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

May 2018

National Institute of Standards and Technology
U.S. Department of Commerce

RTI INTERNATIONAL

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Analysis Brief

The 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[1]. Its aim is to enable U.S. companies to more rapidly and efficiently develop and deploy advanced materials, with applications ranging from consumer goods, 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 briefing provides key findings from economic analysis and interviews with more than 120 industry experts on their needs for new technological infrastructure supporting advanced materials innovation and the potential economic impacts of meeting those needs. We conclude that **an improved Materials Innovation Infrastructure would deliver between $123 billion and $270 billion in value annually.**

ABOUT THE MATERIALS GENOME INITIATIVE

Advanced materials are an increasingly essential—and increasingly complex—component of the manufacturing environment, forming the first tier of advanced manufacturing supply chains.[2] This complexity demands larger, more diversified, and integrated R&D resources, which are not easily defined and implemented.[3]

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.

The aim of the Materials Genome Initiative is to enable U.S. industry to develop and deploy advanced materials more quickly and efficiently.

$123 Billion per year. **$270**

NIST is a key player in supporting the MGI approach and the development of a national Materials Innovation Infrastructure. This analysis presents estimates of potential impacts attributable to improved infrastructure of between $123 billion and $270 billion per year.

1 To make this analysis tractable, the central concept of a Materials Innovation Infrastructure was reduced to the six industry needs summarized in Table 1.

2 Moskowitz, S. L. (2014). The advanced materials revolution: Technology and economic growth in the age of globalization. John Wiley & Sons, Inc., New York.

3 Tassey, G. (2016). The technology element model, path-dependent growth, and innovation policy. Economics of Innovation and New Technology, 25(6), 594-612.

> 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" *(NSTC, 2011).*

Examples include the Industrial Technology Research Institute of Taiwan, the Electronics and Telecommunications Research Institute 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, National Nanotechnology Initiative, the MGI, and other initiatives.[4]

Launched in 2011 as a key enabling element of a strategy 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 materials science and engineering."[5]

Motivating the initiative are two ideas: first, that developing advanced materials is critical to addressing challenges in sectors like energy, supercomputing, national security, and healthcare; second, that accelerating the process of moving an advanced material from laboratory to market could significantly improve U.S. global competitiveness and ensure that the United States remains at the forefront of the advanced materials marketplace.

Released in 2014, the MGI strategic plan sets out four defining goals for the initiative: [6]

- **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.
- **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. 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.
- **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.
- **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.

Leading the MGI are the Department of Defense, Department of Energy, National Science Foundation, and NIST. Other 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.[7]

