moore's Law. As conventional optical lithography reaches its physical limits, new technologies will be needed to sustain this rate of innovation.

Integrated theory, computation, and experimentation have unlocked the promise of block copolymers for semiconductor devices and other applications.

One leading candidate is directed self-assembly (DSA) of block copolymers (Laachi, Shykind, and Fredrickson, 2014; Laachi et al., 2015). The promise of this novel nanoscale patterning technique rests on decades of research in the MGI mode. Well-integrated theory, computation, and experimentation by research teams at universities and in industry has provided the necessary knowledge base (de Pablo et al., 2014). Recently, "integration of computation and experiments between researchers at the University of Chicago, AZ Electronic Materials, Tokyo Electron Ltd., and Imec has resulted in demonstration of the world's first 300-mm fab compatible directed self-assembly (DSA) process line." (de Pablo et al., 2014, p. 112).

2.4 PUBLIC POLICY RATIONALE

The public sector's role in performing basic research is generally understood. Less well understood is the appropriate scope of the public sector's involvement in the process by which fundamental knowledge is translated into commercial technologies. Incentives for private-sector investment do not snap suddenly from inadequate (basic science) to adequate (all subsequent steps).

Technical Infrastructure, a bulwark of public-good technology elements, creates opportunities for productive private-sector R&D investment.

Efficient translation of fundamental knowledge into commercial technology depends on a bulwark of technology elements, having varying degrees of public-good content, that together comprise a technical infrastructure supporting innovative activity in the private sector. As with basic, nonmarket-oriented scientific knowledge, the private sector has weak incentives to supply these quasi-public goods.

The quasi-public-good elements of the technical infrastructure include proof-of-concept research resulting in the creation of "technology platforms" and "infratechnologies" like measurement and test methods, scientific and engineering data, quality control techniques, and the functional and physical basis for interfaces between components of technology systems. Tassey (2008, 2013, 2016) defines these technology elements, explains why their public-good characteristics lead to significant private-sector underinvestment, and analyzes their critical role in an efficient innovation ecosystem.

Technology platforms are precompetitive proof-of-concept technologies on which myriad commercial technologies can be based. Tassey (2008) offers the classic example of Bell Labs' development of the transistor, based on the principles of solid-state physics. A related technology platform is the light-emitting diode (LED), the basis for numerous technologies commercialized over decades (Sanderson and Simons, 2014). Today, LEDs are ubiquitous, found in everything from flat screen televisions to household light bulbs. The scope of different applications of technology platforms is typically much broader than the market strategy of any one company, making it so that a company can only expect to capture a fraction of the value of developing the platform. This difficulty leads to underinvestment in technology platforms by the private sector, a market failure that public investment of the right sort can correct.

Illustrative examples of infratechnologies include "research tools (measurement and test methods), scientific and engineering data, the technical basis for interface standards, quality control techniques" (Tassey, 2008, p. 616).

As technology platforms emerge and birth new commercial technologies, they typically require specialized infratechnologies. For example, the ever-smaller structures of next-generation semiconductor and digital storage devices are "challenging the resolution limits of current analytical and inline metrology tools" (Kline, Sunday, Windover, and Bunday, 2017, p. 014001). For the many solid-state lighting applications of the LED platform now ascendant, NIST is developing specialized metrology and calibration services and working with DOE and national and international standard-setting organizations to develop measurement standards to meet the industry's emerging needs.[5]

Like the value created by investing in technology platforms, the value of developing infratechnologies is difficult for any single company to capture. Moreover, developing infratechnologies often requires highly specialized expertise different from that of the companies that could benefit from using these technologies. For these reasons, developing infratechnologies is typically outside the scope of these companies' market strategies.

The elements of an improved Materials Innovation Infrastructure aligned with the MGI are special examples of technology platforms and infratechnologies. Although it is ultimately through private-sector R&D investments that the potential economic benefits of an improved Materials Innovation Infrastructure will be realized, public investment is needed to create the infrastructure, thereby creating opportunities for productive private-sector investment.

[5] See www.nist.gov/programs-projects/solid-state-lighting-metrology.

3 Methods and Analysis Approach

This section provides an overview of our methods and analytic approach. The section presents the six areas of industry need on which the assessment focuses and describes the process by which they were identified. It presents and explains the quantitative materials R&D process model and describes how structured interviews were used to collect the data needed to calibrate the model. It describes the composition of the group of 121 industry experts interviewed. It describes the methods used to develop economic impact estimates and confidence intervals from the calibrated R&D process model.

3.1 SCOPING INTERVIEWS AND INTERVIEW GUIDE DEVELOPMENT

Review of peer-reviewed literature, white papers, issue briefs, and industry reports, supplemented by 18 scoping interviews with industry experts involved with MGI-aligned efforts, provided the foundation for this study. This initial step identified six broad areas of industry need:

- **access to high-quality data**, nonproprietary experimental data, computational data, and software code;
- **collaborative networks**, efficient means of sharing materials information (e.g., along a supply chain or among research collaborators);
- **materials design methods**, computational approaches providing shorter paths to better starting points for materials discovery and design; application of systems approach to materials;
- **production and scale-up methods**, including model-based and simulation-based alternatives to expensive

physical testing based on trial and error and faster, more cost-effective means of producing advanced materials at pilot scale and full scale;

- **quality assurance and control, and component certification methods**, enabling improved capabilities to model, predict, and control the formation of defects and to forecast manufacturing variation; and
- **model validation and uncertainty quantification**, providing a basis for trust and acceptance of computational models and objective decision-making regarding reliance on computational analysis and simulation at a business level.

After characterizing these six areas of need, RTI developed an interview guide to gather two types of information:

- perspectives of industry experts on the relative importance of these needs and the difficulty of addressing them through private investment, supported with explanation and examples based on these experts' first-hand experience;
- quantitative input on the potential impact of addressing the six areas of need with an improved Materials Innovation Infrastructure.

The interview guide is provided in the appendix to this report. Importance and difficulty ratings, together with qualitative analysis of industry needs distilled from the perspectives industry experts shared, are presented in Section 4. Quantitative analysis of potential economic impacts is presented in Section 5.

3.2 MATERIALS R&D PROCESS MODEL

For the purpose of quantifying the potential impacts an improved Materials Innovation Infrastructure could have on the materials R&D process, we employ a stylized model, breaking the materials R&D process into four successive stages: Discovery/Design, Development, Manufacturing, and Deployment (Figure 3-1).

The ***Discovery and Design*** stage involves experimentation and modeling at the smallest scale, using coin-sized pieces of a metal or polymer, for example. The stage begins with a statement of intent to seek a new material for a given application or end use. It ends when researchers are satisfied that they have identified candidate material compositions and processing methods that are promising enough to justify investing in the next stage, development.

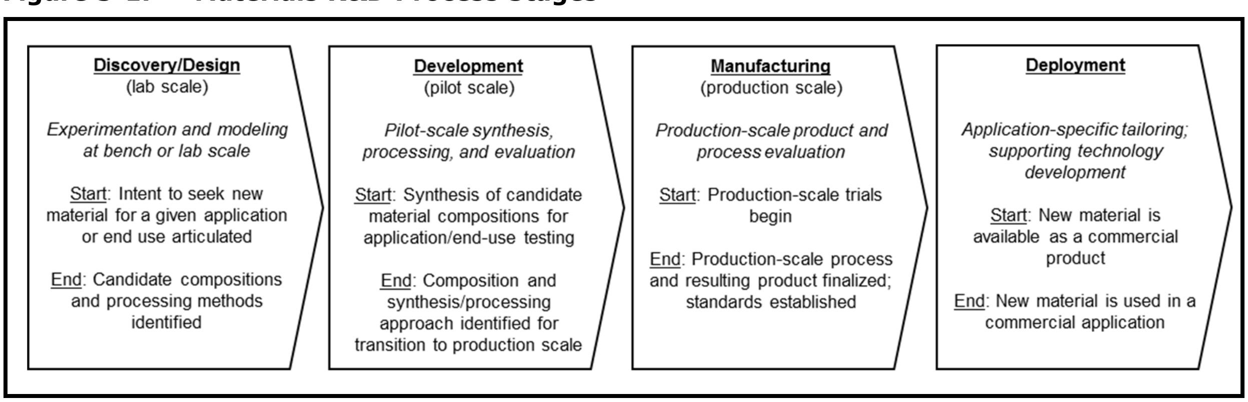
The ***Development*** stage involves pilot-scale synthesis, processing, and evaluation, starting with producing candidate materials in quantities sufficient for application-specific testing and ending when developers are satisfied that they have identified a candidate composition and processing approach that is ready to transition to production scale.

The definition of pilot scale varies depending on the type of material and its intended use. For a new alloy, pilot scale might involve a 1,500-pound heat, compared with production-scale heats of multiple tons (Materials Innovation Case Study, 2016a). In developing Gorilla Glass 3, Corning progressed immediately to a production-scale process in the development stage (Materials Innovation Case Study, 2016b).

The ***Manufacturing*** stage involves production-scale product and process evaluation, starting with the first production-scale trial and ending with a finalized product, produced as it will be produced for use in commercial products.

The ***Deployment*** stage is for integrating the new material into a commercial product—a new alloy into a production automobile engine component, a new glass into a mobile device, block copolymers into a microprocessor. The stage may involve application-specific tailoring of the material and development of supporting technologies needed to integrate the new material into the commercial product.

Figure 3-1. Materials R&D Process Stages



Note: The materials R&D process stages are based on the Quantitative Benchmark for Time to Market (QBTM) analytical framework, developed for NIST by Nexight Group and Energetics (2016).

To complete the materials R&D process model, we assumed that, for a given R&D project, each stage has a duration (the time from start to end) and a cost per year, and that there is a probability of transitioning from one stage to the next. A given R&D project will simply progress from one stage to the next or not, based on the technical success of the R&D performed and business decisions about its market potential and alignment with the company's market strategies. Thinking of transition probabilities governing this process is a tractable way to model the risk a company faces of sinking investment into an R&D project that may never bring in revenue.

RTI made two key simplifying assumptions. First, projects that begin an R&D stage were assumed to complete that stage. Therefore, the probability of deployment, conditional on reaching (starting) the deployment stage, is 100%. Second, we assumed R&D stages do not overlap.

Departing from the first assumption would have complicated the modeling (if a project begins a stage but does not complete it, how much time does it spend in the stage before ending?). Although not strictly true, the assumption is fairly realistic because of the "gated" approach taken by many companies: a stage is green-lighted, completed, its results evaluated, and a determination made about whether to continue into the next stage. In reality, there are more than four such gates, which divide these four broad stages with intermediate gates. Departing from either assumption would have required placing additional burden on interviewees by asking them to provide more detailed descriptions of the R&D process. Lessening this burden enabled us to focus more attention during interviews on qualitative discussions of the identified needs.

The model does not represent the entire technology lifecycle, ending with the first use of a new material in a commercial application. The process of market diffusion, of a new material finding its way into new applications and expanding its share of the market in those applications, is not modeled here. Although this process is important to consider for innovation policy, including public investments in technical infrastructure, it is less directly related to the vision of the MGI. Concentrating on the R&D process from discovery and design through deployment allowed us to focus resources on the most important issues for technical infrastructure and policy related to the MGI.

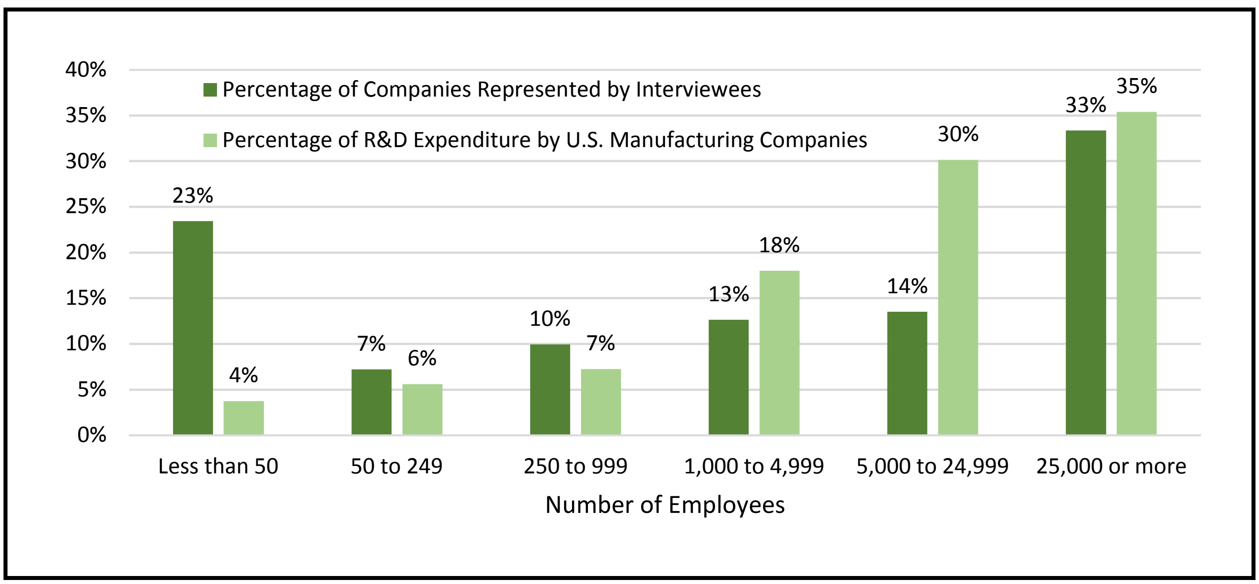
3.3 EXPERT INFORMANT INTERVIEWS

Structured interviews were conducted with 121 experts, 116 of whom worked in industry; of the other 5, 3 had worked for companies and now consulted, and 2 worked in government laboratories doing applied materials research in collaboration with industry partners.

The distribution of interviewees by company size is shown in Figure 3-2, together with the distribution of U.S. manufacturing companies' R&D expenditure. With the exception of companies of less than 50 employees, which are overrepresented among our interviewees, and to a lesser extent companies with 5,000 to 24,999 employees, which are underrepresented, the distributions are similar. Roughly half of interviewees represented companies of fewer than 500 employees, which are 98% of all U.S. manufacturing companies (U.S. Census, 2015 County Business Patterns).

Companies represented by interviewees were, on average, more R&D-focused than typical U.S. manufacturing companies. Based on the R&D employment of these companies, reported by interviewees (Figure 3-3), our interviewees represented companies with a total R&D employment of between 34,000

Figure 3-2. Distribution of Interviewees by Company Size

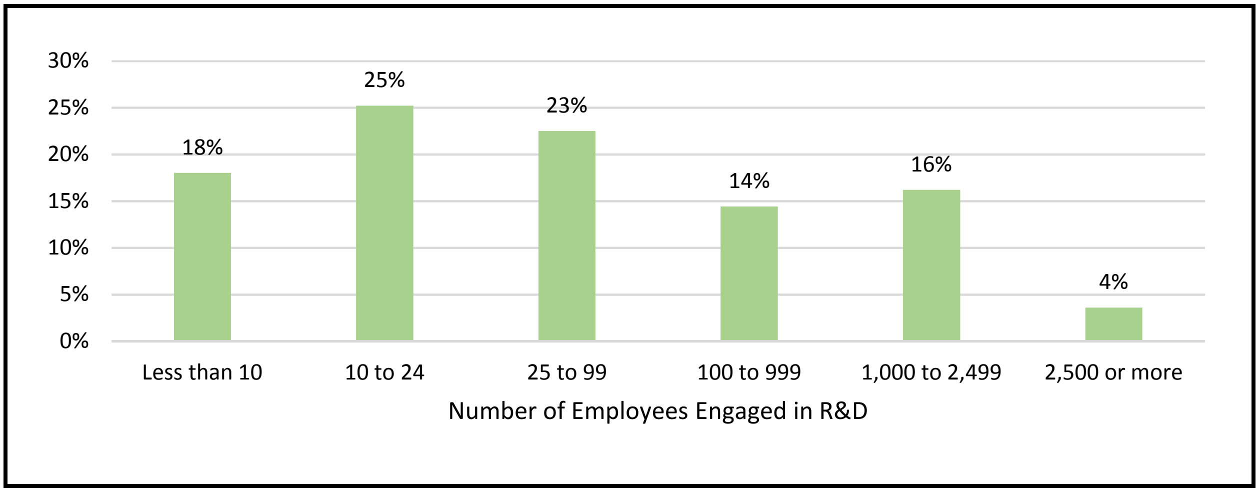


Note: Distribution of U.S. manufacturing companies' R&D expenditure, which is offered for comparison, comes from NSF (2016, Table 21). With the exception of companies with less than 50 employees, which are overrepresented among our interviewees, and to a lesser extent companies with 5,000 to 24,999 employees, which are underrepresented, the distribution of companies represented by experts with whom we spoke is similar to the distribution of U.S. manufacturing companies' R&D expenditure.

and 80,000, or between 4% and 9% of U.S. manufacturing R&D employment (National Science Foundation, 2016). By comparison, our industry experts represented 0.05% of U.S. manufacturing companies and 1.4% of U.S. manufacturing companies with 500 or more employees.

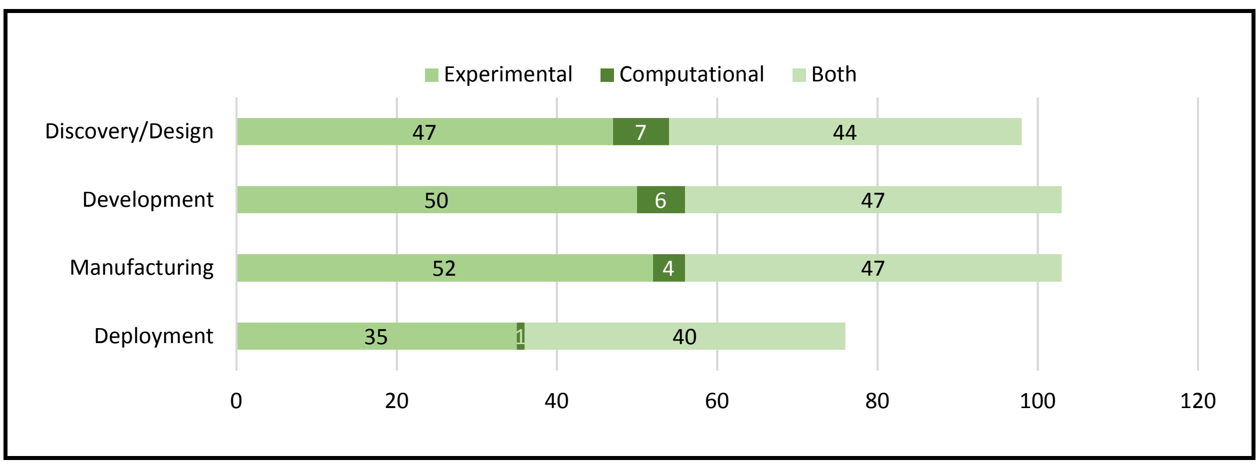
The industry experts who shared their perspectives and opinions for this study come from both experimental and computational backgrounds, and their expertise covers the four stages of the materials R&D process model: discovery/design, development, manufacturing, and deployment (Figures 3-4 and 3-5). Many of these industry experts were also familiar with the

Figure 3-3. Distribution of Interviewees by Companies' R&D Employment



Note: This graph is based on interviewees' responses to question V.1 in the interview guide, which is provided in the appendix.

Figure 3-4. Representation of R&D Stages among Interviewees

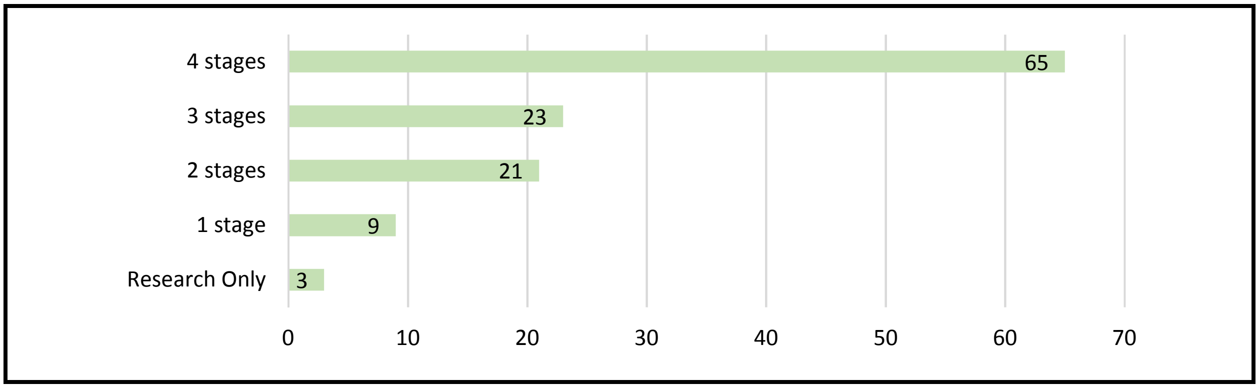


Note: Each interviewee may have expertise in multiple stages. Therefore, figures sum to more than the unique number of interviewees, which is 121.

academic research setting, having completed advanced degrees, worked in academia, or worked with university researchers serving in consulting roles on commercial projects.

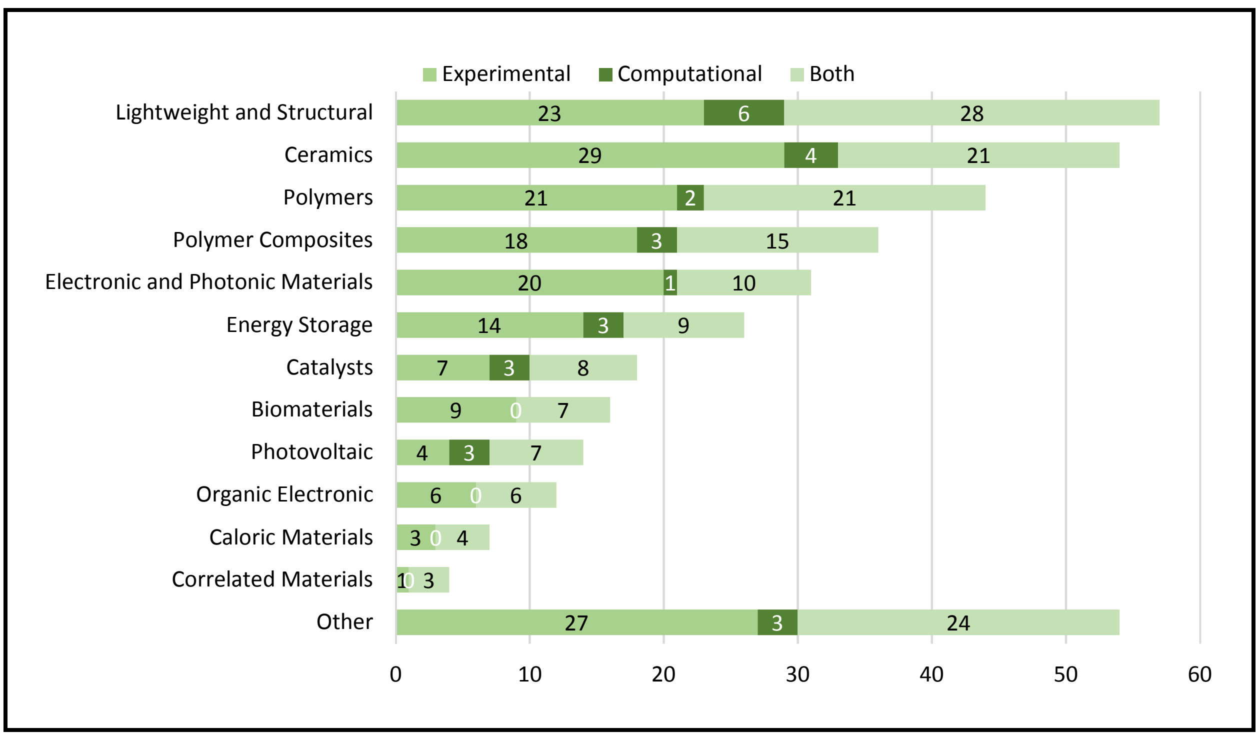
Interviewees' expertise covers a range of materials classes, with the greatest representation for lightweight and structural materials (predominantly alloys), ceramics, polymers, and polymer composites (Figure 3-6).

Figure 3-5. Multiple R&D Stages Represented by Interviewees



Note: The expertise of three non-industry respondents was in fundamental research.

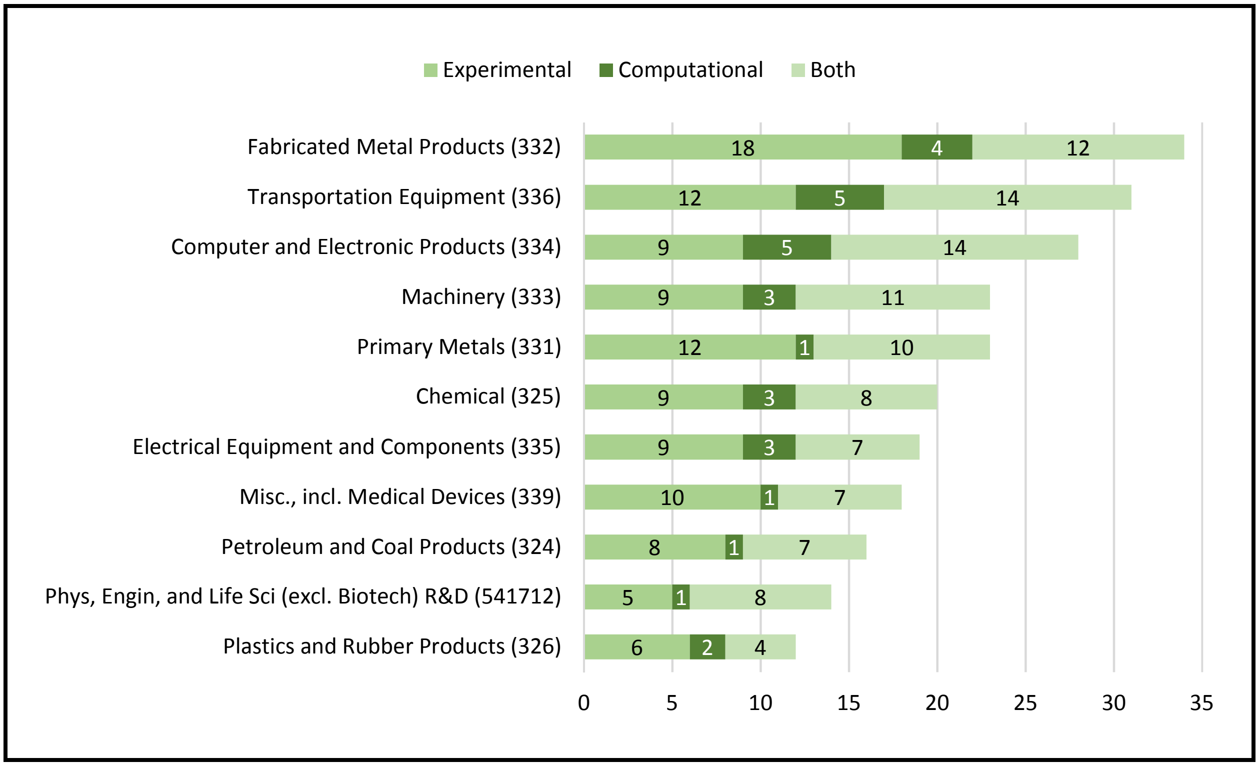
Figure 3-6. Representation of Materials Classes among Interviewees



Note: Each interviewee may have expertise in multiple materials classes. Therefore, figures sum to more than the unique number of interviewees, which is 121.

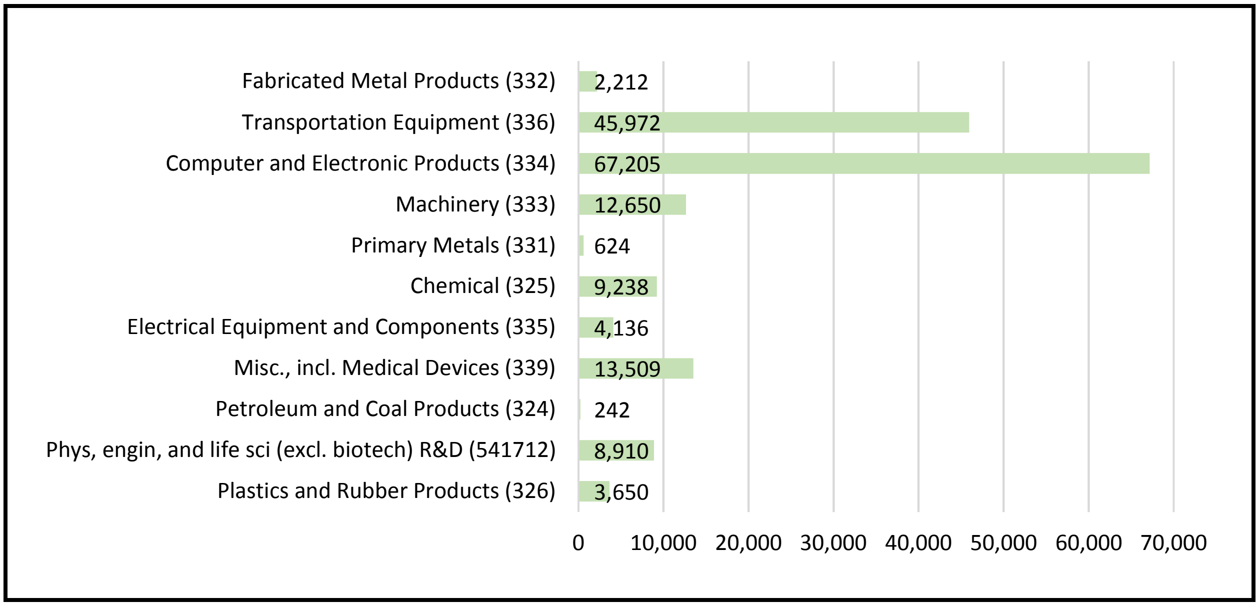
Interviewees represented companies in or developing materials for 10 manufacturing industries and one relevant service industry: physics, engineering, and life sciences R&D (Figure 3-7). Most manufacturing R&D expenditures are concentrated in transportation equipment, which includes aerospace, and in computer and electronic products, which includes semiconductors (Figure 3-8); out of the 121 industry experts interviewed, 51 had expertise in at least one of these two industries.

Figure 3-7. Representation of Industries among Interviewees



Note: Each interviewee may develop materials for multiple industries. Therefore, figures sum to more than the unique number of interviewees, which is 121.

Figure 3-8. Annual R&D Expenditure by Industry (millions of U.S. dollars)



Note: 2013 domestic R&D comes from NSF (2016, Table 23). North American Industry Classification System (NAICS) identifiers are given in parentheses. R&D reported for the chemical industry (325) excludes pharmaceuticals and medicines (3254), which account for $52 billion in R&D.

3.4 ECONOMIC IMPACT ESTIMATION

RTI estimated the potential economic impacts of an improved infrastructure addressing the identified needs of industry by calibrating the materials R&D process model (Section 3.2) in two scenarios: first, in the current environment with existing infrastructure (actual scenario) and then in a hypothetical environment with improved infrastructure (counterfactual scenario). Comparison of the models in the two scenarios yielded estimates of the relative reduction in R&D cost, which was then applied to annual R&D expenditure.

As part of the process of developing potential impact estimates, RTI developed benchmark estimates of the time, risk, and relative costs of developing a new material given the infrastructure that exists today. These benchmark estimates are presented with the impact estimates in Section 5.

The approach to cost estimation explained below is adapted from one that is well established for estimating the costs of developing pharmaceuticals (DiMasi et al., 2003, 2016) and that has been applied to estimate potential impacts of improved infrastructure (Gallaher et al., 2007; Scott et al., 2014).

Defining Costs. The cost to be estimated is the economic cost of successfully deploying a new material, including the cost of failures (candidate materials that go through some R&D stages but are never deployed) and the cost of capital. The cost of capital reflects the opportunity cost of financial capital, which is a significant part of the true economic cost of R&D, regardless of how that R&D is resourced.[6]

In the model, R&D costs are capitalized from the date they are incurred until the end of the deployment stage, when a new material is first used in a commercial product application. This is typically the point at which the stream of revenues attributable to the R&D would begin, and it is a useful benchmark for calculating the real cost of the R&D. For a company to want to invest in R&D, the expected value of the stream of future returns, discounted back to this point, must be greater than the expected cost of the R&D, capitalized to this point.

Consider the choice between investing, say, $100,000 in either an early-stage R&D project, to begin 10 years before the point of deployment, or in a later-stage R&D project, for a material that is only 1 year from deployment. Intuitively, it is more difficult to justify the investment in the early-stage R&D project, because it must generate a greater expected return to justify the longer wait.[7]

This feature of the model is important; omitting the opportunity cost of capital from the model would neglect this important reality and distort the analysis, making impacts on earlier stages of R&D appear less important than they really are.

Stepping Through the Model. The model is presented with an extended example, using the materials R&D process model parameters obtained from interviews, which are presented in Table 3-1. The relative cost per year, per project, in the

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[6] Not only must outside investors or lenders receive an acceptable rate of return when R&D is financed, there is also the need to provide an analogous return on a company's internal resources (as when paying for R&D with retained earnings) so that a company's shareholders are content with the resources being used for R&D instead of being paid out as dividends.

[7] Assuming an 8% cost of capital, the early-stage project would have to generate twice the return of the project that is only 1 year out: The long-term project would have to generate at least $100,000($1.08^{10}$), or $215,892.5, while the other would need to generate only $108,000 to be considered worthwhile.

discovery and design stage is normalized at 1. Heuristically, it may be convenient to think of that cost as $1, but within the model the cost is unitless. The method of conversion to dollars will be explained in a subsequent step.

To explain the model, let us start with the final stage, deployment, and work backward. The average cost per project per year in the deployment stage is 11.9, and the deployment stage lasts an average of 2.5 years (Table 3-1). It was assumed that every project that starts the deployment stage completes it. That is, every new material that is made available as a commercial product (defining the start of the deployment stage in the model) will be used in a commercial product application (defining the end of the deployment stage).

Under these assumptions, the contribution of the deployment stage to total out-of-pocket cost is the product of 11.9 per year and 2.5 years, or 29.8. Recall, this *relative* cost is unitless; it would be $29.8 if the cost of one project for one year in the discovery and design stage were $1.

The calculation of capitalized cost assumed that out-of-pocket costs are incurred at a constant rate of 11.9 per year, and these costs are capitalized to the end of the deployment stage. The capitalized cost is therefore given by the following integral,

Table 3-1. Materials R&D Process Model Parameter Estimates

Model Parameter	R&D Stage			
	Discovery & Design	**Development**	**Manufacturing**	**Deployment**
Relative cost per year	1	3.9	16.5	11.9
Probability of advancing to next stage	29%	48%	72%	N/A
Duration (years)	2.6	3.0	2.0	2.5

Note: The relative cost per year in the discovery and design stage is normalized at 1. For simplicity, projects that begin a stage were assumed to complete that stage. These numbers reflect the average responses from all interviews. For a response related to a given R&D stage to be included in these averages, the respondent must have reported expertise in the R&D stage.

where *e* is the base to the natural logarithms and *r* is the real cost of capital, as a continuously compounded annual rate:[8]

$$11.9 \int_0^{2.5} e^{rt} dt = 11.9\,(e^{2.5r} - e^{0r})/r.$$

We assumed an 8% cost of capital and converted this to a continuously compounded annual rate by letting $r = \ln(1.08) = 0.077$. Feeding in this value for *r*, the contribution of the deployment stage to capitalized cost is 32.8.

Out-of-pocket and capitalized costs can be calculated in a similar way for the manufacturing stage. The difference is that not every project that goes through the manufacturing stage will go through the deployment stage; interview data indicate that, on average, only 72.4% of projects will advance. Therefore, 1.38 projects (the reciprocal of 72.4%) must go through the manufacturing stage for every new material that is successfully deployed. The out-of-pocket cost of the manufacturing stage is therefore $(2.0)(16.5)/0.724 = 46.4$.

The capitalized cost is given by the following integral, where *e* is the base to the natural logarithms and *r* is the real cost of capital, as a continuously compounded annual rate, and *p* is the probability of deployment, conditional on reaching the manufacturing stage:

$$\left(16.5 \int_{2.5}^{2.5+2.0} e^{rt} dt\right)/0.724 = 16.5\,(e^{4.5r} - e^{2.5r})/0.724r$$

Still assuming an 8% cost of capital and converting to a continuously compounded annual rate by letting $r = \ln(1.08) = 0.077$, the contribution of the manufacturing stage to capitalized cost is 60.8.

In general, the contribution of each stage to the out-of-pocket cost per new material deployed is given by $c(t_{start} - t_{end})/p$, where c is the cost per year per project in that stage; t_{start} is the time, in years, from the start of the stage to the end of the deployment stage; t_{end} is the time, in years, from the end of the stage to the end of the deployment stage; and p is the probability of deployment, conditional on reaching the stage.

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[8] Continuous compounding allows tractable calculations with costs that accrue continuously over the durations of R&D stages; it does not result in larger estimates of capital costs because the cost of capital is adjusted: an annually compounded 8% rate is equivalent to a continuously compounded rate of ln(1.08), or 7.7%, because $1.08^t = e^{\ln(1.08)t}$.

The contribution of each stage to the capitalized cost per new material deployed, capitalized to the end of the deployment stage, is given by this integral:

$$c\int_{t_{end}}^{t_{start}} e^{rt}dt/p = c\,(e^{rt_{start}} - e^{rt_{\text{end}}})/pr.$$

Table 3-2 summarizes these parameters for each R&D stage, derived from the parameters given in Table 3-1, and gives the out-of-pocket and capitalized costs for each stage. Note that the probability of deployment, conditional on reaching a given stage, is given by the product of the transition probabilities for that and all subsequent stages. For instance, the probability of deployment, conditional on reaching development, is 48% times 72%.

Table 3-2. Materials R&D Process Model Parameter Estimates

Model Parameter	Definition	R&D Stage: Discovery & Design	R&D Stage: Develop-ment	R&D Stage: Manu-facturing	R&D Stage: Deployment
c	Cost per year per project in that stage	1	3.9	16.5	11.9
t_{start}	Time, in years, from the start of the stage to the end of the deployment stage	10.2	7.5	4.5	2.5
t_{end}	Time, in years, from the end of the stage to the end of the deployment stage	7.5	4.5	2.5	0
p	Probability of deployment, conditional on reaching the stage	10%	35%	72%	100%
Out-of-pocket cost		25.9	33.3	46.4	29.8
Capitalized cost		51.1	53.0	60.8	32.8

Note: The cost per year in the discovery and design stage is normalized at 1. As a result, out-of-pocket and capitalized costs are given in relative terms, as a multiple of the cost per year for a project in the discovery and design stage. For example, the total out-of-pocket cost for the manufacturing stage is 48.5 times the cost of a year in the discovery and design stage. For simplicity, projects that begin a stage were assumed to complete that stage. Therefore, the probability of deployment, conditional on reaching (starting) the deployment stage, is 100%. A further simplifying assumption is that the R&D stages do not overlap. In reality, the start time of one stage need not be the same as the end time of the preceding stage. Departing from this assumption does not complicate the cost calculation but would have required placing additional burden on interviewees by asking them to provide more detailed descriptions of the R&D process.

Several details of the approach to impact estimation are worth noting:

Aggregating Results by Industry. The R&D process model was calibrated separately for each industry for which R&D expenditures are reported by NSF (2016).

The calibrations of the model for a given industry, under actual and counterfactual scenarios, are based on the responses of interviewees whose companies develop materials in or for that industry, based on question V.1 in the interview guide (provided in the appendix). Interviewees were allowed to indicate multiple industries. The responses of an interviewee who indicated a total of *n* industries receive a weight of 1/*n* in the calibration of each of those industries, thus the responses of each interviewee receive a total weight of 1 across all industries in the impact assessment.

Interviewees were not required to answer every question applied to the calibration of the R&D process model in the actual and counterfactual scenarios (Tables 2 and 3 in the interview guide, provided in the appendix), and responses applicable to a given R&D stage were counted only if the respondent indicated experience in that stage, based on question I.1 in the interview guide. Tables 3-3 and 3-4 show the total weights of responses and the number of individuals for each question (R&D process model parameter) and for each industry.

For each industry, actual and counterfactual costs, both out-of-pocket and capitalized, were calculated for each R&D stage; that is, the *relative* cost of each stage, as a multiple of 1 year of out-of-pocket costs in the discovery/design stage. These relative costs were then converted to dollar-denominated costs according to the following two steps:

Step 1. Industry R&D Fraction. A dollar-denominated R&D discount factor was determined for each industry based on the fraction of R&D in each industry interviewees believed was focused on developing and applying new materials, based on question V.5 in the interview guide. Interviewees' responses to question V.5 were combined for each industry as a weighted average, in the same way that the R&D process model parameter responses were combined.

Table 3-3. Total Weights by Industry and R&D Process Model Parameter

Actual Industry	Dev R/C	Mfctr R/C	Deplo R/C	D/D Prob	Dev Prob	Mfctr Prob	D/D Dur	Dev Dur	Mfctr Dur	Deplo Dur
Chemical (325)	7.9	5.6	4.4	8.9	7.9	5.6	8.9	8.9	5.6	4.4
Primary Metal (331)	11.3	11.9	9.4	10.4	10.6	12.7	11.4	11.8	12.9	10.4
Machinery (333)	8.2	7.7	5.4	5.6	7.0	7.5	6.6	8.2	8.7	5.2
Electrical Equip. (335)	3.9	3.4	3.0	4.1	4.9	3.4	4.1	4.9	4.4	3.0
Trnsport. Equip. (336)	12.2	12.3	9.2	11.8	12.0	12.1	11.8	12.2	12.3	8.6
Petro/Coal (324)	4.7	4.5	4.3	5.7	4.7	4.5	5.7	4.7	4.5	4.3
Plastics (326)	2.9	2.7	2.2	3.3	2.9	2.7	3.3	2.9	2.7	2.2
Fabricated Metal (332)	8.7	9.3	5.7	8.9	9.2	9.3	7.9	9.2	8.3	4.9
Computer/Electron (334)	6.5	6.0	3.7	8.2	7.5	6.0	8.2	7.5	6.0	4.7
Misc. (339)	6.4	6.2	3.0	6.5	6.2	6.0	6.5	6.4	6.2	1.8
R&D Services (541712)	3.4	3.4	2.7	3.5	3.2	3.2	3.5	3.4	2.4	1.5
Total	76	73	53	77	76	73	78	80	74	51

Counterfactual Industry	D/D R/C	Dev R/C	Mfctr R/C	Deplo R/C	D/D Prob	Dev Prob	Mfctr Prob	D/D Dur	Dev Dur	Mfctr Dur	Deplo Dur
Chemical (325)	7.9	6.9	4.6	3.4	7.9	7.9	5.6	8.9	8.9	5.6	4.4
Prim. Met. (331)	10.5	9.7	10.4	8.4	10.0	10.2	11.4	10.0	11.2	11.4	9.4
Machinery (333)	4.5	5.8	5.5	3.7	4.5	5.5	6.2	4.5	5.8	6.5	3.7
Elec. Equip. (335)	2.5	3.3	2.9	2.5	3.5	4.3	2.9	3.5	4.3	3.9	2.5
Trnsp. Eqp. (336)	10.1	10.5	11.8	8.6	11.1	11.5	11.8	11.4	11.5	11.8	8.6
Petro/Coal (324)	4.1	3.6	3.5	3.3	4.1	2.2	2.1	4.1	3.6	3.5	3.3
Plastics (326)	2.6	2.8	2.7	2.2	2.6	2.8	2.7	2.6	2.8	2.7	2.2
Fab. Metal (332)	6.5	6.8	7.5	4.9	6.0	5.9	6.2	6.0	7.3	7.5	4.9
Comp. Elec. (334)	6.7	5.9	5.5	3.2	6.7	5.9	5.5	7.1	5.9	5.5	4.2
Misc. (339)	6.4	5.6	5.5	2.3	6.4	5.6	5.5	6.4	5.6	5.5	1.3
R&D (541712)	3.2	3.2	2.2	1.5	3.2	3.2	2.2	3.5	3.2	2.2	1.5
Total	65	64	62	44	66	65	62	68	70	66	46

Note: Interviewees were allowed to indicate multiple industries. The responses of an interviewee who indicated a total of *n* industries receives a weight of 1/*n* in the calibration of each of those industries. Numbers in this table reflect the total of these weights in each industry for interviewees answering each question. The responses of each interviewee received a total weight of 1 across all industries in the impact assessment; therefore, totals in this table match totals in Table 3-4. R&D stages: D/D, discovery/design; Dev, development; Mfctr, manufacturing; Deplo, deployment. Model parameters: R/C, relative cost; Prob, probability of advancing to next stage; Dur, duration. These parameters correspond to Table 2 (Actual Scenario) and Table 3 (Counterfactual Scenario) in the interview guide (provided in the appendix). Industries: 325, Chemical, excluding pharmaceuticals and medicines; 331, Primary metals; 333, Machinery; 335, Electrical Equipment, Appliances, and Components; 336, Transportation Equipment, including aerospace; 324, Petroleum and Coal Products; 326, Plastics and Rubber Products; 332, Fabricated Metal Products; 334, Computer and Electronic Products, including semiconductor and other electronic components; 339, Miscellaneous Manufacturing, including medical devices; 541712, Physical, Engineering, and Life Sciences (except biotechnology) R&D.

Table 3-4. Interviewees Responding by Industry and R&D Process Model Parameter

Actual Industry	Dev R/C	Mfctr R/C	Deplo R/C	D/D Prob	Dev Prob	Mfctr Prob	D/D Dur	Dev Dur	Mfctr Dur	Deplo Dur
Chemical (325)	14	10	8	15	14	10	15	15	10	8
Primary Metal (331)	21	21	16	20	20	21	21	22	22	15
Machinery (333)	17	14	9	13	15	13	14	17	15	8
Electrical Equip. (335)	11	8	5	11	12	8	11	12	9	5
Trnsport. Equip. (336)	20	19	12	20	19	18	20	20	19	10
Petro/Coal (324)	11	9	8	11	11	9	11	11	9	8
Plastics (326)	10	8	5	10	10	8	10	10	8	5
Fabricated Metal (332)	21	21	13	21	22	21	20	22	20	11
Computer/Electron (334)	14	11	7	15	15	11	15	15	11	8
Misc. (339)	13	11	6	11	12	10	11	13	11	4
R&D Services (541712)	7	7	5	7	6	6	7	7	6	3
Unduplicated Total	76	73	53	77	76	73	78	80	74	51

Counterfactual Industry	D/D R/C	Dev R/C	Mfctr R/C	Deplo R/C	D/D Prob	Dev Prob	Mfctr Prob	D/D Dur	Dev Dur	Mfctr Dur	Deplo Dur
Chemical (325)	14	13	9	7	14	14	10	15	15	10	8
Prim. Met. (331)	19	17	18	13	18	18	19	18	19	19	14
Machinery (333)	10	12	10	6	10	11	10	10	12	11	6
Elec. Equip. (335)	8	9	7	4	9	10	7	9	10	8	4
Trnsp. Eqp. (336)	16	16	17	10	17	17	17	18	17	17	10
Petro/Coal (324)	8	9	8	7	8	7	6	8	9	8	7
Plastics (326)	8	9	8	5	8	9	8	8	9	8	5
Fab. Metal (332)	17	17	18	11	16	16	16	16	18	18	11
Comp. Elec. (334)	12	12	10	6	12	12	10	13	12	10	7
Misc. (339)	10	10	9	4	10	10	9	10	10	9	3
R&D (541712)	6	6	5	3	6	6	5	7	6	5	3
Unduplicat. Total	65	64	62	44	66	65	62	68	70	66	46

Note: Interviewees were allowed to indicate multiple industries. Numbers in this table reflect the number of interviewees in each industry answering each question. Totals in this table are unduplicated, counting each interviewee only once, no matter how many industries that interviewee is in; therefore, numbers in each column sum (over industries) to more than the total. R&D stages: D/D, discovery/design; Dev, development; Mfctr, manufacturing; Deplo, deployment. Model parameters: R/C, relative Cost; Prob, probability of advancing to next stage; Dur, duration. These parameters correspond to Table 2 (Actual Scenario) and Table 3 (Counterfactual Scenario) in the interview guide (provided in the appendix). Industries: 325, Chemical, excluding pharmaceuticals and medicines; 331, Primary metals; 333, Machinery; 335, Electrical Equipment, Appliances, and Components; 336, Transportation Equipment, including aerospace; 324, Petroleum and Coal Products; 326, Plastics and Rubber Products; 332, Fabricated Metal Products; 334, Computer and Electronic Products, including semiconductor and other electronic components; 339, Miscellaneous Manufacturing, including medical devices; 541712, Physical, Engineering, and Life Sciences (except biotechnology) R&D. In the calibration of the actual scenario model, relative cost in the discovery/design stage is normalized at 1.

As an example, for transportation equipment, the average of responses to question V.5 was 30.5%. Domestic R&D for this industry was $45.972 billion in 2013, 30.5% of which is $14.019 billion.

Step 2. Converting to Dollar-Denominated Costs: Analogy Principle. For each industry, relative costs for each R&D stage, under the actual and counterfactual scenarios, were converted to dollar-denominated costs by drawing an analogy between the total relative out-of-pocket cost in the calibrated model for an industry and the total annual R&D expenditure for that industry. The method is most easily illustrated by example.