4 See www.manufacturing.gov/programs.

5 National Science and Technology Council (NSTC). (June 2011). Materials Genome Initiative for Global Competitiveness.

6 National Science and Technology Council (NSTC). (December 2014). Materials Genome Initiative Strategic Plan.

7 See https://www.mgi.gov/partners.

Table 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

Table 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

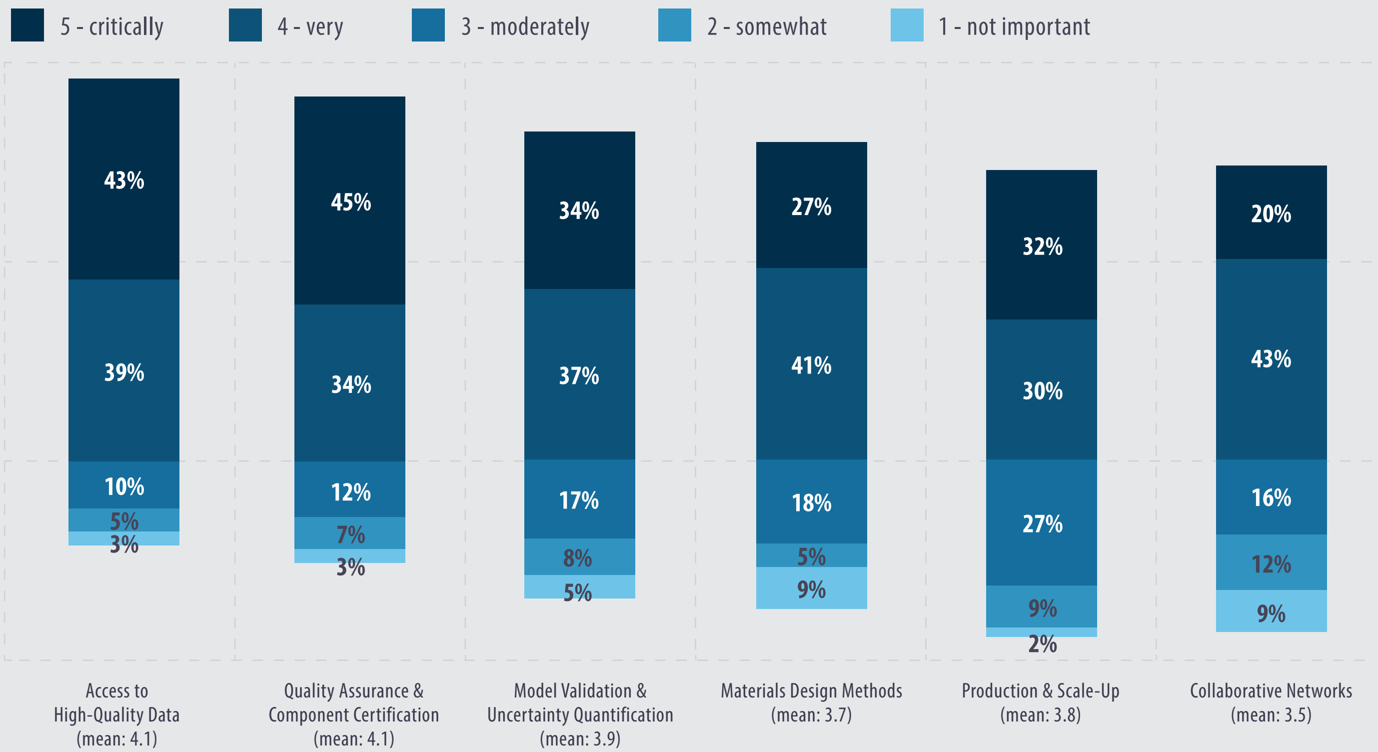
INDUSTRY NEEDS ASSESSMENT

Six identified areas of industry need provided the common basis for the more than 120 interviews that support this analysis:

- access to high-quality data;
- collaborative networks;
- material design methods;
- production and scale-up;
- quality assurance, quality control, and component certification; and
- model validation and uncertainty quantification (Figures 1 and 2).

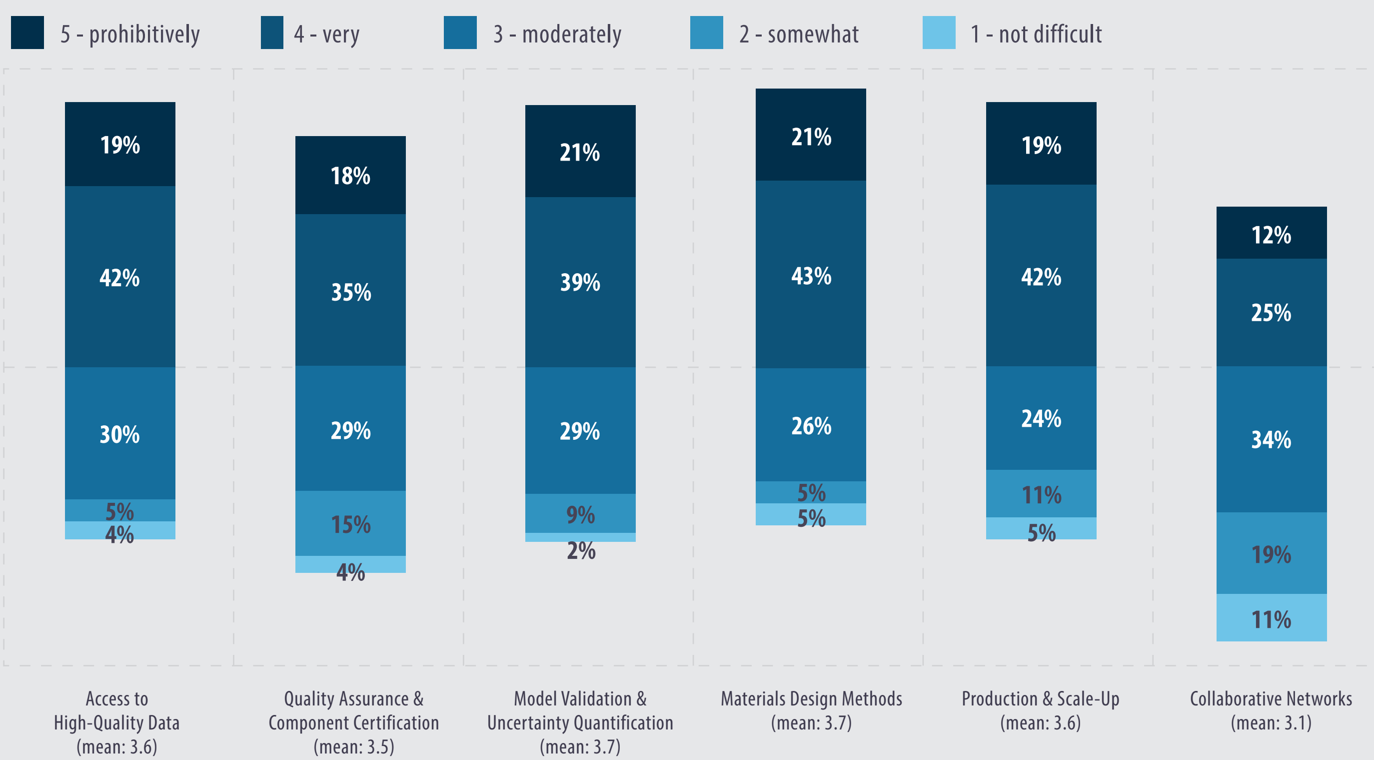
Access to high-quality data emerged as a linchpin of a Materials Innovation Infrastructure. Industry experts stressed the strong complementarity among the six areas of need and the consequent overlap among the types of infrastructure and potential impacts: efforts to address one need tend to increase the return on efforts to address the others. 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 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 2. Interviewees' Rating of Difficulty of Meeting Needs through Private Investment