Continuing with the example of transportation equipment, (unitless) relative costs are shown together with dollar-denominated costs in Table 3-5. Dollar-denominated costs were calculated based on an analogy: Total relative out-of-pocket costs of 159.6 in the calibrated model representing the current environment with existing infrastructure (actual scenario) were assumed to be analogous to actual R&D expenditures of $14,019 million per year. Then, every other cell in the table of dollar-denominated costs is obtained by multiplying the corresponding relative cost by the ratio of $14,019 to 159.6.

Table 3-5. Converting to Dollar-Denominated R&D Costs, Transportation Equipment

Type of Costs	Discovery & Design	Development	Manufacturing	Deployment	Total
Relative (unitless)					
Out-of-pocket, actual	46.6	35.7	40.3	36.9	159.6
Capitalized, actual	110.8	65.4	57.9	41.8	275.9
Out-of-pocket, counterfactual	8.8	8.0	12.7	25.5	54.9
Capitalized, counterfactual	15.6	12.2	16.6	27.9	72.2
Dollar-denominated (millions of 2013 U.S. dollars), based on $13.895 billion annual out-of-pocket R&D expenditure					
Out-of-pocket, actual	4,091	3,137	3,545	3,246	14,019
Capitalized, actual	9,734	5,746	5,090	3,670	24,240
Out-of-pocket, counterfactual	774	699	1,113	2,237	4,823
Capitalized, counterfactual	1,367	1,070	1,455	2,454	6,346

Note: Dollar-denominated costs in the lower part of the table were calculated based on an analogy: Total relative out-of-pocket costs of 134.2 in the calibrated model representing the current environment with existing infrastructure (actual scenario) were assumed to be analogous to actual R&D expenditures of $13,895 per year. Then, every other cell in the table of dollar-denominated costs is obtained by multiplying the corresponding relative cost by the ratio of $13,895 to 134.2.

For example, in the "Discovery & Design" column, multiplying a relative capitalized actual cost of 110.8 by $14,019 and dividing by 159.6 yields a capitalized actual cost of $9,734. Completing the table and comparing total capitalized costs, actual with counterfactual, improved infrastructure is estimated to save $17.9 billion in capitalized R&D costs per year for the transportation industry (the difference between $24.2 billion actual and $6.3 billion counterfactual).

Adding Value to R&D Outcomes. The value of R&D efficiency impacts is only part of the total value of an improved Materials Innovation Infrastructure. This value, as we have estimated it, is the value companies could realize by targeting the same R&D outcomes they would have without the improved infrastructure. But when companies are faced with opportunities to perform R&D more efficiently (at lower cost for a given outcome), it stands to reason that they would respond by targeting more ambitious R&D outcomes, aiming to deploy superior materials at a higher rate. By choosing this response, companies would reveal that they can realize greater value that way.

Through interviews with industry experts, we were able to test this hypothesis and quantify the additional value improved R&D infrastructure could enable companies to capture—by undertaking R&D projects they would not otherwise have done, leveraging that R&D to commercialize improved products and new product lines, and expand into new markets (Section IV of the interview guide, provided in the appendix).

3.5 CALCULATING CONFIDENCE INTERVALS

As is clear from the description in Section 3.2 of the R&D cost model, key measurements of interest are nonlinear functions of interviewees' quantitative responses. What is more, at least some of these quantitative responses are unlikely to be normally distributed. For example, transition probabilities are constrained to be between 0 and 1. These features complicate the calculation of confidence intervals.

A bootstrap approach is therefore used to provide confidence intervals for all quantitative measures of interest. The bootstrap approach involves generating additional (pseudo) data using the information from the original data, then drawing inferences from the pseudo data about the distribution of a measure of interest. The pseudo data are generated by resampling with replacement from the actual data to generate a large number (1,000 in this case) of pseudo samples. The measure of interest is then calculated from each of those samples, generating 1,000 pseudo observations of the measure. A confidence interval for the measure of interest can then be calculated from those 1,000 pseudo observations.

Recall from Section 3.3 that improved infrastructure is estimated to save $16.8 billion in capitalized R&D costs per year for the transportation industry. The bootstrap procedure can be explained by example, by deriving the 95% confidence interval for this estimate step by step.

Step 1. Each of our 121 observations was assigned an integer weight (i.e., 0, 1, 2, …), drawn from the binomial distribution, which is a convenient way of simulating sampling with replacement. The weight assigned to an observation represents the number of times the observation is "drawn" or selected into the pseudo sample. One set of 121 weights defines one pseudo sample.

Step 2. We performed a full analysis on the pseudo sample, deriving averages of each parameter of the R&D process model, total out-of-pocket and capitalized costs for both the actual and counterfactual scenarios, the differences between the costs in the two scenarios, etc. Each measure of interest for that pseudo sample was stored.

Step 3. Steps 1 and 2 were repeated 1,000 times, resulting in 1,000 pseudo observations of each measure of interest. For example, after completing Step 3, we had generated 1,000 pseudo observations of the capitalized R&D cost savings (i.e., the difference in capitalized R&D cost between the actual and counterfactual scenarios) for the transportation industry. These pseudo observations fell on either side of our actual observation of $17.9 billion. For the calculations that follow, it is helpful to use the more exact figure of $17.894 billion.

Step 4. The 1,000 pseudo observations were sorted, and the 25th and 976th largest for each measure of interest were stored. For capitalized cost savings for the transportation industry, x_{25} = $11.341 billion ($6.553 billion less than our estimate) and x_{976} = $25.509 billion ($7.615 billion more than our estimate).

Because the true expected value of the 1,000 pseudo observations is equal to our estimate of $17.894 billion, we can say that there is a 2.5% chance that a given observation is at least $6.553 billion less than the true expected value and also a 2.5% chance that a given observation is at least $7.615 billion more than the true expected value.

That is equivalent to saying there is a 2.5% chance that the true expected value is at least $6.553 billion more than a given observation and also a 2.5% chance that the true expected value is at least $7.615 billion less than a given observation. Therefore, a 95% confidence interval for our point estimate of $17.894 billion would be between $10.279 billion ($7.615 less than $17.894) and $24.447 billion ($6.553 more than $17.894).

4 Industry Needs Assessment

Access to high-quality data emerged as a linchpin of a Materials Innovation Infrastructure. Access to high-quality data is a prerequisite for model validation and uncertainty quantification and for the productive application of machine learning, modeling and simulation, and many other elements of an envisioned Materials Innovation Infrastructure.

Through preliminary scoping interviews with industry experts and review of the relevant literature, issue briefs, and industry reports, as discussed in Section 3.1, we identified six broad areas of industry need to be addressed by an improved Materials Innovation Infrastructure. Table 4-1 presents these areas of need and provides illustrative examples of the types of infrastructure technology that could address each one and the types of potential impacts improved infrastructure could be expected to have.

Experts interviewed—both for the preliminary scoping interviews and the more structured, guided interviews—stressed the strong complementarity among the six areas of need and the consequent overlap among the types of infrastructure and potential impacts. One important policy implication of this complementarity is that infrastructure investments should be planned with all of the six areas in mind; to ignore any one of the six would reduce the value realized from investments aimed at addressing the others.

Access to high-quality data emerged as the most important need and one of the most difficult for industry to address exclusively through private investment (Figures 4-1 and 4-2). Moreover, through qualitative discussions, access to high-quality data emerged as a linchpin of a Materials Innovation Infrastructure. Access to high-quality data is a prerequisite for model validation and uncertainty quantification and for the productive application of machine learning, modeling and simulation, and many other elements of an envisioned Materials Innovation Infrastructure. In discussions of the other five identified needs and the kinds of infrastructure that could help address them, interviewees often returned to the primacy of high-quality data to emphasize that "this other thing [i.e., the specific infrastructure technology under discussion] does not work without it."

Table 4-1. Technology Infrastructure Needs for Advanced Materials Innovation

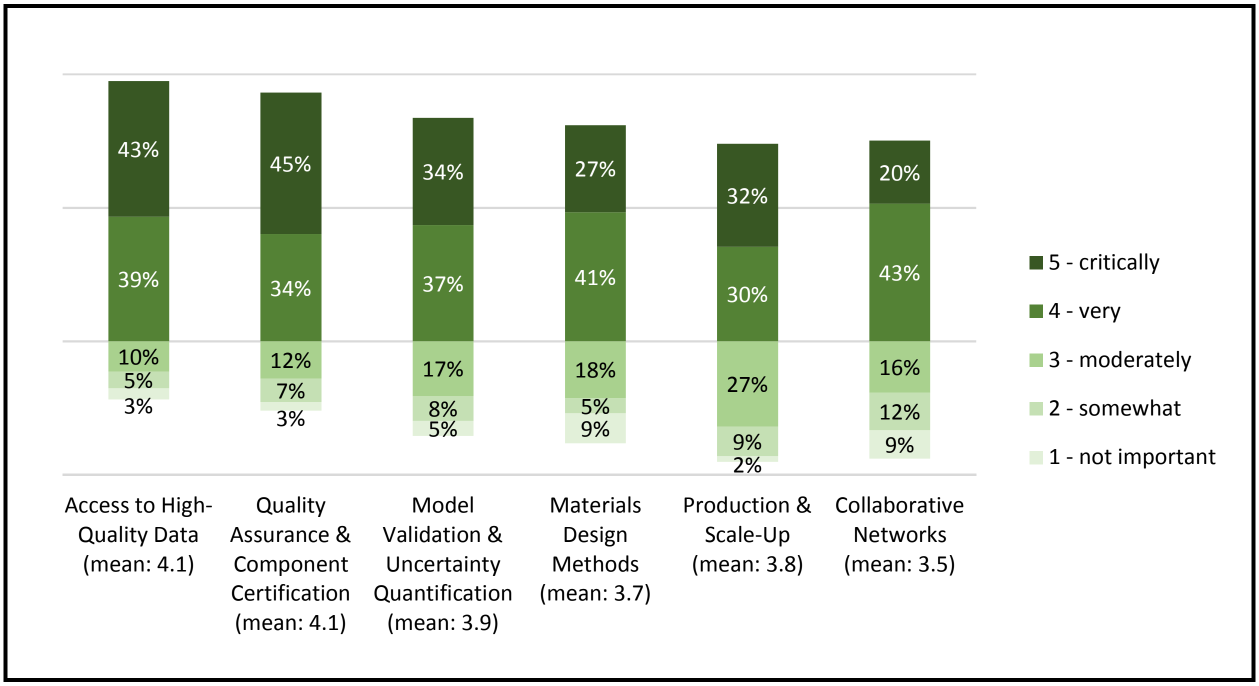
Industry Need	Examples of Infrastructure Technology to Address Need	Potential Impacts
Access to High-Quality Data		
Nonproprietary experimental data, computational data, and software code	▪ Fundamental materials data ▪ Data standardization and curation ▪ Models underpinning accurate and repeatable material measurement	▪ More easily leverage prior research with less duplication of effort ▪ Enable greater reliance on more efficient computational approaches
Collaborative Networks		
Efficient means of sharing materials information (e.g., along a supply chain, among research collaborators)	▪ Methods for capturing, characterizing, and sharing materials data in structured formats ▪ Communication standards and translators ("MT Connect for material measurement equipment")	▪ Align academic and public-sector research to industry-relevant challenges ▪ Integrate experimental measurement and computational modeling to improve model fidelity and overall utility ▪ Realize network externalities
Material Design Methods		
Shorter paths to better starting points Inverse modeling capability	▪ Models, simulations, and metrologies for advanced materials design ▪ Machine learning tools	▪ Enable more targeted searches of design space for promising candidate materials ▪ Identify more novel materials, breaking out of the search for incremental improvements to find more distant global optima
Production & Scale-Up		
Model-based alternatives to expensive physical testing, trial and error–based approaches Faster, cost-effective means of producing advanced materials at pilot and full scales	▪ Multiscale modeling frameworks (integrating macroscopic process models with microscopic materials simulation) ▪ Process technology platforms (e.g., cold sintering, additive manufacturing, roll-to-roll printing, directed self-assembly)	▪ Reduce trial and error when scaling up (from lab scale to pilot scale, from pilot scale to production scale) ▪ Overcome the "Valley of Death" between lab scale and production scale: pilot-scale manufacturing services and facilities are underprovided by the market

(continued)

Table 4-1. Technology Infrastructure Needs for Advanced Materials Innovation (continued)

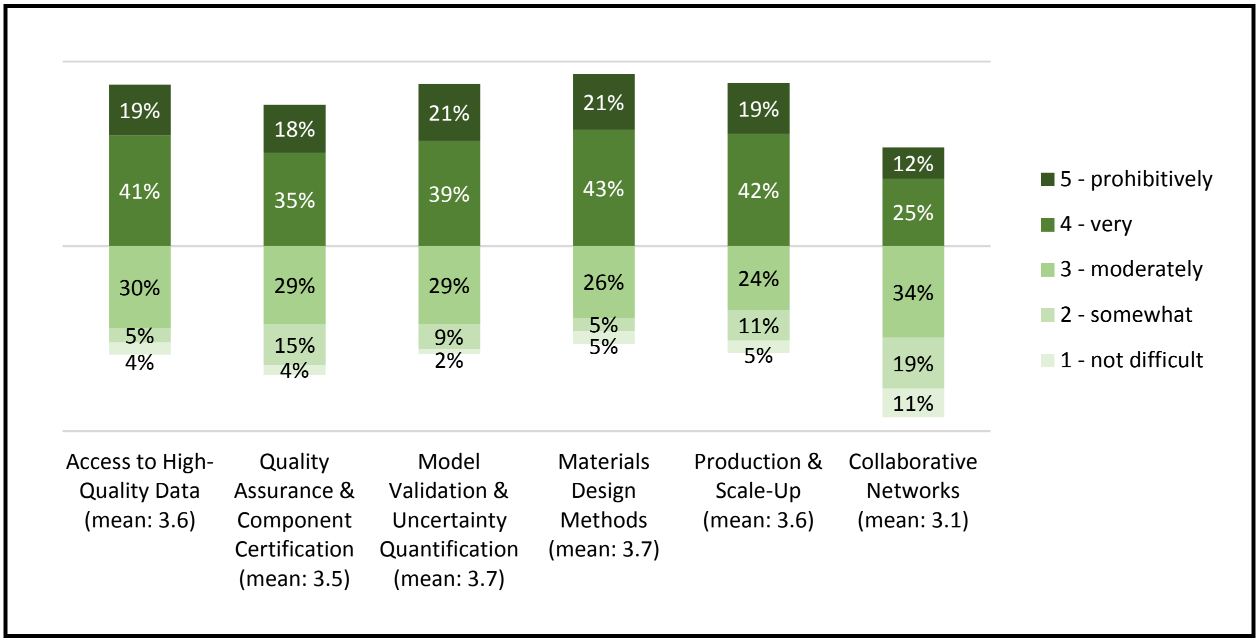
Industry Need	Examples of Infrastructure Technology to Address Need	Potential Impacts
Quality Assurance, Quality Control & Component Certification		
Ability to model, predict, and control formation of defects Ability to forecast manufacturing variation	▪ Performance metrics (benchmarks, reference data, testbeds to characterize performance of systems and components) ▪ Process control tools (test protocols, objective scientific and engineering data, reference databases)	▪ Reduce the cost of controlling and verifying the performance attributes of materials—and components and products embodying those materials ▪ Reduce the risk of large costs incurred if defects are not detected and lead to product failures in use (e.g., lithium-ion battery fires)
Model Validation & Uncertainty Quantification		
Basis for trust and acceptance of computational models Basis for objective decision-making regarding reliance on computational analysis and simulation at a business level	▪ Generally accepted and easily applied methods for uncertainty quantification for both experimental and computational data ▪ Validation of analytical methods and procedures, emphasizing industrially relevant systems, comparing predicted and measured properties from multiple sources	▪ Enhance the utility of computational approaches from an engineering perspective ▪ Enable rational decision-making regarding computational approaches from a business perspective ▪ Advance industry’s reliance on computational approaches in situations where they can save cost and add value

Figure 4-1. Interviewees' Rating of Importance of Technology Infrastructure Needs



Note: Percentages shown reflect the distribution of ratings. Average ratings are given in parentheses below each area of industry need.

Figure 4-2. Interviewees' Rating of Difficulty of Meeting Needs through Private Investment



Note: Percentages shown reflect the distribution of ratings. Average ratings are given in parentheses below each area of industry need.

To justify the need for public investment in Materials Innovation Infrastructure, industry experts emphasized its public-good content and the multidisciplinarity required to develop it.

All of the elements of the envisioned Materials Innovation Infrastructure have strong public-good content. Companies therefore have weak incentives to develop these technologies themselves. This essential insight was borne out in interviews with industry experts. Beyond the public-good content of infrastructure technologies, the principal cross-cutting justification for public investment, voiced most often by industry experts as the reason identified needs could not be effectively addressed through private investment, was the multidisciplinarity required to meet the needs. Collaboration is needed among computer scientists, statisticians, data analysts, and materials engineers with both computational and experimental expertise. This multidisciplinary expertise is found only in some larger companies. Industry experts, even those at large, diversified companies, stressed that the depth of expertise and close collaboration across multiple disciplines required to develop a Materials Innovation Infrastructure is more than they have in-house and is a reason they value the involvement of the national laboratories.

The difficulty of meeting a need through private investment, for which ratings are summarized by Figure 4-2, could reflect either technical difficulty (i.e., the difficulty of developing a solution with the R&D facilities and personnel at the company's disposal) or the difficulty of justifying investment in developing a solution or buying a solution from outside the company. The difficulty rating is intended to capture industry experts' perceptions of the importance of public investment: Is this a need that the private sector can adequately address on its own (reflected in a lower difficulty rating), or is there a compelling argument for public investment in infrastructure technology (reflected in a higher difficulty rating)?

All six areas of need were perceived to be "very" or "critically" important by at least 60% of respondents, led by access to high-quality data (82%) and quality assurance, quality control, and component certification (78%). Five of the six needs were perceived to be "very" or "prohibitively" difficult to address through private investment by at least 50% of respondents, led by materials design methods (64%), followed by production and scale-up, model validation and uncertainty quantification, and access to high-quality data (all tied at 60%). Figures 4-1 and 4-2 summarize these results.

When respondents rated something as being relatively unimportant to them, one or more of three broad reasons was typically offered, no matter which area of need they are discussing:

1. They deem the technology to be underdeveloped for their purposes, either because they are unaware of recent data and model improvements or because they work with materials for which these tools are less fully developed (this viewpoint was especially common for ceramics, electronics, and biomaterials).

   To paraphrase one interviewee: "Computational methods have difficulty dealing with the statistical probability of defects, their location, and the statistical imprecision of manufacturing processes, whether making aluminum or composites."

2. They think that their status quo of operations is efficient enough. This attitude seemed to come most often from respondents with exclusively experimental backgrounds.

3. They are worried about keeping information proprietary and protecting their intellectual property (although we tried to emphasize voluntary exchange of precompetitive, or nonproprietary, information and data in follow-up questions with these respondents, it was still a concern often heard).

Common themes and key takeaways from the qualitative insights provided by respondents are discussed below for each identified area of need.

4.1 ACCESS TO HIGH-QUALITY DATA

The identified need for access to high-quality data refers to precompetitive as opposed to proprietary data. Although companies must also produce data specific to proprietary materials they are developing, they can often benefit from nonproprietary, or nonmarket-oriented, data on related generic materials, which companies can use to develop computational models. For instance, a company could use high-quality data on a generic material (like the now standard 4130 steel alloy) to develop and calibrate a computational model, verify that its predictions are accurate, and quantify the uncertainty or variability associated with its predictions. The company could then use the model to simulate the properties of a proprietary material it is developing (like a new alloy that strives to offer improvements in terms of performance characteristics or cost).

In general, improved access to high-quality data will enable companies to rely increasingly on computational approaches to materials design in situations where doing so can reduce costs, accelerate timelines, and improve outcomes.

Fundamental materials data can be generated by experiments (experimental data, which are generated from observations on actual physical materials) or by computer simulations (computational data, which are generated by computational models). High-quality data include not only measured quantities but also information about the precision of the measurements and the methods by which they were obtained. Computational data are most useful when accompanied by the software code used to generate the data.

Besides fundamental materials data, organized in standard reference datasets, examples of infrastructure that could improve access to high-quality materials data include methods for data standardization and curation and the models underpinning accurate and repeatable material measurement. For example, several respondents noted the need for improved sensors that are able to automatically collect and upload data generated through experiments or in production lines. Such tools would automate the data generation and organization process, improving the quality and efficiency of data collection and reducing the cost of contributing to private or common high-quality materials databases.

A shortage of high-quality data "drives conservatism" and slows down the innovation process.

Industry experts indicated that a shortage of high-quality data "drives conservatism" and slows down the innovation process. Without high-quality data that could be used to evaluate new candidate materials early on in the discovery/design phase when the cost of failure is lower, companies are unwilling to take chances for fear that technical failures in later R&D stages will be too costly. Without the ability to effectively screen candidate materials early on, the expected cost of attempting to develop a new material is prohibitive, and companies are more likely to stay with materials they know. Materials innovation then tends to be limited to incremental improvements without attempts at breakthrough innovation.

One materials engineer described it as "local optimization" as opposed to "global optimization"—locating slightly higher ground near where you are already standing (on the surface of an objective function) instead of striking out to find a higher hilltop farther away. In his analogy, high-quality data are (an essential part of) the telescope that helps you find the higher hilltop in the distance. Improved access to high-quality data would lead to a greater number and diversity of ideas being explored in the discovery/design stage.

A common remark was that "the data are out there" but not really accessible. Either the data are not in digital form (e.g., underlying published results and represented in tables and figures in online articles, and therefore prohibitively costly to extract on a useful scale, given currently available tools) or else they are behind a pay wall. The upshot is that only very large companies can afford to access high-quality digital data.[9] Small companies are shut out of ("can't play" in) certain markets because their customers want them to be using the same data and models as the larger companies. This point was emphasized not only by small companies but also by downstream customers who felt locked into buying from a few large companies. For these downstream customers, the difficulty faced by smaller prospective suppliers in accessing high-quality data represented a "weakness in their supply chain."

With improved access to high-quality data, companies could better leverage published research without needing to replicate experiments, enabling them to more quickly focus on the most promising compositions and processes as the starting point for developing a new material.

With improved access to high-quality data, companies could better leverage published research with less need to replicate the underlying experiments, enabling them to more quickly focus on the most promising compositions and processes as the starting point for developing a new material. In the current environment, the same experiments are being repeated again and again by different researchers, each extracting only the information they need. Variations in experimental conditions—without the means to combine data across all of the different experiments—reduce the quality, or information content, of the body of published results produced by these experiments. In these conditions, replication wastes resources. With standardization of experimental conditions—not necessarily making all experiments the same but rather enabling experimenters to measure and record all relevant differences in a standardized way—and the means of measuring, recording, and digitally publishing all of the information that can be captured from a given experiment, this situation would change:

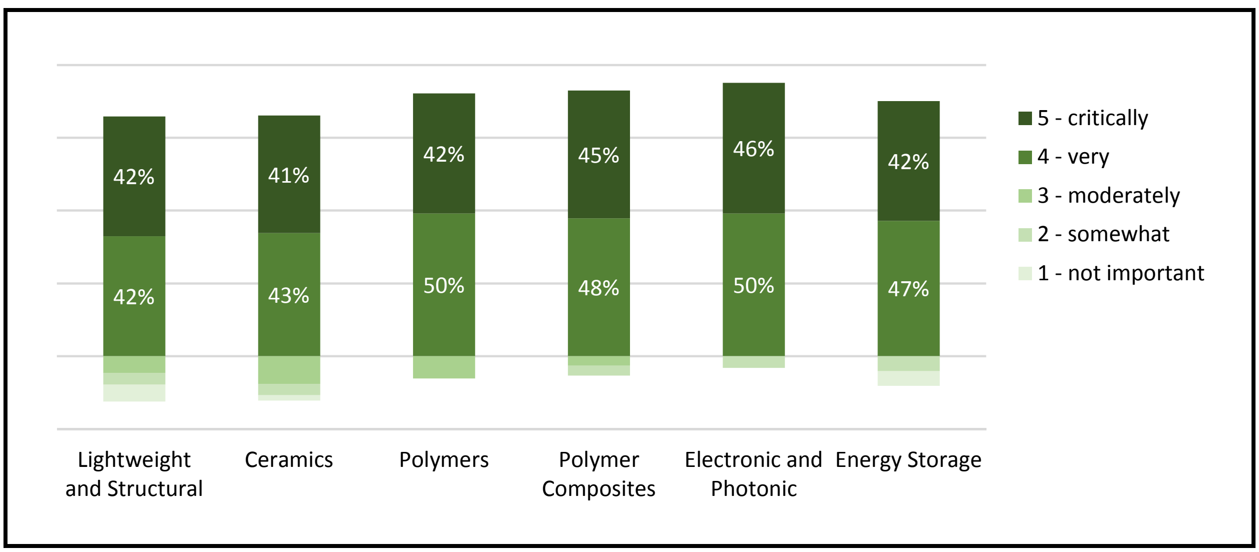
[9] Notable exceptions exist where small companies focusing on lab-scale discovery and design rely heavily on commercial data and modeling tools.