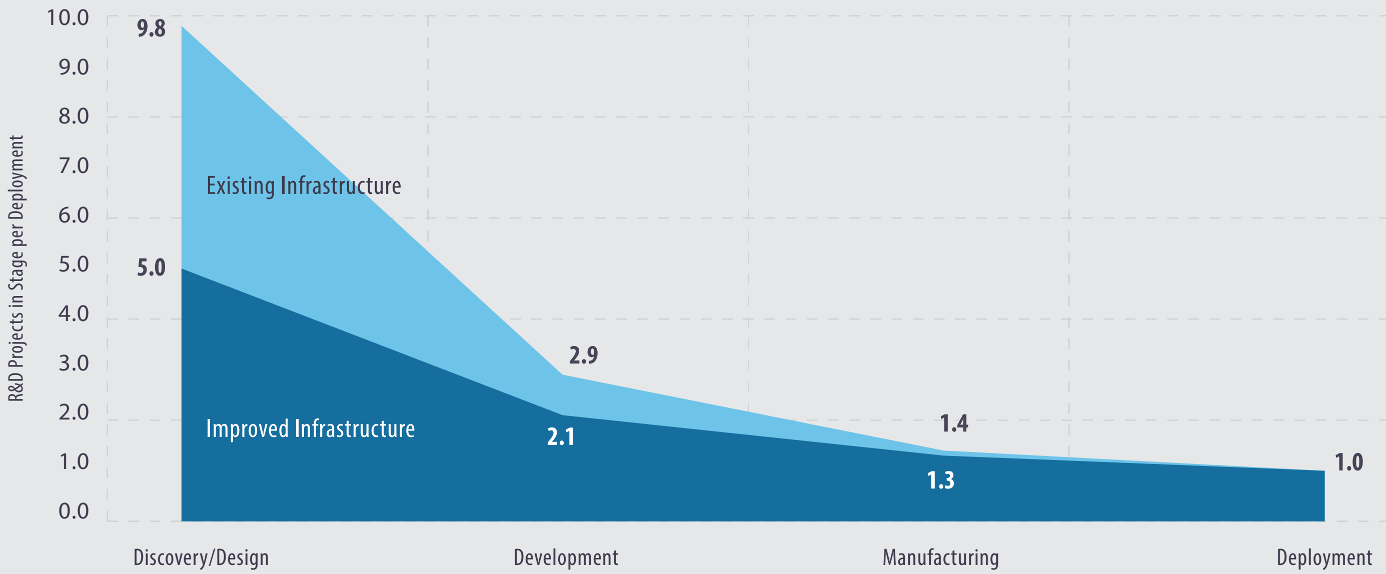


Note: Percentages shown reflect the distribution of ratings. Average ratings are given in parentheses below each area of industry need.

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 3).