Some degree of replication would be productive, because the data from each experiment could be combined with that from related experiments to yield better information (e.g., improving the accuracy and precision of a given measurement or prediction); truly redundant experiments (doing the same experiment again only to capture information that was not collected from previous ones) would become unnecessary, freeing research resources for more productive uses.

Industry experts emphasized that being able to trust and use published research is critically important to companies, for which the replication of published research can be a significant—and for some potential R&D projects a prohibitive—cost at the discovery/design stage. From structural alloys to nanomaterials, industry researchers reported roughly a 50% "hit rate" when trying to reproduce published results. The other half of the time, misses were generally attributable to an omitted step or an incorrect interpretation in the published research. In nanomaterials, where results can depend on atom-level purity, researchers have encountered published results of "successful" experiments that were later found to have been the result of contaminants.

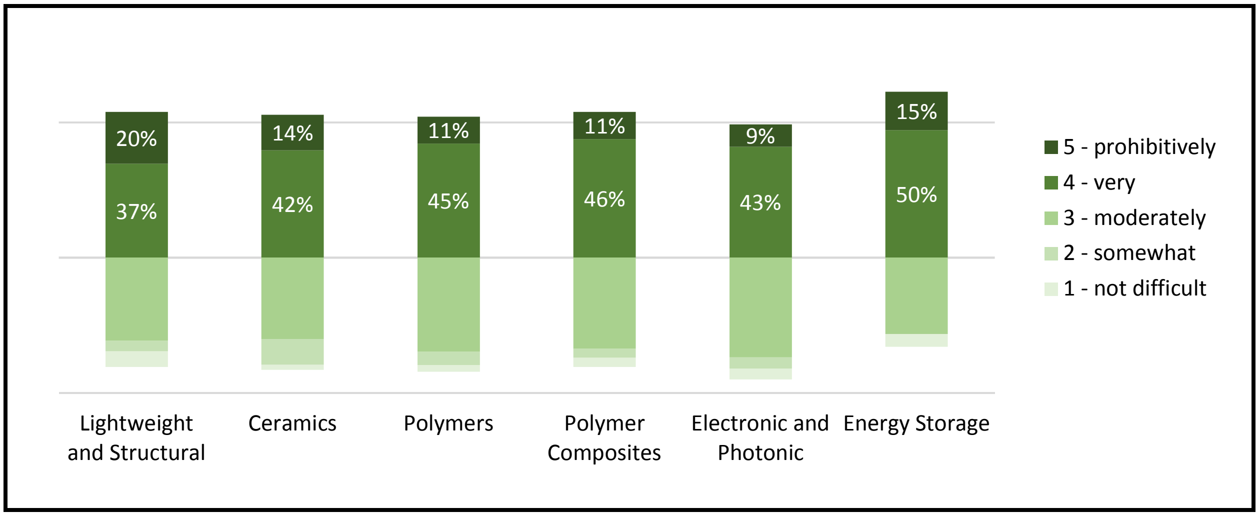
Interviewees' ratings of the importance and difficulty of meeting this need did not vary significantly across materials classes (Figures 4-3 and 4-4).

Figure 4-3. Interviewees' Rating of Importance of Access to High-Quality Data



Note: The distribution of ratings is shown for the six materials classes represented by at least 20 interviewees.

Figure 4-4. Interviewees' Rating of Difficulty of Addressing the Need for High-Quality Data through Private Investment



Note: The distribution of ratings is shown for the six materials classes represented by at least 20 interviewees.

4.2 COLLABORATION NETWORKS

The collaborative networks envisioned as part of an improved Materials Innovation Infrastructure would provide an efficient means of voluntarily sharing materials information across tiers of supply chains or among research collaborators. As envisioned, these networks would help address industry's need for high-quality experimental data, computational data, and software code by providing a means of connecting disparate but related datasets and making it possible to locate relevant data with targeted searches.[10]

Ultimately, collaborative networks could alter the incentives facing academic researchers, with positive impacts on the translation of public science into commercial applications. Proponents envision a means of tracking the use of digital data and software code that attaches credit to its originator. In this way, researchers who produce relevant, well-interpreted, reproducible data and results, which are then used by others, will receive recognition analogous to that which attaches to publication and citation today. The idea is that by providing a

[10] Collaboration networks envisioned as part of the MGI are distinct from the similar-sounding "innovation clusters" much discussed in innovation policy circles. Innovation clusters are physically collocated firms and universities, whereas collaboration networks are virtual, geographically dispersed, having nodes connected by the internet.

means of recognizing more relevant contributions to materials science and engineering, collaborative networks can alter incentives and thereby change behavior, increasing the productivity of research, measured in terms of its translation into commercial applications and ultimate impacts.

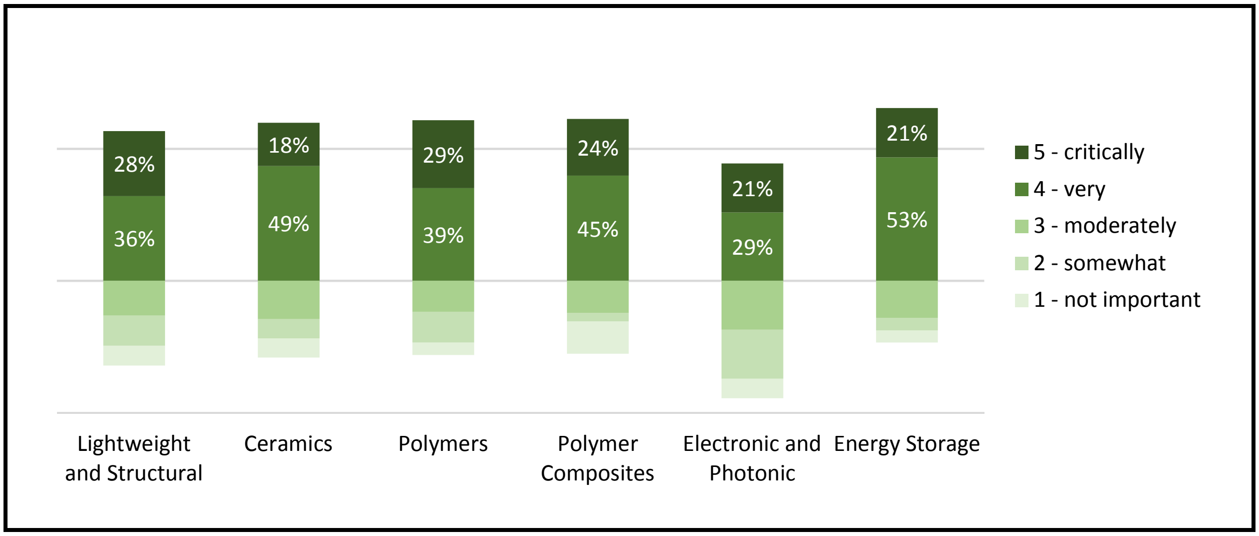
Keeping proprietary information private and protecting their intellectual property was highlighted by many respondents as the key deterrent to taking part in collaborative networks, even among those who considered improved collaborative networks to be important. For example, a company producing a range of metal alloy materials stated that collaborative networks have a direct benefit for companies like theirs, but only if they can protect their intellectual property while contributing. Respondents generally perceived a useful role for a neutral body with technical expertise in facilitating interactions between potentially competing entities.

Respondents who rated collaborative networks highly were more likely to emphasize the importance of network externalities in realizing the benefits of MGI approaches: the more other organizations in their supply chains invested in MGI approaches, the greater the return on their own investments.

Collaborative networks were less likely to receive the highest ratings for importance or difficulty. Notably, however, respondents who did rate collaborative networks highly in both respects were more likely to emphasize the importance of network externalities in realizing the benefits of MGI approaches: the more other organizations in their supply chains invested in MGI approaches, the greater the return on their own investments. In the context of these discussions, respondents counted universities among these organizations in two important respects, both of which could be enhanced by collaborative networks. First, academic research was a source of fundamental knowledge, which collaborative networks could enhance by making digital data more available and its quality (especially its reproducibility) easier to assess. Second, these respondents emphasized the importance of universities as a source of talented scientists and engineers: new hires out of graduate programs and consultants and collaborators among faculty.

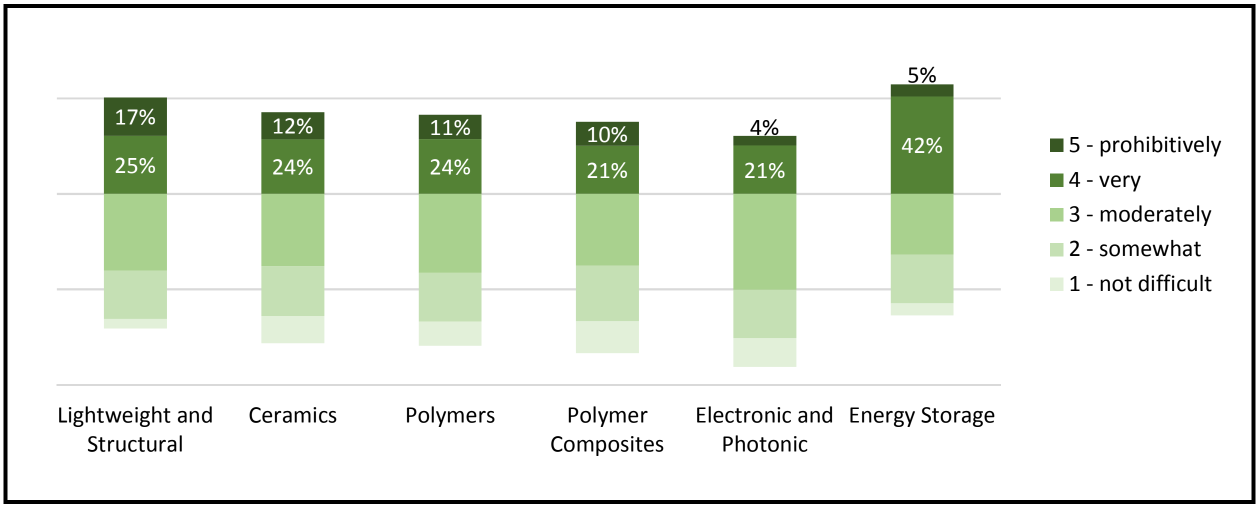
Interviewees’ ratings of the importance and difficulty of meeting this need vary only slightly across materials classes (Figures 4-5 and 4-6). Differences were not statistically significant, and qualitative discussions in interviews revealed no notable justification for them, so these differences among materials classes should not be overinterpreted.

Figure 4-5. Interviewees' Rating of Importance of Collaborative Networks



Note: The distribution of ratings is shown for the six materials classes represented by at least 20 interviewees.

Figure 4-6. Interviewees' Rating of Difficulty of Provisioning Collaborative Networks through Private Investment



Note: The distribution of ratings is shown for the six materials classes represented by at least 20 interviewees.

4.3 MATERIALS DESIGN METHODS

High-quality materials data are food for computational modeling and simulations. These computational materials design methods are needed to analyze the data and generate testable hypotheses and predictions that aid the process of designing and developing new materials.

Commercial computational software packages are available but expensive, making them accessible only to (typically larger) companies with large R&D budgets. Many respondents indicated that even if their companies were able to afford the tools needed for improved materials design, they lack the internal expertise to use such tools. A typical comment was that "the tools exist, but they require a highly specialized modeler to use them, and our company's business model, or the business model of a typical company in our supply chain, does not support a dedicated full-time employee who is so highly specialized."

Realizing a vision of using machine learning approaches for materials discovery requires collaboration among computer scientists, statisticians, data analysts, and materials scientists and engineers.

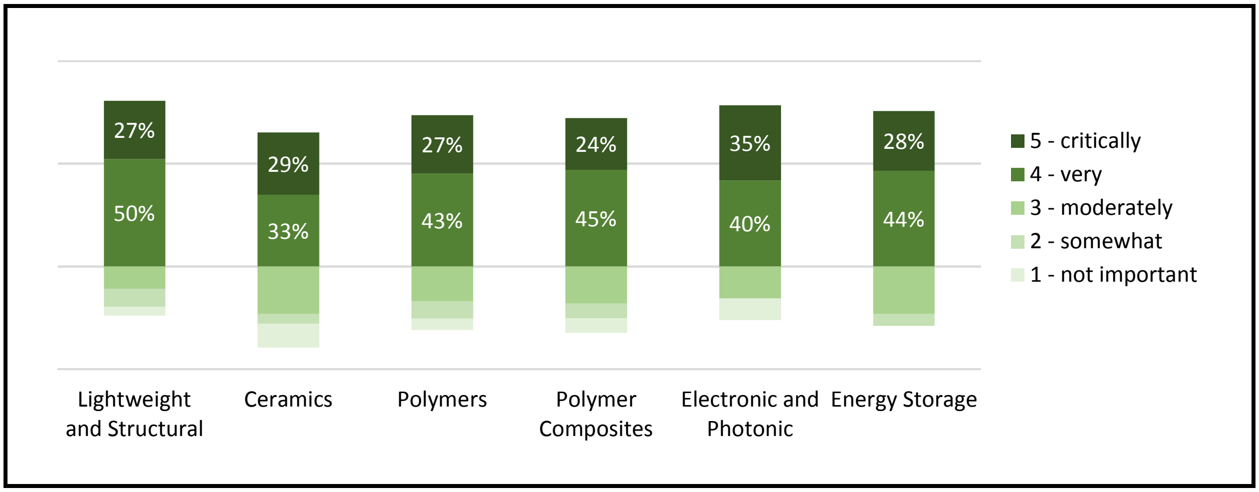
Moreover, the need for materials design methods is broader than modeling software. As industry's needs for high-quality data and collaborative networks are met, the potential increases for machine learning (i.e., artificial intelligence) to identify related datasets, uncover correlations, and generate new hypotheses by analyzing massive amounts of data.

Realizing this vision requires collaboration among computer scientists, statisticians, data analysts, and materials scientists and engineers. This breadth of expertise is rarely found all in one place in U.S. industry, but it is found in U.S. national laboratories. One industry expert was especially blunt: "No U.S. company can develop multiscale modeling frameworks,[11] nor would they have the incentive to attempt to do so. But many companies would benefit from having this capability."

Interviewees' ratings of the importance and difficulty of meeting this need vary only slightly across materials classes (Figures 4-7 and 4-8). Differences were not statistically significant, and qualitative discussions in interviews revealed no notable justification for them. Therefore, these differences among materials classes should not be overinterpreted.

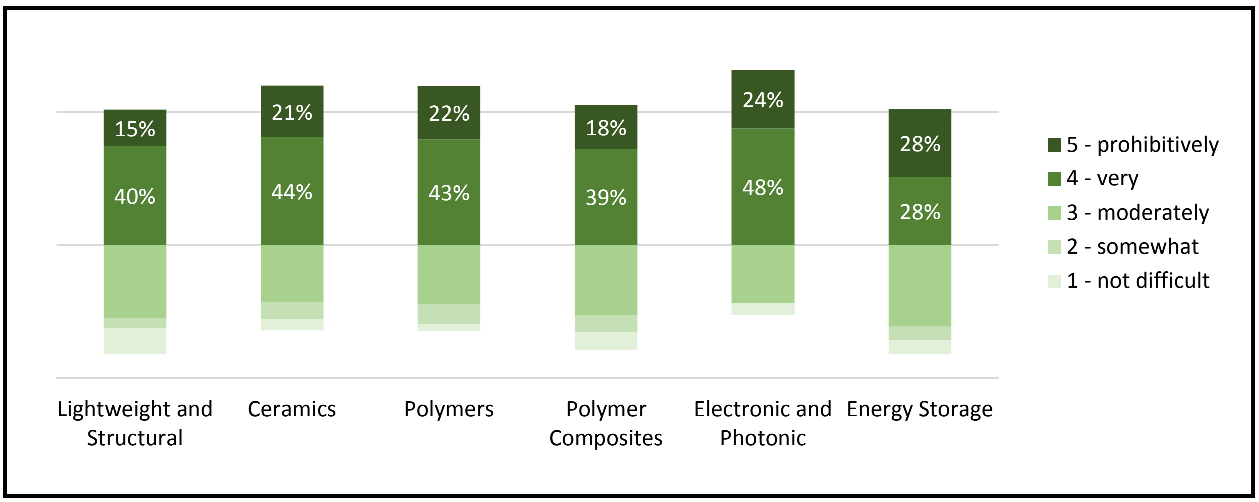
[11] An example of infrastructure technology offered in the interview guide, multiscale modeling frameworks are analytic means of linking macroscopic process models with microscopic materials simulations.

Figure 4-7. Interviewees' Rating of Importance of Materials Design Methods



Note: The distribution of ratings is shown for the six materials classes represented by at least 20 interviewees.

Figure 4-8. Interviewees' Rating of Difficulty of Provisioning Infrastructure for Materials Design Methods through Private Investment



Note: The distribution of ratings is shown for the six materials classes represented by at least 20 interviewees.

4.4 PRODUCTION AND SCALE-UP

Computational approaches that could reduce failure rates in later R&D stages, especially the scale-up that happens in the manufacturing stage, could have enormous impact. Failures at this stage can be extremely costly because of the amounts of materials used and the costs of setting up large-scale production runs. There is also the large sunk cost of earlier R&D stages at stake.

Key to preventing costly failures at this stage is to be able to predict them and then go forward with expensive physical testing only when computational models predict a high likelihood of success. For some materials classes, like metal alloys, good process models are available and commonly used. In others, like polymer composites or biomaterials, such models are less well developed. Typical of materials classes and applications where models are available and widely used is that the properties of the bulk materials are more readily translated into good predictions of the materials' performance characteristics in a product application. Models of the way a material behaves at a molecular level (e.g., in nanotechnology applications) or of material behavior at interfaces between thin layers of different materials are comparatively less mature and therefore less widely used in industry.

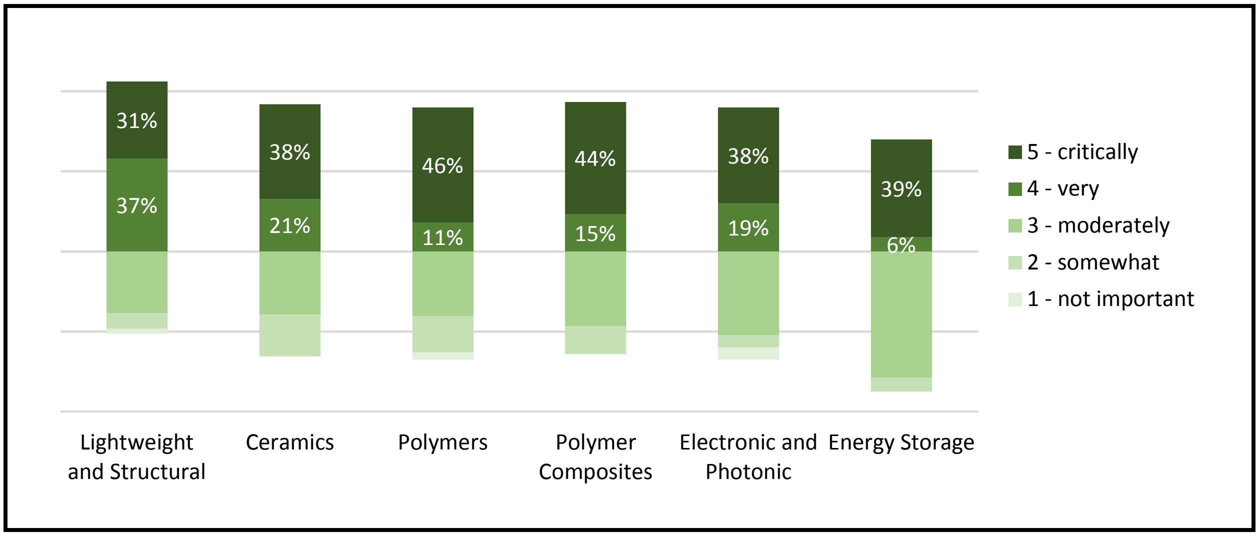
Interviewees across seemingly very different industries and applications emphasized the difficulty of scaling the production of a new material.

Interviewees across seemingly very different industries and applications emphasized the difficulty of scaling the production of a new material. The common denominator here seemed to be the company's size. Small, innovative startups, whether developing advanced structural alloys or nanotechnology components for flexible touchscreens or batteries, typically need to partner with other companies after the discovery/ design stage. For the metal alloy developer, the challenge is finding a foundry that will do pilot-scale runs. For the developer of a touchscreen or flexible battery material, the challenge is putting their product into a prototype device with all of the other components it needs to function, if only in a rudimentary way for demonstration purposes.

As examples of other countries' proactive efforts to address this issue, interviewees referenced the Industrial Technology Research Institute (ITRI) of Taiwan, the Electronics and Telecommunications Research Institute (ETRI) of South Korea, and the Fraunhofer institutes in Germany. Fraunhofer's 67 institutes had a research budget in 2015 of more than 2.1 billion euros ($2.2 to $2.4 billion U.S. dollars in 2015), 30% of which comes from German state and federal governments; by comparison, U.S. government investment in the Manufacturing Innovation Institutes of Manufacturing USA is roughly one-tenth that amount.[12] Although the respective policy scopes of Fraunhofer and Manufacturing USA are not perfectly analogous, the magnitude of the funding difference loomed large for many industry respondents.

Interviewees' ratings of the importance and difficulty of meeting this need did not vary significantly across materials classes (Figures 4-9 and 4-10).

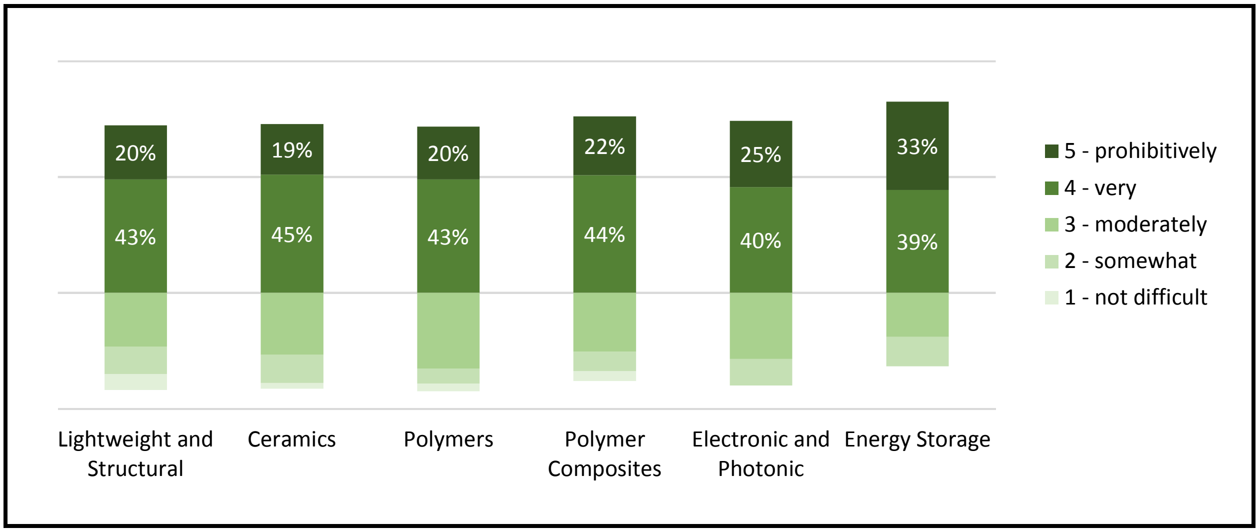
Figure 4-9. Interviewees' Rating of Importance of Provisioning Infrastructure for Production and Scale-Up



Note: The distribution of ratings is shown for the six materials classes represented by at least 20 interviewees.

[12] According to the 2015 annual report of Fraunhofer-Gesellschaft, almost 30% of its 2.1-billion-euro annual research budget "is contributed by the German federal and state governments in the form of base funding, enabling the institutes to work ahead on solutions to problems that will not become relevant to industry and society until five or ten years from now." Manufacturing USA institutes are funded by the U.S. government through cooperative agreements, with the federal funding level between $70 million and $110 million (https://www.manufacturing.gov/funding/).

Figure 4-10. Interviewees' Rating of Difficulty of Provisioning Infrastructure for Production and Scale-Up through Private Investment



Note: The distribution of ratings is shown for the six materials classes represented by at least 20 interviewees.