Figure 3. Potential Impact on Risk

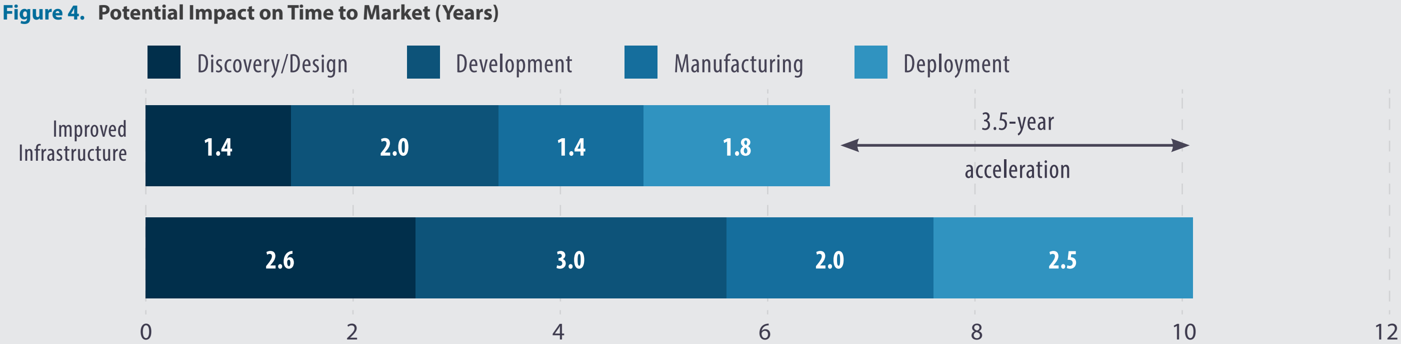


Note: With improved infrastructure, materials R&D projects are more likely to transition to successive stages. The number of projects that must enter the R&D pipeline at the discovery/design stage for each one that successfully reaches the final deployment stage improves from 9.8 to 5.0 (a 20% chance 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).

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 4).

Figure 4. Potential Impact on Time to Market (Years)



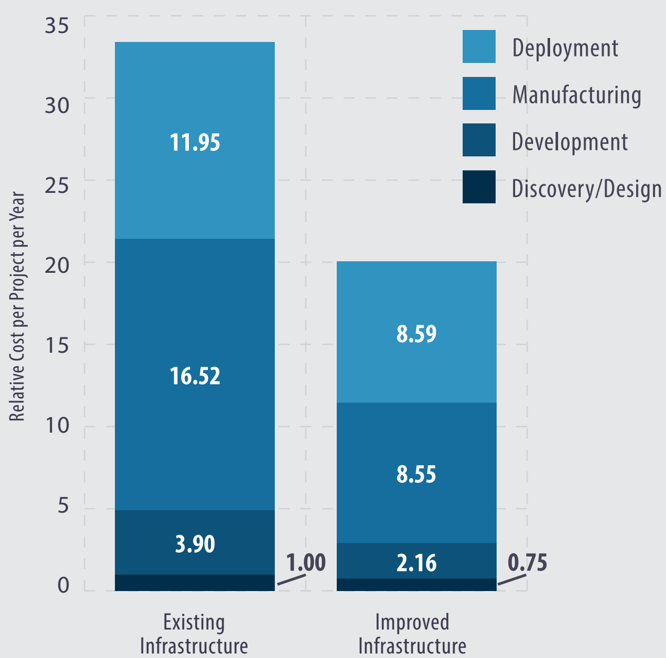
Note: U.S. manufacturers would be able to bring new materials to market faster with the benefit of improved infrastructure. Average time to market is estimated to be 6.6 years with improved infrastructure compared with 10.2 years in the current environment.

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 5).

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 2).[8]

Figure 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.

> 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.

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.

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' contributions to U.S. gross domestic product).

8 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.

TOTAL ECONOMIC IMPACTS

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 2).

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.

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

TYPE OF POTENTIAL IMPACT	DESCRIPTION	POINT ESTIMATE	95% CONFIDENCE INTERVAL
R&D Efficiency	R&D cost savings	56,421	(38,846 to 68,836)
Improved R&D Outcomes	Superior performance of products emerging from R&D	151,447	(82,515 to 203,036)
Total		**207,869**	**(123,229 to 270,047)**

Note: Potential R&D efficiency impact estimates are based on interview-based estimated impacts to the R&D process, summarized in Figures 3, 4, and 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.

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