4.5 QUALITY ASSURANCE AND CONTROL AND COMPONENT CERTIFICATION

Before a new material can be made available as a commercial product and used in commercial applications, its manufacturer must develop quality-control practices. For applications critical to health and safety, such as implantable medical devices and aerospace, new products must undergo certification or qualification testing. New materials may themselves be subjected to certification or qualification testing before being used in the actual product.

Computational modeling and simulation can help reduce the cost of quality assurance, quality control, and qualification and certification testing. Application of computational approaches for this purpose begins in the discovery/design R&D stage, where researchers working with small amounts of material can gain early insight into its susceptibility to defects at manufacturing scale.

For example, if it is difficult to completely eliminate variation in a material's composition or microstructure at manufacturing scale, early research may look for materials with performance characteristics (such as strength and conductivity) that are comparatively robust to small variations in those attributes that are difficult or expensive to control at manufacturing scale.

Modeling and simulation could not only find the "hilltops" of an objective function in design-attribute space but also describe how steeply that hilltop falls away in different dimensions. If certain dimensions are difficult or expensive to control at manufacturing scale, the best material might be one that attains a slightly lower hilltop that falls away gradually instead of the highest peak with a precipitous drop off.

In later stages of R&D, computational models can be used to forecast manufacturing variation and, by understanding its determinants, better control it.

Computational modeling and simulation can reduce the overall cost of physical testing by reducing failure rates, enabling companies to better predict the outcomes of physical testing and go forward only when there is high confidence of success.

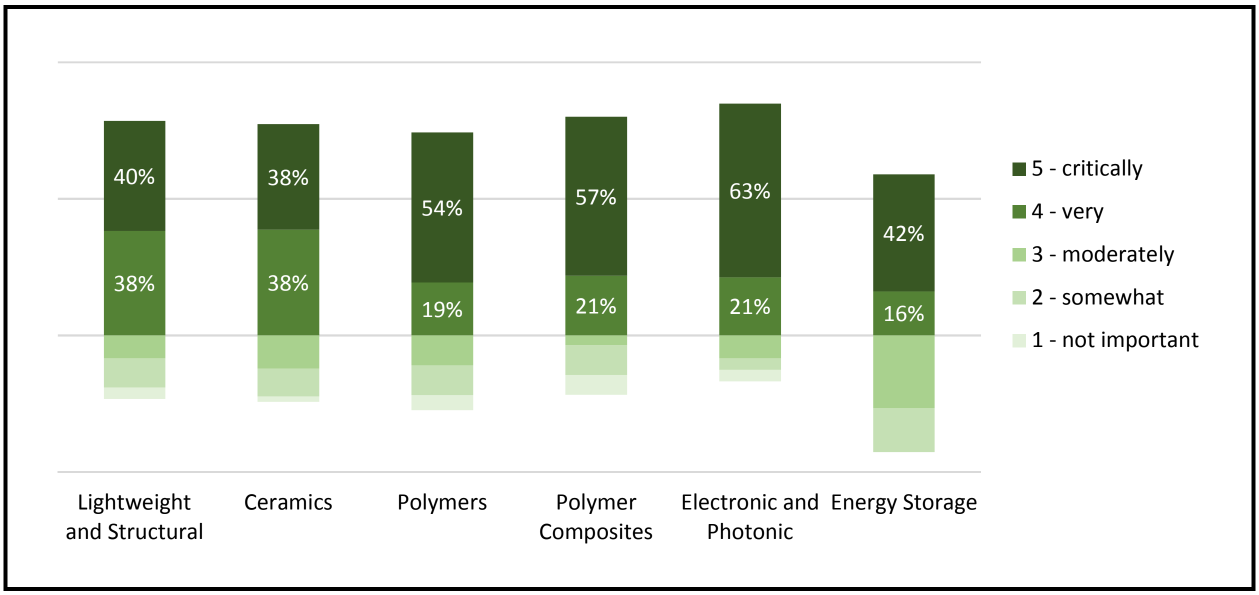
Physical testing of materials is expensive. Material samples, batches, or parts must be manufactured, often on a large scale, to undergo testing. Computational modeling and simulation can reduce the overall cost of physical testing by reducing failure rates. A common misconception is that the objective is to reduce the need for physical testing—to actually reduce the number of successful tests that must be performed before the material is accepted—by relying instead on high-fidelity simulations. Although reducing the need for physical testing may be a part of the story in some applications, it is generally not where the greatest potential impact is to be found. Rather, the proposition is to be more certain of a successful outcome before beginning the expensive process of physical testing, saving time and material that would otherwise be wasted on failed tests.

These points apply equally to product acceptance testing at the point of market transactions as well as to R&D operations. As part of the manufacturing stage of R&D, a company will perform tests to ensure a newly developed manufacturing process is producing the new material to the correct specifications. Buyers must likewise be satisfied that the material's performance characteristics meet their specifications. Being able to accurately and efficiently measure compliance with performance specifications therefore has important implications even after a material's first use in a commercial application, which defined the end of the deployment stage in our R&D process model; it affects a new material's rate of diffusion into multiple commercial applications.

A common theme, especially notable for additive manufacturing, semiconductors, and nanomaterials, was the need to assess the quality, in terms of purity or other attributes, of incoming raw materials. Nanomaterials manufacturing, for instance, requires extremely high purity for reagents, and it is typical to have to rely on suppliers who are focused on larger customers with less stringent requirements, making it necessary for nanomaterials developers to do their own quality control testing on raw materials after acquiring them from upstream suppliers.

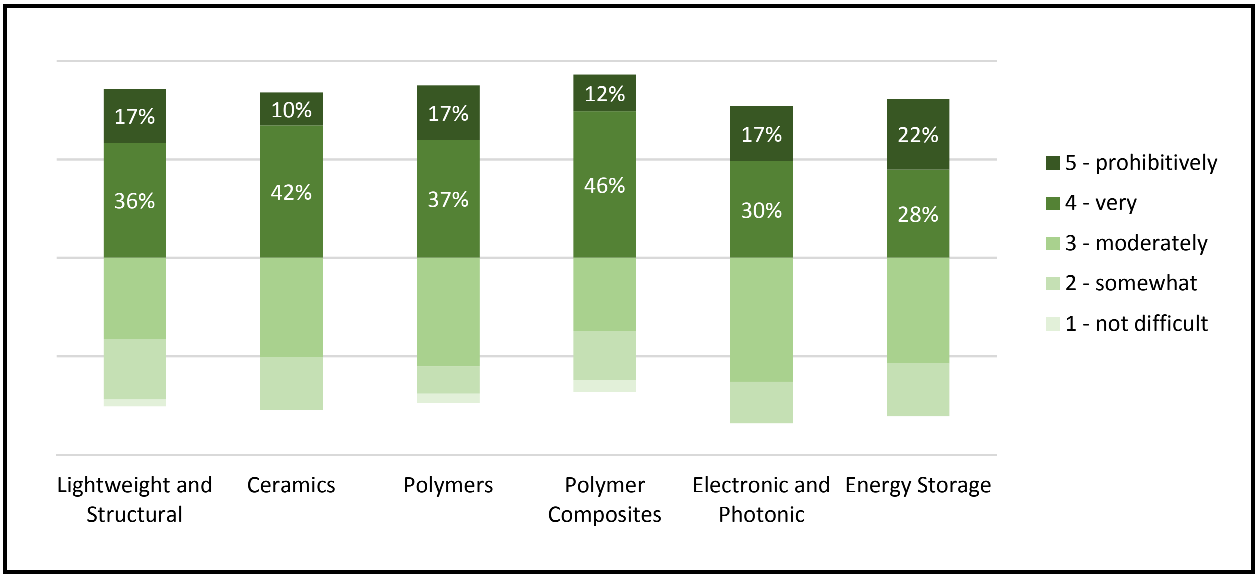
Interviewees' ratings of the importance and difficulty of meeting this need did not vary significantly across materials classes (Figures 4-11 and 4-12). Although its importance rating is lower for energy storage materials, no justification for such a difference emerged from the interviews, so it should not be overinterpreted.

Figure 4-11. Interviewees' Rating of Importance of Quality Assurance/Control and Component Certification



Note: The distribution of ratings is shown for the six materials classes represented by at least 20 interviewees.

Figure 4-12. Interviewees' Rating of Difficulty of Provisioning Infrastructure for Quality Assurance/Control and Component Certification through Private Investment



Note: The distribution of ratings is shown for the six materials classes represented by at least 20 interviewees.

4.6 MODEL VALIDATION AND VERIFICATION AND UNCERTAINTY QUANTIFICATION

Computational models and simulations are only useful if they make good predictions. No model makes predictions with perfect accuracy and precision. Being able to understand and quantify a model's accuracy and precision is therefore critical for making good use of it.[13]

Developing a general architecture and specific tools for uncertainty quantification to address this need requires a combination of statistical analytic and materials engineering expertise that is not typically required by the business model of any one company. Even when the multidisciplinary expertise does reside within a company, companies have weak incentives to develop and disseminate general purpose tools and methods for model validation and uncertainty quantification. Industry experts who characterized this issue saw the potential to address it by leveraging "significant untapped capabilities" in national laboratories.

[13] Although uncertainty quantification, or UQ, is the term that has taken hold, its meaning is actually closer to precision quantification: describing in quantitative terms how far an estimate or prediction is likely to be from the "true" value of something.

Industry experts expressed a keen interest in better tools to meet this need. Materials scientists and engineers who perceive the benefits of computational modeling and simulation in their work said that better tools in this area would be a “force multiplier,” greatly enhancing the value they can leverage from computational approaches to materials design.

Lack of validation data presents a bottleneck. A repository of measured basic properties (e.g., band gaps, conductivities, structural properties) of different materials classes would be enormously valuable.

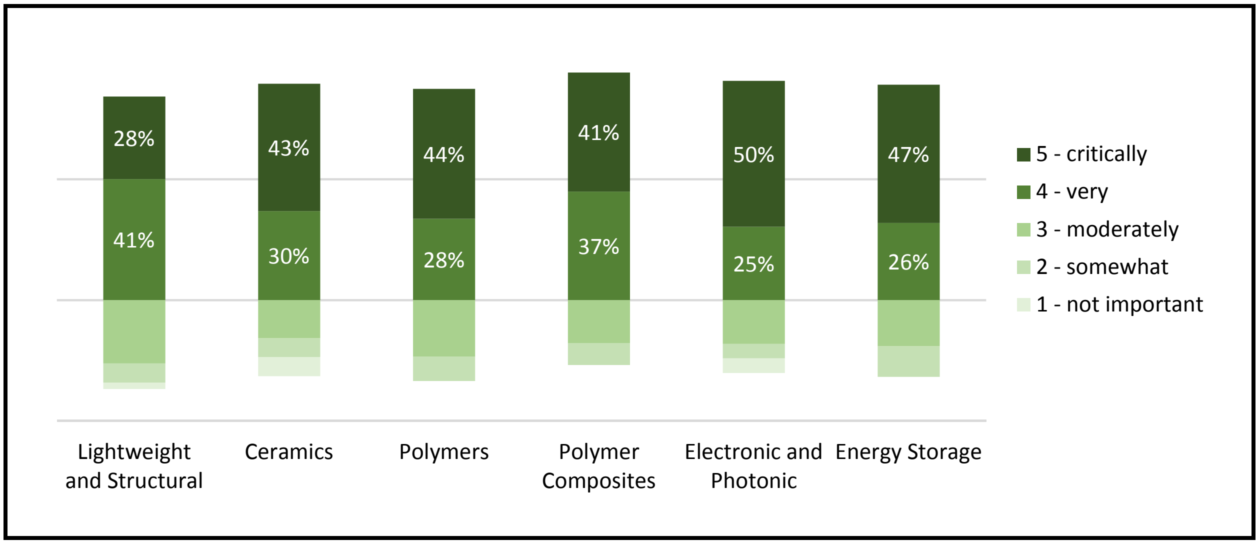
On a pragmatic note, many emphasized the need to make a business case for investment in computation; they see uncertainty quantification and model validation and verification as key to securing the buy-in of business leadership in their companies. As one interviewee put it (to paraphrase), “these capabilities are critical because, when you are asking for funding, management has to be able to evaluate the expected return on investment. You have to be able to demonstrate tangible value and also identify the risks and uncertainties.”

From the interviews, it was clear that this need has significant overlap with the need for high-quality materials data. A typical comment was that lack of validation data presented a bottleneck. A repository of measured basic properties (e.g., band gaps, conductivities, structural properties) of different materials classes would be enormously valuable. Materials used for validation are nonproprietary. Even the largest companies (large, diversified multinational manufacturers with R&D laboratory capacity) have weak incentives to direct their experimental groups to generate this kind of basic data, but it is an essential step to be able to trust computational models. Clean, verified characterization data for different materials classes from an unimpeachable source are absolutely critical.

To paraphrase one interviewee: “If you want to predict ionic transport in a polymer, there’s a shortage of papers that reliably and reproducibly provide all the data we need to validate our models. We therefore have to ask for experiments to be done again and again. A central repository of many properties for many materials classes would fill this need.”

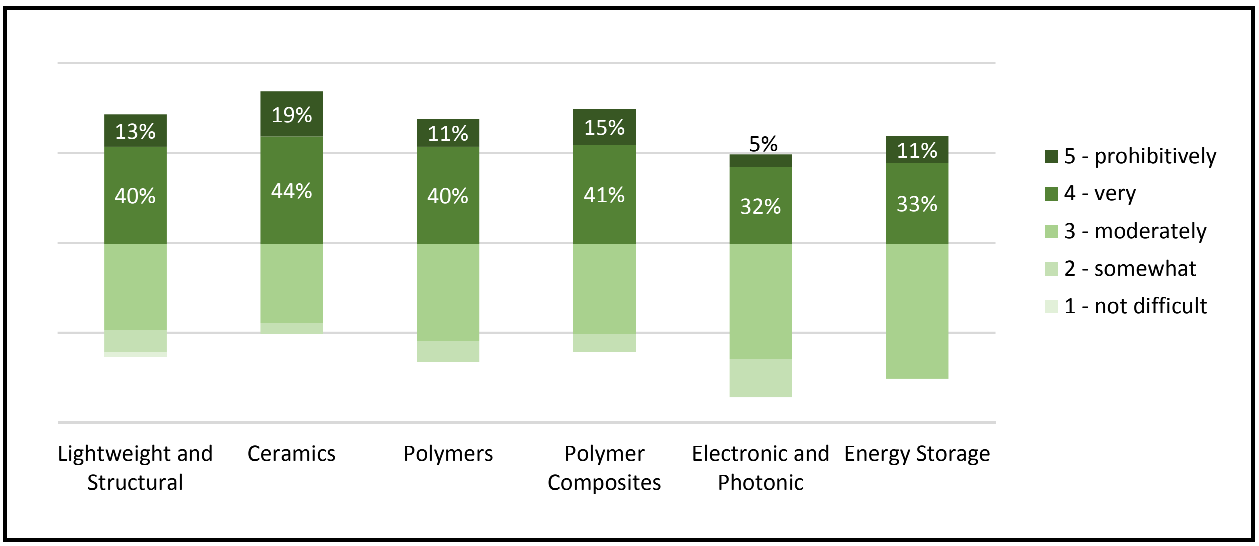
Interviewees’ ratings of the importance and difficulty of meeting this need vary only slightly across materials classes (Figures 4-13 and 4-14). Differences were not statistically significant, and qualitative discussions in interviews revealed no notable justification for them, so these differences among materials classes should not be viewed as significant.

Figure 4-13. Interviewees' Rating of Importance of Model Validation/Verification and Uncertainty Quantification



Note: The distribution of ratings is shown for the six materials classes represented by at least 20 interviewees.

Figure 4-14. Interviewees' Rating of Difficulty of Provisioning Infrastructure for Model Validation/Verification and Uncertainty Quantification through Private Investment



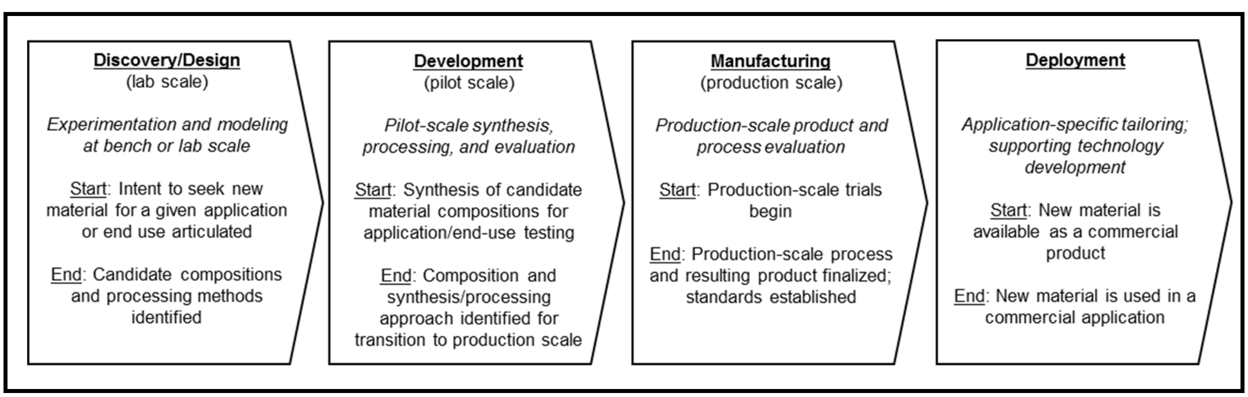
Note: The distribution of ratings is shown for the six materials classes represented by at least 20 interviewees.

5 Economic Impact Assessment

The potential economic impact estimates reported here are based on a comparison of the materials R&D process in the current environment (actual scenario) with the process in a hypothetical environment with an improved Materials Innovation Infrastructure (counterfactual scenario). The actual and counterfactual scenarios were characterized by assigning values to the parameters of the R&D process model (Figure 5-1) based on the opinions and perceptions of industry experts.

Section 5.1 presents the model calibrations in the actual and counterfactual scenarios, looking at overall averages (across industries and materials classes) of R&D model parameters. Section 5.2 presents overall economic impact estimates. Section 5.3 presents results for individual industries and materials classes.

Figure 5-1. Materials R&D Process Stages



Note: Reprised from Figure 3-1 for ease of reference, the materials R&D process stages are based on the Quantitative Benchmark for Time to Market (QBTM) analytical framework, developed for NIST by Nexight Group and Energetics (2016).

5.1 CALIBRATED R&D PROCESS MODEL

Tables 5-1 and 5-2 show estimated parameters of the R&D process model in the actual scenario (Table 5-1) and in the counterfactual scenario with improved infrastructure (Table 5-2). Confidence intervals were estimated using the bootstrap approach explained in Section 3.5.

Potential Impacts on Risk. Companies developing new materials face the risk that an R&D project will fail to reach deployment and generate investment returns. We estimate that the total risk could be reduced by almost half with improved infrastructure: for every new material deployed, only 5 R&D projects would need to enter the R&D pipeline at the discovery/design stage, down from an estimated 9.8 in the current environment (Figure 5-2).

Estimated potential impacts on transition probabilities are greater earlier in the R&D process. The number of projects that must enter the development stage for every one that reaches the deployment stage improves from 2.9 to 2.1; that is a 48% chance of deployment, conditional on reaching the development stage, with improved infrastructure versus a 35% chance in the current environment.

Table 5-1. Materials R&D Process Model Parameter Estimates: Actual Scenario

Model Parameter	R&D Stage			
	Discovery & Design	Development	Manufacturing	Deployment
Relative cost per year	1	3.9 (3.3, 4.5)	16.5 (9.1, 23.4)	11.9 (5.5, 19.8)
Probability of advancing to next stage	29% (25%, 34%)	48% (44%, 54%)	72% (67%, 78%)	N/A
Duration (Years)	2.6 (2.1, 3.2)	3.0 (2.5, 3.6)	2.0 (1.6, 2.4)	2.5 (1.8, 3.3)

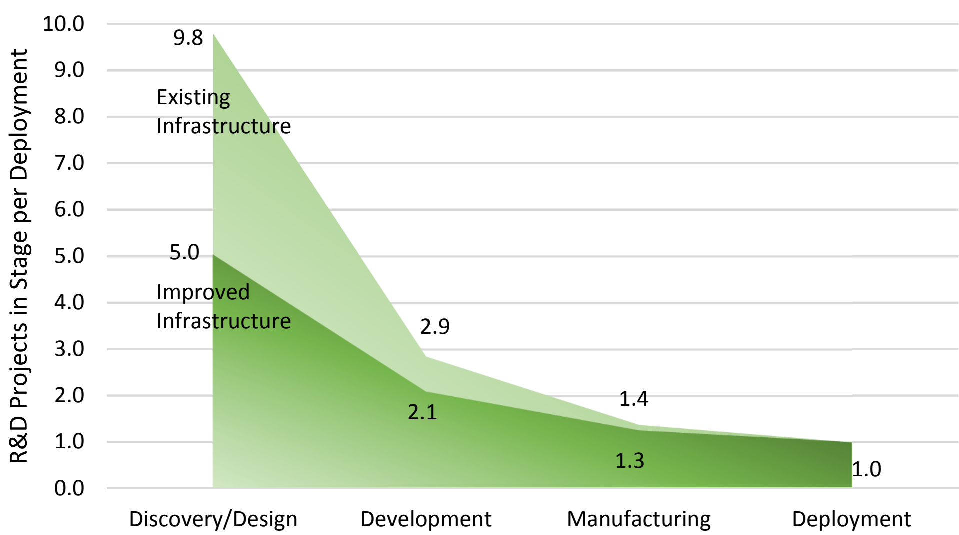
Note: The relative cost per year in the discovery and design stage is normalized at 1. For simplicity, projects that begin a stage are assumed to complete that stage. These numbers reflect the average responses from all interviews. For a response related to a given R&D stage to be included in these averages, the respondent must have reported expertise in the R&D stage. In parentheses are 95% confidence intervals.

Table 5-2. Materials R&D Process Model Parameter Estimates: Counterfactual Scenario

	R&D Stage			
Model Parameter	**Discovery & Design**	**Development**	**Manufacturing**	**Deployment**
Relative cost per year	0.7 (0.6, 0.8)	2.2 (1.8, 2.6)	8.5 (3.9, 13.1)	8.6 (3.7, 13.7)
Probability of advancing to next stage	42% (36%, 47%)	60% (55%, 65%)	80% (74%, 85%)	N/A
Duration (years)	1.4 (1.1, 1.7)	2.0 (1.5, 2.6)	1.4 (1.2, 1.7)	1.8 (1.3, 2.4)

Note: For simplicity, projects that begin a stage are assumed to complete that stage. These numbers reflect the average responses from all interviews. For a response related to a given R&D stage to be included in these averages, the respondent must have reported expertise in the R&D stage. In parentheses are 95% confidence intervals.

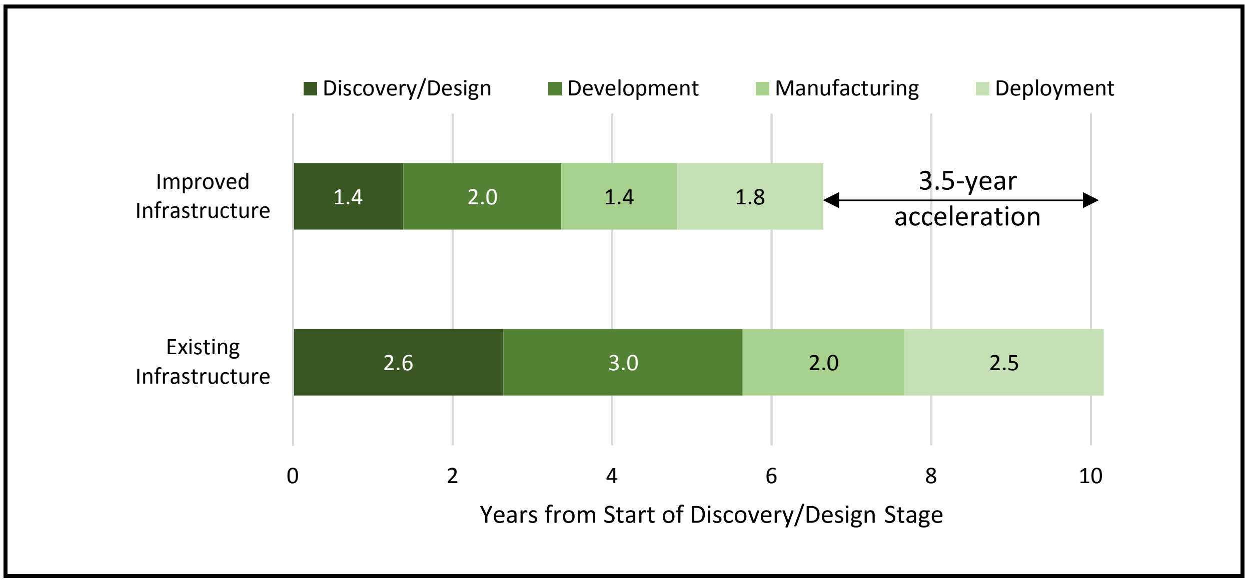
Figure 5-2. Potential Impact on Successful Transition Rates



Note: With improved infrastructure, materials R&D projects are more likely to transition to successive stages. The number of projects that must enter the R&D pipeline at the discovery/design stage for each one that successfully reaches the final deployment stage improves from 9.7 to 4.8 (a 21% chance of deployment with improved infrastructure versus a 10% chance currently). The number of projects that must enter the development stage for every one that reaches the deployment stage improves from 2.7 to 2.0 (a 50% chance of deployment, conditional on reaching the development stage, with improved infrastructure versus a 36% chance currently).

Potential Impacts on Timelines. We estimate that development of a new material takes on average 10.2 years and that an acceleration of 3.5 years could be possible with improved infrastructure (Figure 5-3). That is an estimated potential 35% acceleration (95% C.I. 29% to 41%). We estimate that the duration of the discovery and design stage could be cut from 2.6 years to 1.4 years, an average potential acceleration of 48% (95% C.I. 39% to 59%) Our results suggest that the first stage of materials R&D may be done in half the time with improved infrastructure but that the three subsequent stages cannot be accelerated as much, at least not on average in the cross section of industries represented by our group of experts.

Figure 5-3. Potential Impact on Time to Market



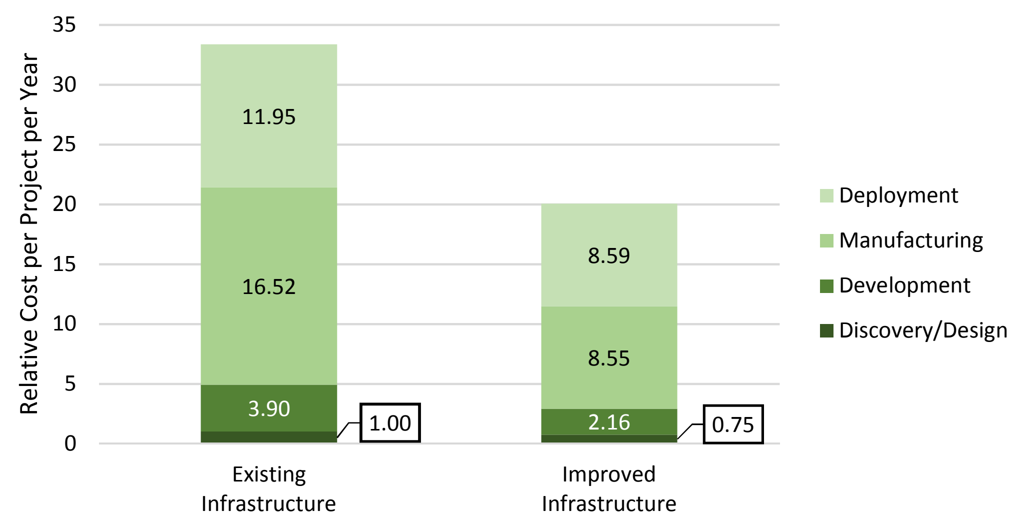
Note: U.S. manufacturers would be able to bring new materials to market faster with the benefit of improved infrastructure. Average time to market is estimated to be 6.6 years with improved infrastructure compared with 10.2 years in the current environment.

Potential Impacts on Relative Costs per Project per Year.

To enable aggregation across respondents and avoid potentially sensitive questions of actual R&D expenditure focused on materials innovation, the cost per project per year in the discovery/design stage in the current environment was normalized at 1.0. Then, respondents were asked to quantify the cost per project per year in the other stages, both in the current environment and the counterfactual environment with improved infrastructure, in relative terms.

We estimate that improved infrastructure has the potential to reduce relative costs by an average of 25% in the discovery/design stage, 45% in the development stage, 48% in the manufacturing stage, and 28% in the deployment stage (Figure 5-4).

Figure 5-4. Potential Impact on Relative R&D Cost per Project per Year



Note: Cost per project, per year, in the discovery/design stage in the current environment was normalized at 1.0. In the current environment, manufacturing and deployment stages are, respectively, roughly four times and three times more cost-intensive than the development stage, which is, in turn, roughly four times more cost-intensive than the discovery/design stage. Improved infrastructure is estimated to reduce relative costs by an average of 25% in the discovery/design stage, 45% in the development stage, 48% in the manufacturing stage, and 28% in the deployment stage.

5.2 POTENTIAL ECONOMIC IMPACT ESTIMATES

The R&D process model was calibrated separately for each industry for which R&D expenditures are reported in the NSF R&D survey (National Science Foundation, 2016). Industry-specific potential impacts were estimated from these calibrations, following the steps described in Section 3.3, and then summed to obtain total economic impact estimates.

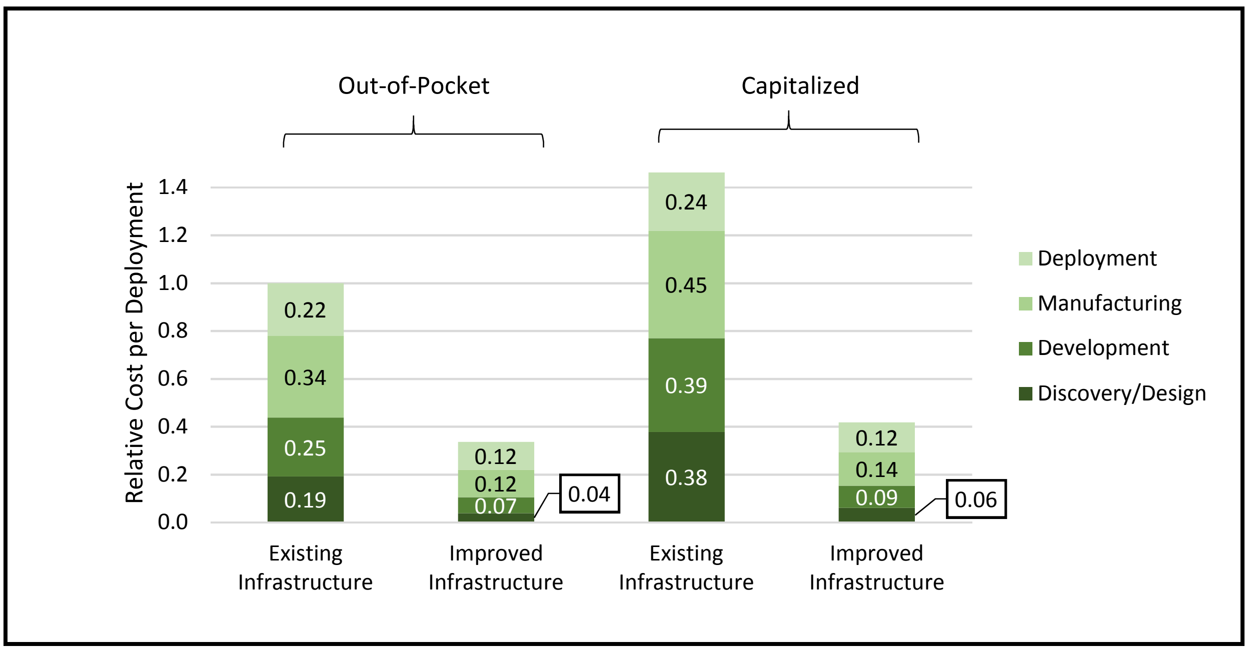
Overall, the potential impacts in transition rates, time to market, and relative costs attributed to an improved Materials Innovation Infrastructure achieve a 65% reduction in out-of-pocket R&D cost (95% confidence interval [C.I.] 56% to 74%) and a 71% reduction in the capitalized cost per successful deployment (95% C.I. 62% to 79%).

On average, in the current environment, $1 million in out-of-pocket R&D cost represents $1.46 million in capitalized R&D cost (95% C.I. 1.37 to 1.54), assuming an 8% cost of capital. With improved infrastructure, under the same assumptions, $1 million in out-of-pocket cost represents $1.24 million in capitalized cost (95% C.I. 1.19 to 1.29).

The relative burden of financial capital cost is lower with improved infrastructure for two main reasons. First, improved infrastructure shortens development time, reducing the time over which capital costs accrue. Second, improved infrastructure reduces risk; a disproportionate share of this potential impact is realized in the earlier stages, discovery/design and development, which carry relatively more capital costs because of their longer time to market (Figure 5-5).

To estimate the economic value of these relative R&D cost savings to the U.S. economy, we multiplied percentage savings by that part of U.S. R&D expenditure focused on materials innovation.[14] Out of a total U.S. R&D expenditure of $168.3

Figure 5-5. Potential Impact on Out-of-Pocket and Capitalized R&D Cost per Deployment



Note: Out-of-pocket R&D cost per new material deployment in the current environment is normalized at 1.0. Capitalized costs include the opportunity cost of financial capital.

[14] These steps are explained in Section 3.4.

billion per year[15] across 10 manufacturing industries and one relevant service industry (Physical, Engineering, and Life Sciences R&D, excluding biotechnology), between $41.2 billion and $60.8 billion was estimated to be the subset to which the relative impacts attributable to improved infrastructure could be applied. Based on the perceptions of the industry experts interviewed, this is the total R&D effort, summed across their respective industries, focused on advanced materials innovation. These out-of-pocket R&D expenditures translate to capitalized R&D costs of between $60.0 billion and $93.6 billion.

Table 5-3. R&D Expenditure and Savings by Industry (Millions of 2013 U.S. Dollars/Year)

Industry	R&D Expenditure	Materials R&D Expenditure	Out-of-Pocket R&D Cost Savings	Capitalized R&D Cost Savings
Computer/Electron (334)	67,205	19,186 (11,462, 27,321)	12,611 (6,211, 18,275)	21,390 (8,791, 30,275)
Transport. Equip. (336)	45,972	14,019 (10,743, 17,588)	9,196 (5,050, 12,924)	17,894 (10,279, 24,447)
Chemical (325)	9,238	4,973 (3,650, 6,228)	3,690 (2,620, 5,375)	4,584 (3,107, 6,262)
R&D Services (541712)	8,910	3,734 (2,052, 5,398)	3,072 (1,892, 4,783)	5,326 (2,937, 8,090)
Machinery (333)	12,650	3,644 (1,831, 5,677)	1,444 (-420, 2,860)	2,101 (-685, 4,372)
Misc. (339)	13,509	2,845 (1,565, 4,076)	1,713 (645, 2,662)	2,501 (1,118, 3,826)
Electrical Equip. (335)	4,136	1,135 (610, 1,660)	639 (170, 1,071)	955 (211, 1,574)
Plastics (326)	3,650	693 (316, 999)	491 (110, 893)	627 (124, 1,081)
Fabricated Metal (332)	2,212	635 (415, 839)	433 (226, 625)	742 (322, 1,101)
Primary Metal (331)	624	231 (160, 301)	163 (99, 241)	253 (163, 366)
Petroleum and Coal (324)	242	76 (41, 110)	34 (0, 69)	50 (-1, 96)
Total	168,348	51,172 (41,219, 60,762)	33,486 (25,253, 42,150)	56,421 (38,846, 68,836)

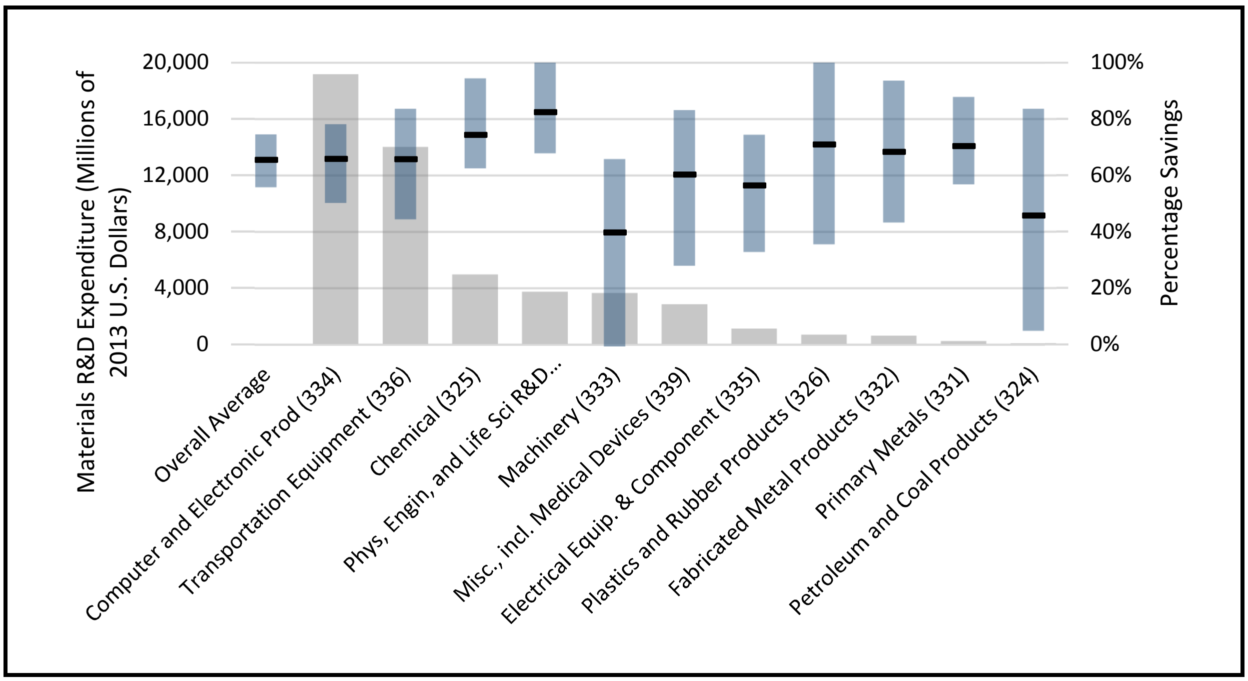
Note: In parentheses are 95% confidence intervals. Industries: 325, Chemical, excluding pharmaceuticals and medicines; 331, Primary metals; 333, Machinery; 335, Electrical Equipment, Appliances, and Components; 336, Transportation Equipment, including aerospace; 324, Petroleum and Coal Products; 326, Plastics and Rubber Products; 332, Fabricated Metal Products; 334, Computer and Electronic Products, including semiconductor and other electronic components; 339, Miscellaneous Manufacturing, including medical devices; 541712, Physical, Engineering, and Life Sciences (except biotechnology) R&D. R&D expenditure is 2013 domestic R&D, from NSF (2016, Table 23).

[15] Based on 2013 BRDIS (National Science Foundation, 2016).

For each industry, Table 5-3 shows total R&D expenditure, estimated R&D expenditure related to developing and applying new materials, estimated out-of-pocket R&D cost savings, and estimated capitalized R&D cost savings. Overall, R&D efficiencies attributable to improved infrastructure are estimated to generate cost savings of between $39 billion and $69 billion per year, or between 62% and 79%.

Percentage savings, in terms of out-of-pocket costs (the ratio of estimated out-of-pocket R&D cost savings to estimated R&D expenditure related to developing and applying new materials), range from 40% to 80% (Figure 5-6). Overall savings are dominated by the two largest industries in terms of R&D: Computer and Electronic Products (334), which includes semiconductor and other electronic components, and Transportation Equipment (336), which includes aerospace.

Figure 5-6. Materials R&D Expenditure and Percentage Savings



Note: Estimated materials R&D expenditures are indicated by gray bars situated on the horizontal axis (confidence intervals are provided in Table 5-3). Estimated percentage savings are indicated by the black tick marks, with 95% confidence intervals indicated by floating blue bars.

Adding Value to R&D Outcomes. Potential R&D efficiency impact estimates are calculated by holding R&D outcomes constant; these are estimates of how much less it could cost, with improved Materials Innovation Infrastructure, to generate the same number and quality of new materials deployed per year on average.

This is not the whole story because it does not account for the increase in the rate of innovation we would expect to see as companies respond to the new environment in which R&D is more efficient. As the cost of developing and deploying new materials falls, U.S. companies would be expected to develop and deploy new materials at a higher rate. The resulting benefits, for the innovating companies and for downstream companies and end users of the products made from those new materials, would stem from the R&D efficiency impact and so multiply the total potential impact associated with improved infrastructure.

To address this issue, structured interviews explored the ways in which an improved Materials Innovation Infrastructure would enable companies to undertake R&D projects they would not otherwise have done, leverage that R&D to commercialize improved products and new product lines, and expand into new markets (see Section IV of the interview guide, provided in the appendix).

The following few examples are broadly representative of industry experts' justification for multiplying the potential R&D efficiency impacts:[16]

- Better models would enable targeted materials design, which would allow manufacturers to design new products faster and incorporate new materials into the product design process earlier on. Taking this idea even further, improved modeling capability could enable the processes of designing of new materials and new product applications to be integrated, so the new material is designed to meet the emerging requirements of the new product as the new product is designed to take fullest advantage of the properties of the new material.
- Models help in understanding the underlying physics and designing better, more focused experiments. Not only

[16] These comments are paraphrased.

can these benefits of modeling reduce the cost of developing and deploying a new material, but they can also improve the performance attributes of the new material. For example, consider an R&D project to develop lighter alloys for engine components. With improved infrastructure, we would expect to be able to achieve the same R&D outcome at lower cost, but our approach in this new environment would more likely be to invest the same amount in R&D and get a better outcome—a lighter and more durable material for lighter and more durable engines.

- Better ways of finding new materials with unique properties would enable companies to expand their design portfolio, which could significantly enhance the quality of the products they supply or open up new markets. Transformative research is much more important than the ability to improve the efficiency of research efforts.
- For small startups especially, built around a new advanced material that may take upwards of 10 years to develop, securing investment capital is often difficult. Shorter time to market and lower risk (i.e. lower attrition rates) could make new materials more attractive investments for U.S. venture capitalists, increasing the number of materials R&D projects that can be sustained through deployment.

Overall, interviewees estimated the value of such potential impacts to be 2 to 3 times as large as the value of the R&D efficiency impacts. Taken together with the R&D efficiency impacts, the potential economic benefit of an improved Materials Innovation Infrastructure is estimated to be between $123 billion and $270 billion per year.

Table 5-4 provides estimates of potential R&D cost savings and the added value of improved R&D outcomes broken out by industry.

Table 5-4. Potential Economic Impacts by Industry (Millions of 2013 U.S. Dollars Per Year)

Industry	Capitalized R&D Cost Savings	Added Value of Improved R&D Outcomes	Total Potential Economic Impact
Computer/Electron (334)	21,390 (8,791, 30,275)	62,771 (18,251, 102,105)	84,160 (29,899, 129,310)
Transport. Equip. (336)	17,894 (10,279, 24,447)	36,913 (15,323, 56,037)	54,807 (28,058, 78,315)
Chemical (325)	4,584 (3,107, 6,262)	11,506 (5,397, 19,564)	16,091 (8,828, 25,206)
R&D Services (541712)	5,326 (2,937, 8,090)	17,263 (8,087, 33,668)	22,589 (12,787, 39,295)
Machinery (333)	2,101 (-685, 4,372)	7,983 (-5,523, 19,267)	10,083 (-5,557, 23,677)
Misc. (339)	2,501 (1,118, 3,826)	8,698 (1,677, 17,922)	11,199 (3,265, 21,142)
Electrical Equip. (335)	955 (211, 1,574)	2,070 (-77, 3,677)	3,025 (274, 5,171)
Plastics (326)	627 (124, 1,081)	2,020 (-1,572, 4,430)	2,646 (-1,433, 5,440)
Fabricated Metal (332)	742 (322, 1,101)	1,876 (797, 3,240)	2,618 (1,146, 4,262)
Primary Metal (331)	253 (163, 366)	251 (142, 385)	504 (322, 716)
Petroleum and Coal (324)	50 (-1, 96)	97 (-41, 221)	147 (-44, 311)
Total	**56,421** **(38,846, 68,836)**	**151,447** **(82,515, 203,036)**	**207,869** **(123,229, 270,047)**

Note: In parentheses are 95% confidence intervals. Industries: 325, Chemical, excluding pharmaceuticals and medicines; 331, Primary metals; 333, Machinery; 335, Electrical Equipment, Appliances, and Components; 336, Transportation Equipment, including aerospace; 324, Petroleum and Coal Products; 326, Plastics and Rubber Products; 332, Fabricated Metal Products; 334, Computer and Electronic Products, including semiconductor and other electronic components; 339, Miscellaneous Manufacturing, including medical devices; 541712, Physical, Engineering, and Life Sciences (except biotechnology) R&D.

5.3 INDUSTRY AND MATERIALS CLASS RESULTS

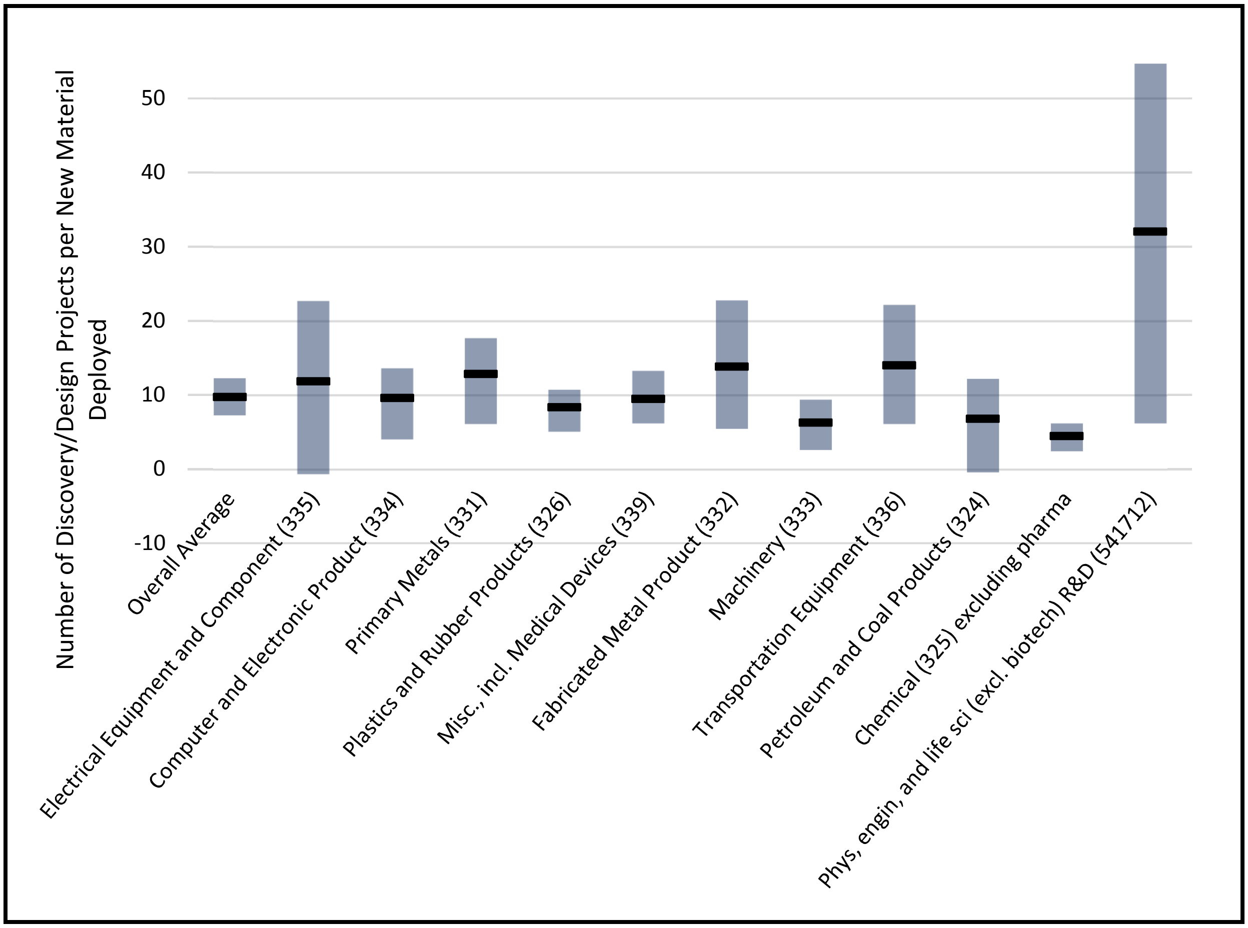
The R&D process model was calibrated separately for industries and for materials classes.[17] This section gives an overview of some of those industry-specific and material-specific results.

R&D is inherently risky in that the outcomes of R&D trials are uncertain. The risk associated with R&D outcomes in the present environment was found not to vary significantly across industries (Figure 5-7). Responses of interviewees developing chemicals and new materials for machinery suggest that these industries' average attrition rates, reflected in the number of projects that must enter the discovery/design stage for every

[17] The steps of this process are explained in Section 3.3.

new material successfully deployed, are less than other industries' rates. The number of materials development projects entering the pipeline for every new material deployed is 4.5 for chemicals (95% confidence interval 2.4 to 6.2) and 6.3 for machinery (95% confidence interval 2.6 to 9.4) compared with the overall average of 9.7 (95% confidence interval 7.3 to 12.2). For the one nonmanufacturing industry considered—physics, engineering, and life sciences R&D—the number of projects per deployment is 32.0, but with a 95% confidence interval of 16.2 to 54.7 it is not significantly different from the overall average. For all other industries, 95% confidence intervals also include 9.7.

Figure 5-7. Number of Discovery/Design Projects per New Material Deployed by Industry

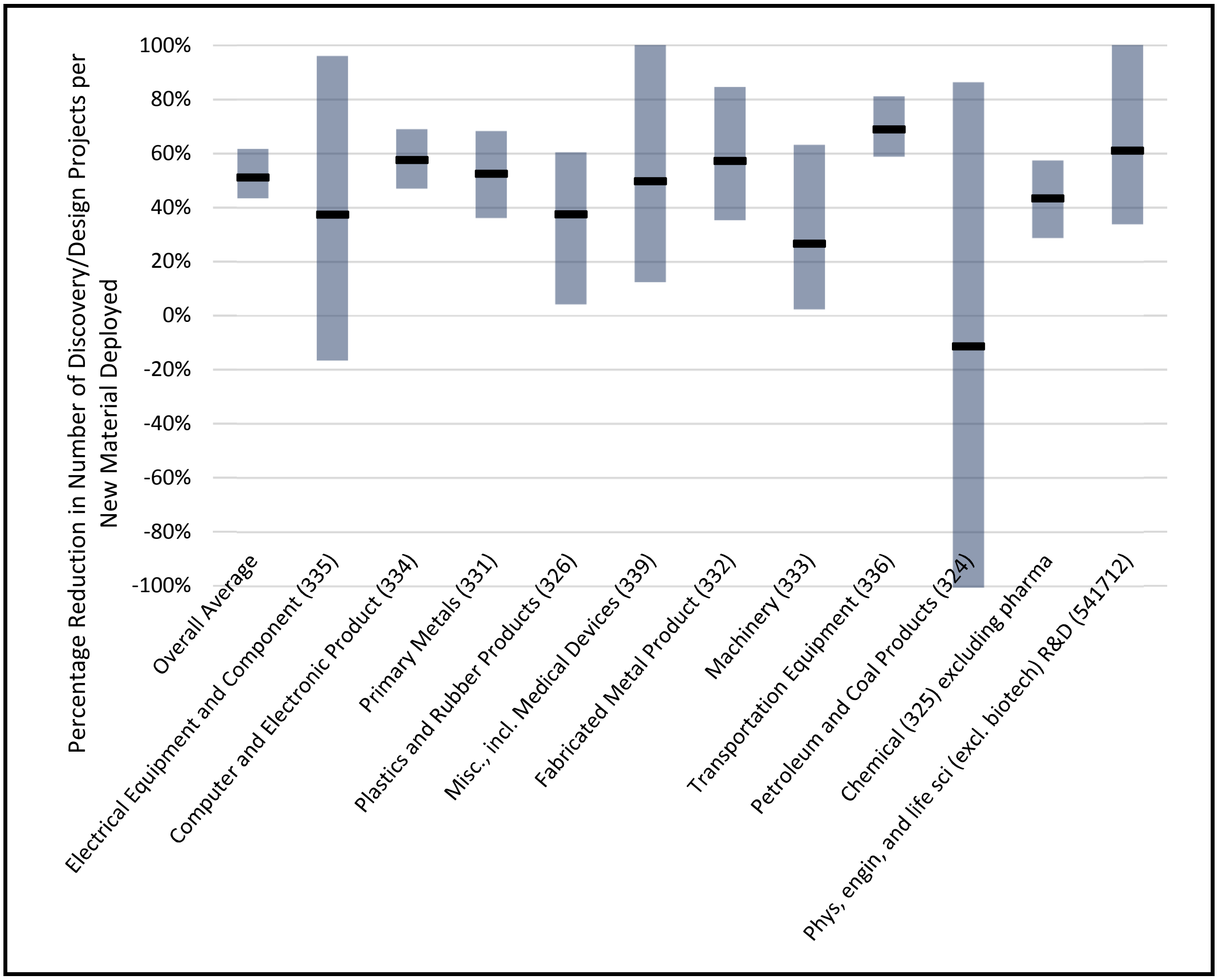


Note: Points are indicated by the black tick marks, with 95% confidence intervals indicated by floating bars.

The average risk reduction—or attrition reduction, reflected in a lower number of projects needing to enter the R&D pipeline for every new material deployed—is 51% fewer projects overall

(95% confidence interval 43% to 62%). Transportation equipment is the only industry to differ significantly from the overall average, with a 69% reduction (95% confidence interval 59% to 81%); all other industries' confidence intervals contain the overall average of 51%. For two industries, electrical equipment and components and petroleum and coal products, the reduction is not significantly different from zero (Figure 5-8).

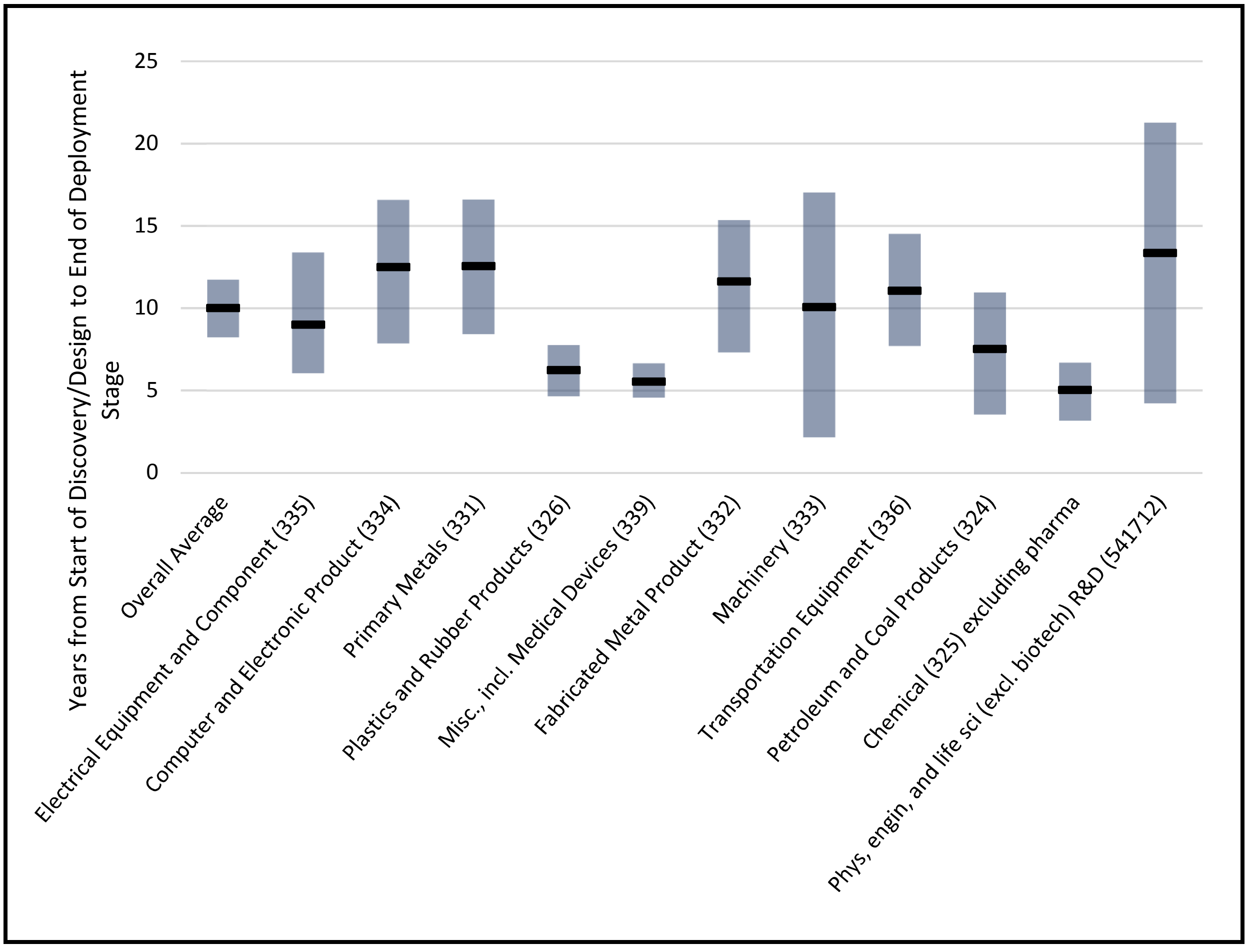
Figure 5-8. Percentage Reduction in Number of Discovery/Design Projects by Industry



Note: Points are indicated by the black tick marks, with 95% confidence intervals indicated by floating bars.

Across all industries, the average total duration of the four R&D stages is 10.0 years (95% confidence interval 8.2 years to 11.7 years). Three industries have significantly shorter average durations, shown in Figure 5-9: chemicals, at 5.0 years (95% confidence interval 3.1 years to 6.7 years), miscellaneous, including medical devices, at 5.5 years (95% confidence interval 4.6 years to 6.6 years), and plastics, at 6.2 years (95% confidence interval 4.6 years to 7.7 years).

Figure 5-9. Total Duration of R&D Stages by Industry

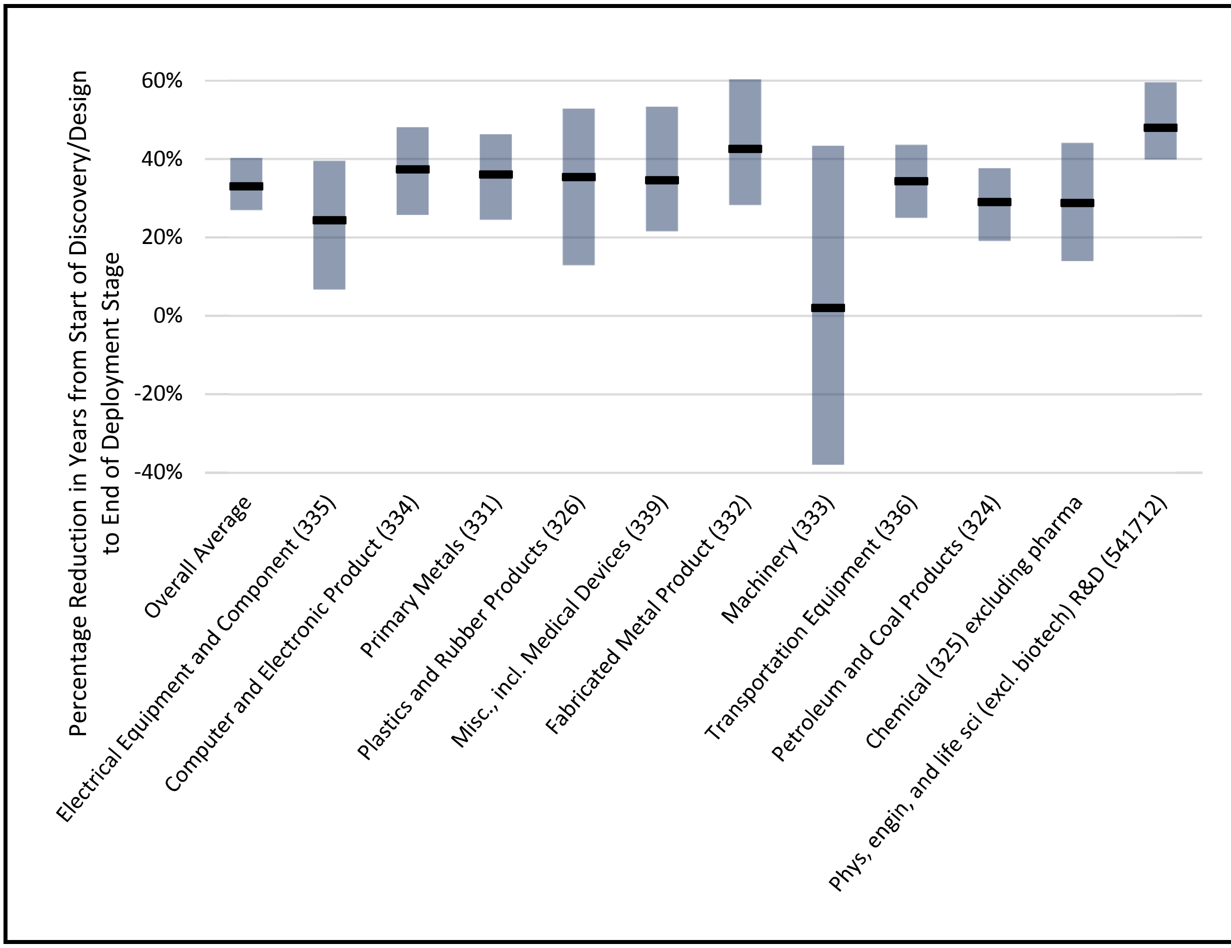


Note: Points are indicated by the black tick marks, with 95% confidence intervals indicated by floating bars.

The relative acceleration averages 33% across industries (95% confidence interval 27% to 40%). Although the relative acceleration varies across industries, as shown in Figure 5-10, the difference is only significant for physics, engineering, and life sciences R&D, with a 48% reduction (95% confidence interval 40% to 59%). The estimated improvement is not significant for the machinery industry.

The data underlying Figures 5-7, 5-8, 5-9, and 5-10 are shown in Table 5-5.

Figure 5-10. Percentage Reduction in Total Duration of R&D Stages by Industry



Note: Points are indicated by the black tick marks, with 95% confidence intervals indicated by floating bars.

Table 5-5. R&D Risk and Duration, Baseline and Potential Impact, by Industry

Industry	Baseline Number of Discovery/ Design Projects per New Material Deployed	Percentage Reduction in Number of Discovery/Design Projects per New Material Deployed	Baseline Total Duration of R&D Stages (Years)	Percentage Reduction in Total Duration of R&D Stages
Overall Average	9.7 (7.3, 12.2)	51% (43%, 62%)	10.0 (8.2, 11.7)	33% (27%, 40%)
Electrical Equip. (335)	11.8 (−0.7, 22.7)	37% (−17%, 96%)	9.0 (6.0, 13.4)	24% (7%, 39%)
Computer/Electron (334)	9.6 (4.0, 13.6)	58% (47%, 69%)	12.5 (7.8, 16.6)	37% (26%, 48%)
Primary Metal (331)	12.8 (6.1, 17.6)	52% (36%, 68%)	12.5 (8.4, 16.6)	36% (24%, 46%)

(continued)

Table 5-5. R&D Risk and Duration, Baseline and Potential Impact, by Industry (continued)

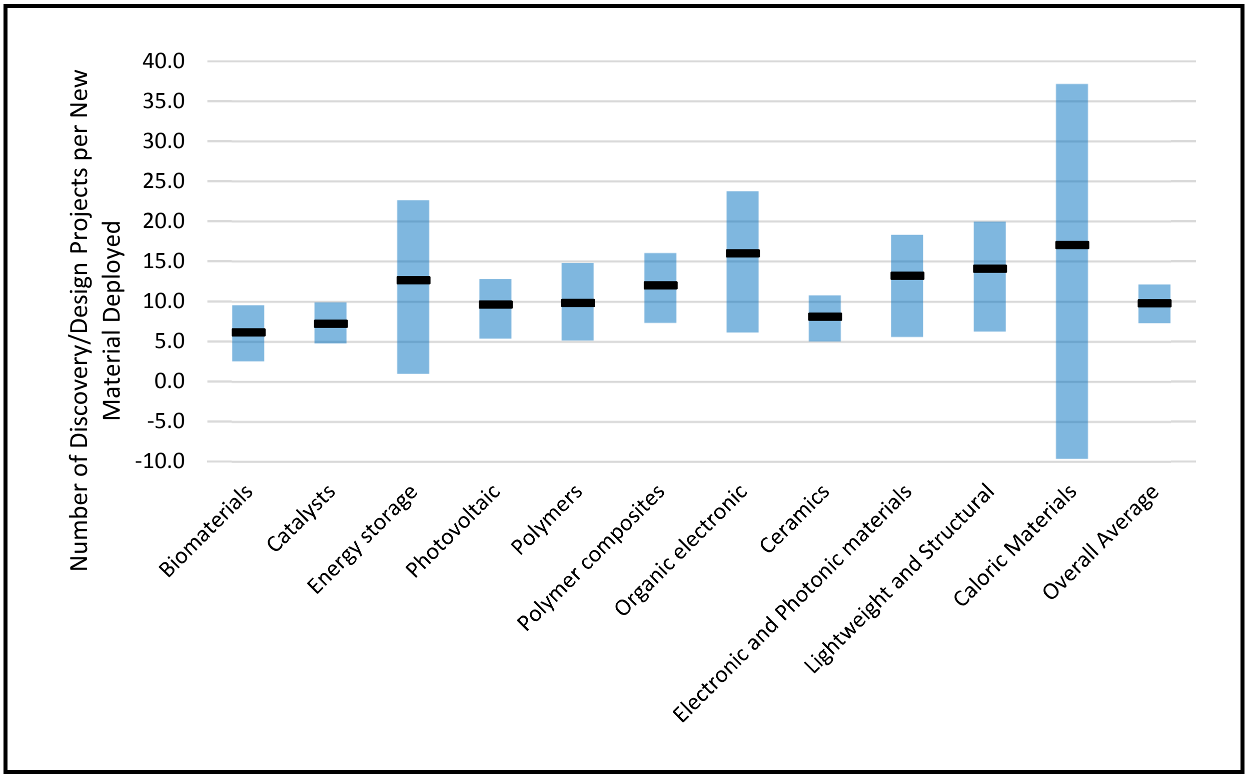
Industry	Baseline Number of Discovery/ Design Projects per New Material Deployed	Percentage Reduction in Number of Discovery/Design Projects per New Material Deployed	Baseline Total Duration of R&D Stages (Years)	Percentage Reduction in Total Duration of R&D Stages
Plastics (326)	8.3 (5.1, 10.7)	37% (4%, 60%)	6.2 (4.6, 7.7)	35% (13%, 53%)
Misc. (339)	9.5 (6.2, 13.3)	50% (12%, 109%)	5.5 (4.6, 6.6)	35% (21%, 53%)
Fabricated Metal (332)	13.8 (5.4, 22.7)	57% (35%, 85%)	11.6 (7.3, 15.3)	43% (28%, 60%)
Machinery (333)	6.3 (2.6, 9.4)	27% (2%, 63%)	10.1 (2.2, 17.0)	2% (−38%, 43%)
Transport. Equip. (336)	14.0 (6.1, 22.2)	69% (59%, 81%)	11.1 (7.7, 14.5)	34% (25%, 44%)
Petroleum and Coal (324)	6.8 (−0.4, 12.2)	−11% (−118%, 86%)	7.5 (3.5, 10.9)	29% (19%, 38%)
Chemical (325)	4.5 (2.4, 6.2)	43% (29%, 57%)	5.0 (3.1, 6.7)	29% (14%, 44%)
R&D Services (541712)	32.0 (6.2, 54.7)	61% (34%, 100%)	13.4 (4.2, 21.3)	48% (40%, 59%)

Note: In parentheses are 95% confidence intervals. Industries: 325, Chemical, excluding pharmaceuticals and medicines; 331, Primary metals; 333, Machinery; 335, Electrical Equipment, Appliances, and Components; 336, Transportation Equipment, including aerospace; 324, Petroleum and Coal Products; 326, Plastics and Rubber Products; 332, Fabricated Metal Products; 334, Computer and Electronic Products, including semiconductor and other electronic components; 339, Miscellaneous Manufacturing, including medical devices; 541712, Physical, Engineering, and Life Sciences (except biotechnology) R&D.

Turning to materials classes, we note that catalysts and biomaterials are estimated to have lower attrition rates across R&D stages, while other materials classes are not significantly different from the overall average (Figure 5-11). The improvement (i.e., percentage reduction) in attrition rates that could be achieved with improved infrastructure is estimated to be significantly higher for two materials classes: polymer composites and caloric materials (Figure 5-12). The total duration of R&D stages is estimated to be significantly different only for biomaterials (Figure 5-13), and the potential improvement (i.e., acceleration) is significantly higher for caloric materials and organic electronics and photovoltaic materials and significantly lower for biomaterials (Figure 5-14).

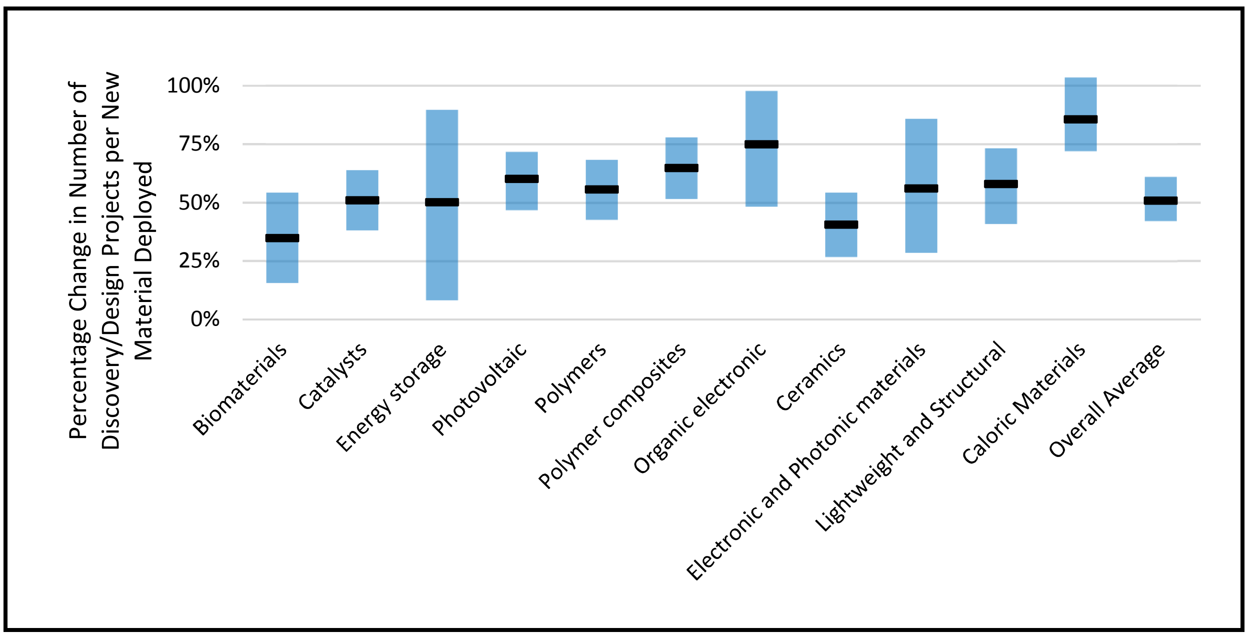
The data underlying Figures 5-11, 5-12, 5-13, and 5-14 are shown in Table 5-6.

Figure 5-11. Number of Discovery/Design Projects per New Material Deployed by Materials Class



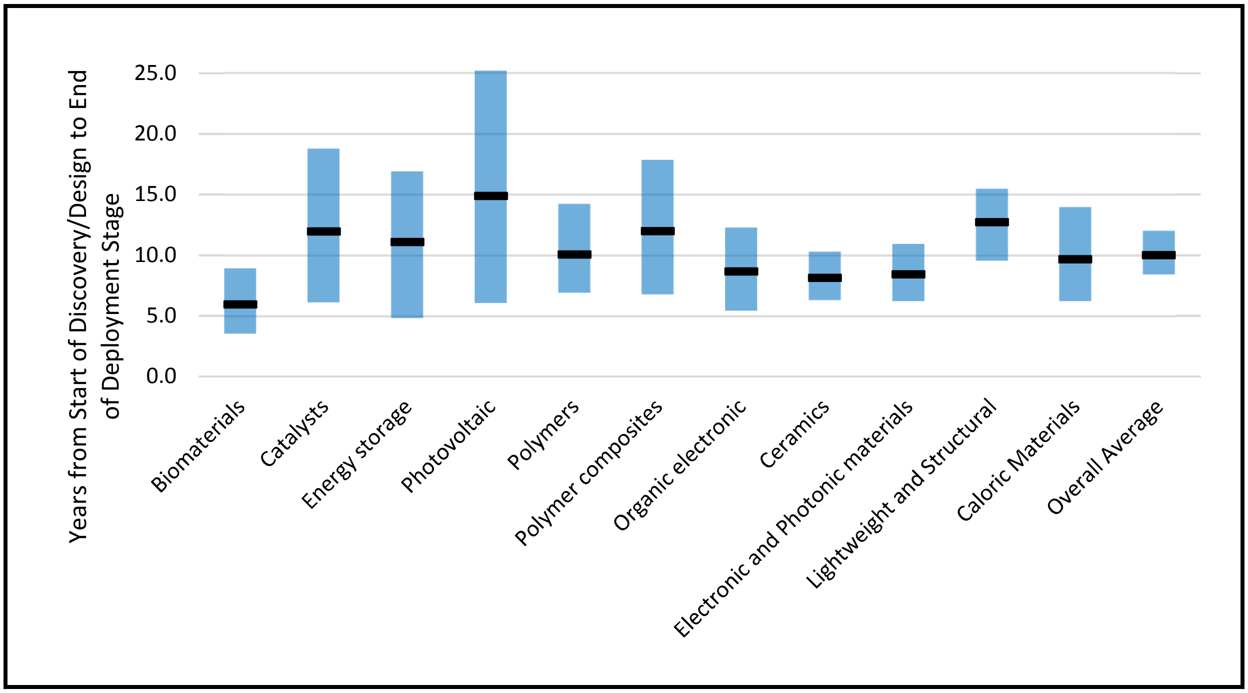
Note: Points are indicated by the black tick marks, with 95% confidence intervals indicated by floating bars.

Figure 5-12. Percentage Reduction in Number of Discovery/Design Projects by Materials Class



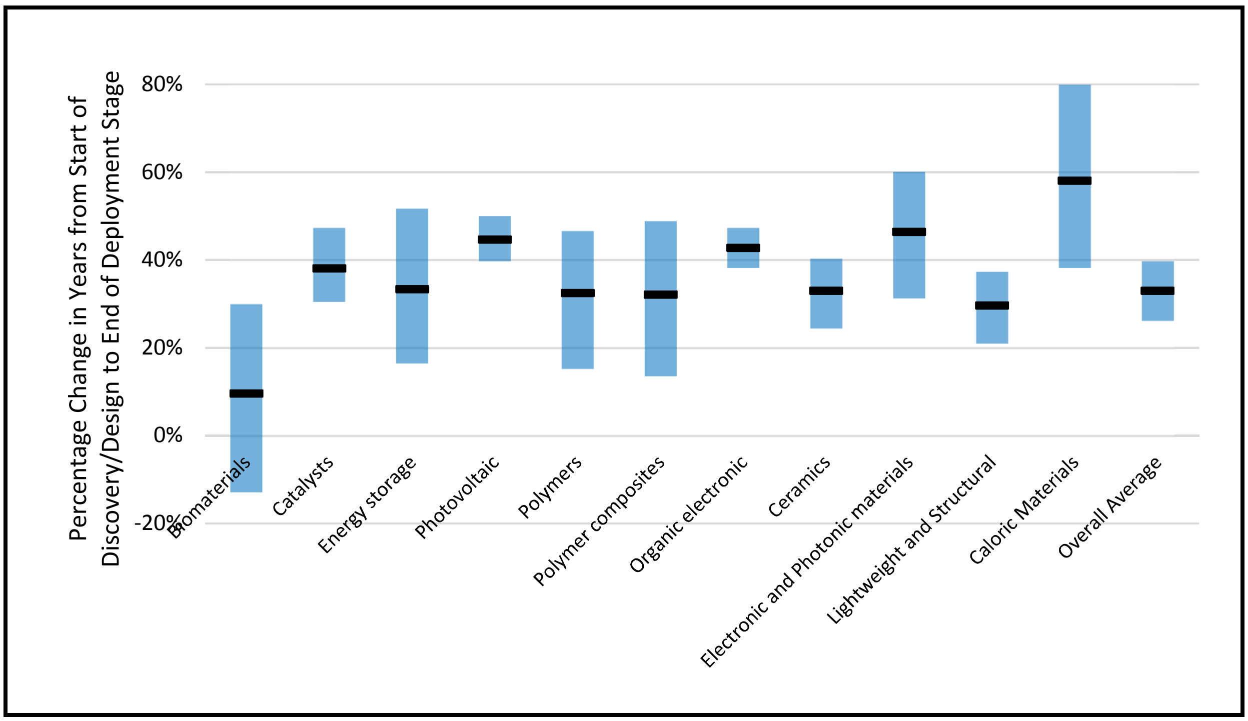
Note: Points are indicated by the black tick marks, with 95% confidence intervals indicated by floating bars.

Figure 5-13. Total Duration of R&D Stages by Materials Class



Note: Points are indicated by the black tick marks, with 95% confidence intervals indicated by floating bars.

Figure 5-14. Percentage Reduction in Total Duration of R&D Stages by Materials Class



Note: Points are indicated by the black tick marks, with 95% confidence intervals indicated by floating bars.

Table 5-6. R&D Risk and Duration, Baseline and Potential Impact, by Materials Class

Industry	Baseline Number of Discovery/ Design Projects per New Material Deployed	Percentage Reduction in Number of Discovery/Design Projects per New Material Deployed	Baseline Total Duration of R&D Stages (Years)	Percentage Reduction in Total Duration of R&D Stages
Biomaterials	6.1 (2.5, 9.5)	35% (16%, 54%)	5.9 (3.5, 8.9)	10% (-13%, 30%)
Catalysts	7.2 (4.7, 9.9)	51% (38%, 64%)	11.9 (6.1, 18.7)	38% (30%, 47%)
Energy storage	12.6 (0.9, 22.6)	50% (8%, 90%)	11.1 (4.8, 16.9)	33% (16%, 52%)
Photovoltaic	9.6 (5.3, 12.8)	60% (47%, 72%)	14.9 (6.1, 25.2)	45% (40%, 50%)
Polymers	9.8 (5.1, 14.8)	56% (43%, 68%)	10.0 (6.9, 14.2)	33% (15%, 47%)
Polymer composites	12.0 (7.3, 16.0)	65% (52%, 78%)	12.0 (6.8, 17.8)	32% (14%, 49%)
Organic electronic	16.0 (6.1, 23.7)	75% (48%, 98%)	8.7 (5.4, 12.3)	43% (38%, 47%)
Ceramics	8.1 (5.0, 10.8)	41% (27%, 54%)	8.1 (6.3, 10.3)	33% (24%, 40%)
Electronic and Photonic materials	13.2 (5.5, 18.3)	56% (29%, 86%)	8.4 (6.2, 10.9)	46% (31%, 60%)
Lightweight and Structural	14.1 (6.2, 19.9)	58% (41%, 73%)	12.7 (9.5, 15.5)	30% (21%, 37%)
Caloric Materials	17.0 (-9.7, 37.2)	86% (72%, 104%)	9.6 (6.2, 14.0)	58% (38%, 80%)
Overall Average	9.7 (7.2, 12.1)	51% (42%, 61%)	10.0 (8.4, 12.0)	33% (26%, 40%)

Note: In parentheses are 95% confidence intervals.

6 Conclusions

This report presents estimates of the potential economic benefit of an improved Materials Innovation Infrastructure of between $123 billion and $270 billion per year, based on structured interviews with more than 100 industry experts (Table 6-1). Roughly a quarter these estimated benefits come from making the R&D process more efficient, saving time and reducing risk. The rest of the potential benefits are projected to come from companies responding to the new environment by targeting more ambitious R&D outcomes: undertaking R&D projects they would not otherwise have done, leveraging that R&D to commercialize improved products and new product lines, and expanding into new markets. The wide range of these estimates is to be expected for this type of analysis, asking a diverse group of experts to share their perceptions and opinions about the potential impact of improvements in infrastructure they can envision to meet their existing and emerging needs.

Table 6-1. Potential Economic Impact Estimates (Millions of 2013 U.S. Dollars Per Year)

Type of Potential Impact	Point Estimate	95% Confidence Interval
R&D Efficiency	56,421	(38,846, 68,836)
Improved R&D Outcomes	151,447	(82,515, 203,036)
Total	**207,869**	**(123,229, 270,047)**

Note: Potential R&D efficiency impact estimates are based on interview-based estimated impacts to the R&D process, summarized in Figures ES-3, ES-4, and ES-5, combined with industry R&D expenditure data (National Science Foundation, 2016) and interview-based estimates of the fraction of that expenditure related to developing new materials. Estimates of the value of improved R&D outcomes were also interview-based. Confidence intervals were calculated based on the variability of industry experts' responses to interview questions, using a bootstrap approach described in Section 3.5. The larger confidence interval for improved R&D outcomes (80% of the point estimate compared with 53% for R&D efficiency) reflects greater variability among experts' opinions and therefore greater uncertainty in the estimate. Point estimates of R&D efficiency and improved R&D outcomes impacts add to the total (the difference of 1 is due to rounding error). Confidence intervals cannot be added because the sources of uncertainty for the two types of potential impact are different and not perfectly correlated; the probability that both estimates (R&D efficiency and improved R&D outcomes) fall outside their respective confidence intervals is lower than the probability that either one does so.

The full economic benefits of improved infrastructure could be worth considerably more than the estimates provided here. Because these estimates were based on interviews with representatives of U.S. materials developers and manufacturers, the estimates reflect only that part of the benefits these companies expect to capture; these estimates exclude the additional benefits to consumers over and above the prices they pay for new products. For example, a new lightweight engine built of advanced alloys may cost more than a heavier conventional engine, but that price difference is likely to be much less than the fuel cost savings over the life of the lighter engine. This extra benefit to consumers of the lightweight engine is an example of consumer surplus not captured in the potential impact estimates presented here.

Interviewees emphasized the need for **high-quality materials data**. The need for **collaborative networks** was most appreciated by those who viewed these networks as a means of improving access to high-quality data. Access to high-quality data was seen as the linchpin (necessary, albeit not sufficient by itself) to meeting the other four identified needs:

- **material design methods**, enabling application of a systems approach to materials development, from discovery and design all the way through to deployment;
- **production and scale-up methods**, including model-based and simulation-based alternatives to expensive physical testing based on trial and error and faster, more cost-effective means of producing advanced materials at pilot scale and full scale;
- **quality assurance and control and component certification methods**, enabling improved capabilities to model, predict, and control the formation of defects and to forecast manufacturing variation; and
- **model validation and uncertainty quantification**, providing a basis for trust and acceptance of computational models and objective decision-making regarding reliance on computational analysis and simulation at a business level.

A typical comment was that a lack of validation data presented a bottleneck, which could be improved by a publicly available repository of measured basic properties (e.g., band gaps, conductivities, structural properties) of different materials classes. Materials used for validation are nonproprietary. Even at the largest companies (large, diversified multinational manufacturers with R&D laboratory capacity and the capability to generate this kind of data), companies have weak incentives to direct their experimental groups to generate basic, nonproprietary data, but it is an essential step to be able to trust computational models. Clean, verified characterization data for different materials classes from an unimpeachable source are absolutely critical.

All six areas of need were rated very or critically important by at least 60% of respondents, led by access to high-quality data and quality assurance, quality control, and component certification. Five of the six needs were rated very or prohibitively difficult to address through private investment by at least 50% of respondents, led by materials design methods, production and scale-up, model validation and uncertainty quantification, and access to high-quality data.

In Section 5, we provided what we believe to be the best available quantitative information on the materials innovation process: relative costs, attrition rates, and durations of four successive R&D stages. Out of more than 100 interviewees, 80 provided quantitative estimates of these parameters, based on their experience and perceptions. These estimates provide a useful benchmark for analyzing a range of policy options.

The policy focus of the present study was a range of infrastructure technology investments aimed at addressing the six identified needs. The exact nature of the technologies springing from those investments and the extent and speed of their impact on the identified needs were necessarily speculative. Nevertheless, out of the 80 interviewees offering parameter estimates for the R&D process model in the current environment, 70 also provided parameter estimates in a hypothetical environment with an enhanced Materials Innovation Infrastructure.

Industry experts anticipated that computational approaches to materials discovery and design will become increasingly universal. Although today companies can gain an advantage by being among the early adopters of these approaches, they foresee a future in which these approaches will become the standard in many manufacturing industries, and companies will not be able to survive without them.

Although these industry experts envision a future in which using computational approaches is part of most if not all manufacturers' business models, they stressed that building the technological infrastructure—developing the tools and standards companies must have to be able to use these approaches—is not part of their business models. Therefore, public investment in Materials Innovation Infrastructure will become increasingly important for a globally competitive U.S. manufacturing sector.

This report has documented the perceptions and opinions of experts in materials innovation, mostly representing U.S. industry, regarding gaps in the Materials Innovation Infrastructure that encumber innovation aimed at realizing many important next-generation applications and industries. The process of discovering, developing, and deploying advanced materials is complex and heterogeneous. So too is the array of public-good infrastructure technologies that are needed for a vibrant, innovative, globally competitive U.S. manufacturing sector to flourish.

This report has taken a broad brush to these complex issues. Its intent is to draw out high-level insights that for the most part cut across specific industries and materials classes. Insights into specific stages of the materials innovation process, specific elements of an improved Materials Innovation Infrastructure, and needs specific to certain industries or company characteristics have been explored qualitatively to the extent possible within the scope of the study.

Accordingly, this analysis can in no way substitute for the close interaction between NIST scientists and industry representatives by which the sorts of high-level needs characterized here can be translated into specific projects, programs, and initiatives within the national laboratories.

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Appendix: Interview Guide

NIST Materials Genome Initiative Strategic Planning Study: Economic Analysis of National Needs for Technology Infrastructure to Support the Materials Genome Initiative

Interview Guide

The National Institute of Standards and Technology (NIST) in the U.S. Department of Commerce has contracted with RTI International to conduct an economic analysis of standards, measurement, and general purpose technology needs that inhibit efficient development and deployment of advanced materials by U.S. manufacturers.

The objectives of this critical strategic planning study include:

- Identify industry needs related to Materials Innovation Infrastructure.
- Identify barriers/challenges to meeting these needs.
- Estimate the economic impact of meeting these needs.
- Review and prioritize public policy and investment options.

Your perspectives will help guide NIST's strategic planning and program development process. Participation in this analysis is confidential; only aggregated information will be included in any deliverables or communications. Your name and your company's name will not be disclosed. We do not wish to discuss specific products, strategies, or technologies, but rather your thoughts about industry needs and how investments in technology infrastructure to meet those needs would affect your company and companies like yours.

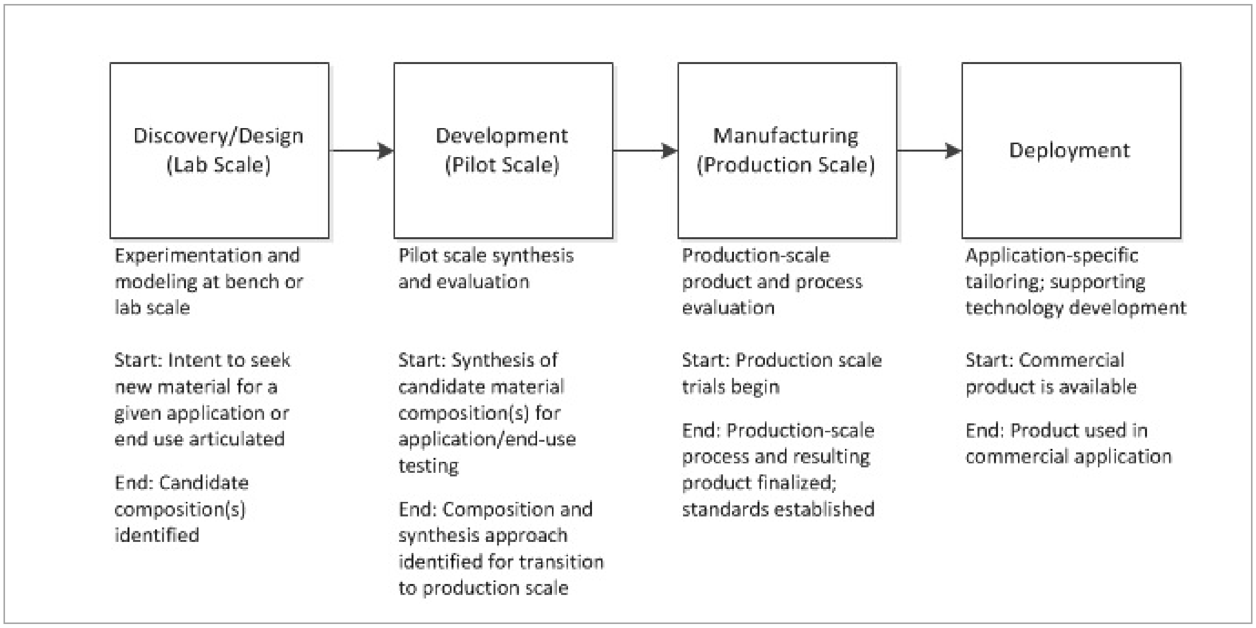
Our research products will be an economic analysis, final report, and presentation materials. All deliverables will be publicly available in 2018 and these will be shared with you as soon as they are released.

If you have questions, please contact:

- Alan O'Connor, Principal Investigator, RTI, 919-541-8841 or oconnor@rti.org
- Courtney Silverthorn, NIST Project Officer, NIST, 301-975-4189 or courtney.silverthorn@nist.gov.

I. RESPONDENT BACKGROUND

We will be referring to a stylized depiction of the materials innovation process:[18]



1. Does your perspective cover all four stages, or is it focused within a subset of these stages?

   [ ] All stages

   [ ] Only the following stages (check all that apply)

   [ ] Discovery/Design [ ] Development [ ] Manufacturing [ ] Deployment

   Briefly describe the lifecycle of a typical project with which you are involved:

2. What types of materials does your work involve? (check all that apply)

   [ ] Biomaterials [ ] Polymers [ ] Correlated Materials

   [ ] Catalysts [ ] Polymer Composites [ ] Electronic and Photonic Materials

   [ ] Energy storage [ ] Organic Electronic [ ] Lightweight and Structural

   [ ] Photovoltaic [ ] Ceramics [ ] Caloric Materials

   [ ] Other ____

   Briefly describe the types of materials and broad applications (we do not need specific information about any proprietary material or product):

3. Is your background primarily experimental or computational?

   [ ] Experimental [ ] Computational [ ] Spans both experimental and computational

Briefly describe the roles of experimental and computational approaches in your work:

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[18] Based on *Quantitative Benchmark for Time to Market (QBTM) for New Materials Innovation: An Analytical Framework*. mgi.nist.gov/sites/default/files/uploads/user124/QBTM%20Final%20Analytical%20Framework_011216.pdf.

II. INDUSTRY NEEDS ASSESSMENT

Table 1 summarizes industry needs identified through scoping interviews.

1. Please rate the importance to your company of addressing each area of unmet need.

   (Please briefly explain the relative importance of meeting these needs.)

2. Please rate the difficulty for your company of meeting each need on its own, in terms of both the technical difficulty and the business difficulty (i.e., difficulty justifying investment within the business model).

   (Please briefly explain the relative difficulty of meeting these needs.)

3. Are there other needs, of equal or greater importance, not included in Table 1?

   (If so, please describe the need, rate its importance and difficulty, and briefly explain.)

Table 1. Industry Needs: Rating Importance and Difficulty

Areas of Industry Need	Examples of Infrastructure Technology to Address Need	**Importance:** 5 = critically 4 = very 3 = moderately 2 = somewhat 1 = not important	**Difficulty:** 5 = prohibitively 4 = very 3 = moderately 2 = somewhat 1 = not difficult
i. Access to High-Quality Data: – Precompetitive experimental data, computational data, and software code	– Data standardization and curation – Models underpinning accurate and repeatable material measurement		
ii. Collaborative Networks: – Efficient means of sharing materials information (e.g., along a supply chain, among research collaborators)	– Methods for capturing, characterizing, and sharing materials data in structured formats – Communication standards & translators (“MT Connect for material measurement equipment”)		
iii. Material Design Methods: – Inverse modeling capability – Shorter paths to better starting points	– Models, simulations, metrologies for advanced materials design – Machine learning tools		
iv. Production & Scale Up: – Model-based alternatives to expensive physical testing/trial & error for scale-up – Faster, cost-effective means of producing advanced materials at pilot and full scale	– Multiscale modeling frameworks (integrating macroscopic process models with microscopic materials simulation) – Process technology platforms (e.g., cold sintering, additive, roll-to-roll, directed self-assembly)		
v. Quality Assurance/Control & Component Certification: – Ability to model, predict, and control formation of defects – Ability to forecast manufacturing variation	– Performance metrics (benchmarks, reference data, testbeds to characterize performance of systems and components) – Process control tools (test protocols, objective scientific and engineering data, reference databases)		
vi. Model Validation/Verification & Uncertainty Quantification: – Basis for trust & acceptance of computational models – Basis for objective decision making regarding reliance on computational analysis/simulation at a business level	– Generally accepted and easily applied methods for uncertainty quantification for both experimental and computational data – Validation of analytical methods and procedures, emphasizing industrially relevant systems, comparing predicted and measured properties from multiple sources		

III. IMPACTS ON MATERIALS DEVELOPMENT PROCESS

1. Given the current environment, please provide generic estimates (i.e., for a typical project) of the relative costs, transition probabilities, and durations of the four stages of materials innovation (Table 2).

    a. How costly is a year of each stage relative to the cost of a year of Discovery/Design? Assume the cost of a year in Discovery/Design is 1.

    (For example: A relative cost of 2 at the Development stage would indicate that a year of Development is twice as expensive as a year of Discovery/Design.)

    b. What is the probability that a project that starts a given stage advances to the next stage?

    (For example, 0.75 at Development stage implies that a project that starts the Development stage has a 75% chance of advancing to enter the Manufacturing stage.)

    c. About how many years does it take to complete each stage?

2. How would your answers change in an improved environment where the needs discussed in Section II are addressed? (Table 3).

    Note that Relative Cost is not necessarily 1 at the Discovery/Design stage in Table 3. Entering a value of 1 would indicate that the cost per year in the Discovery/Design stage would be unaffected by improvements in infrastructure.

3. Finally, please describe how changes would come about. How are potential impacts tied to improved infrastructure?

Table 2. Materials Innovation Process in the <u>Current</u> Environment (<u>Existing</u> Technology Infrastructure)

	Discovery/Design	Development	Manufacturing	Deployment
a. Relative Cost (per year)	1			
b. Probability of Advancing				N/A
c. Duration (years)				

Table 3. Materials Innovation Process in the <u>Improved</u> Environment (<u>Improved</u> Technology Infrastructure)

	Discovery/Design	Development	Manufacturing	Deployment
a. Relative Cost (per year)				
b. Probability of Advancing				N/A
c. Duration (years)				

IV. IMPACTS ON NEW AND IMPROVED PRODUCTS

1. In addition to the impacts on the development process discussed in Section III, would the improved infrastructure lead to new opportunities to provide value to your customers or reach new markets?

   If so, how?

2. Broadly speaking, would these impacts be more or less important to your company than the R&D impacts discussed in Section III?

   Could you quantify the relative importance?

   [ ] More important. Enter a number greater than 1: ____________

   [ ] Equally important.

   [ ] Less important. Enter a number between 0 and 1: ____________

V. COMPANY CHARACTERISTICS

To help us aggregate responses and control for differences in company characteristics, please provide the following information for your company:

1. Industry (NAICS)

   [ ] Food (311)

   [ ] Petroleum and Coal Products (324)

   [ ] Chemical (325)

   [ ] Plastics and Rubber Products (326)

   [ ] Primary Metals (331)

   [ ] Fabricated Metal Product (332)

   [ ] Machinery (333)

   [ ] Computer and Electronic Product (334)

   [ ] Electrical Equipment, Appliance, and Component (335)

   [ ] Transportation Equipment (336)

   [ ] Miscellaneous, incl. medical equipment and supplies (339)

2. Company Size (Total Number of Employees)

   [ ] less than 50

   [ ] 50–99

   [ ] 100–249

   [ ] 250–499

   [ ] 500–999

   [ ] 1,000–4,999

   [ ] 5,000–9,999

   [ ] 10,000–24,999

   [ ] 25,000 or more

V. COMPANY CHARACTERISTICS CONTINUED

1. R&D Size (Total Number of R&D Employees)

   [ ] less than 5

   [ ] 5–9

   [ ] 10–24

   [ ] 25–49

   [ ] 50–99

   [ ] 100–499

   [ ] 500–999

   [ ] 1,000–2,499

   [ ] 2,500 or more

2. What percentage of your company's R&D effort is related to developing and applying advanced materials?

0% to 20%	20% to 40%	40% to 60%	60% to 80%	80% to 100%
[ ]	[ ]	[ ]	[ ]	[ ]

3. On average, for companies in your industry, roughly what percentage of R&D effort do you think is related to developing and applying advanced materials?

0% to 20%	20% to 40%	40% to 60%	60% to 80%	80% to 100%
[ ]	[ ]	[ ]	[ ]	[ ]

VI. CONCLUDING THOUGHTS

Is there anything else that we have not covered that you think is important for us to know?

Is there anyone else that you would recommend we reach out to for our analysis?

Many thanks for your input!