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Technology Infrastructure to support Advanced Materials:
Economic Analysis of Needs and Opportunities

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This presentation is based on a study conducted by RTI International:
Scott, T., Walsh, A., Anderson, B., O'Connor, A. and Tassey, G. (2018). ***Economic Analysis of National Needs for Technology Infrastructure to Support the Materials Genome Initiative*****. Full report and analysis brief available at: https://www.nist.gov/mgi/mgi-reports**

Technology Infrastructure to support Advanced Materials:
Economic Analysis of Needs and Opportunities

1. Study Background: Materials Genome Initiative (MGI) and the role of the National Institute of Standards and Technology (NIST)

2. Materials Innovation Infrastructure: examples of industry needs, the role of materials modelling, and practical ways companies are engaging

3. Interview methodology

4. Potential impact estimates if needs are met

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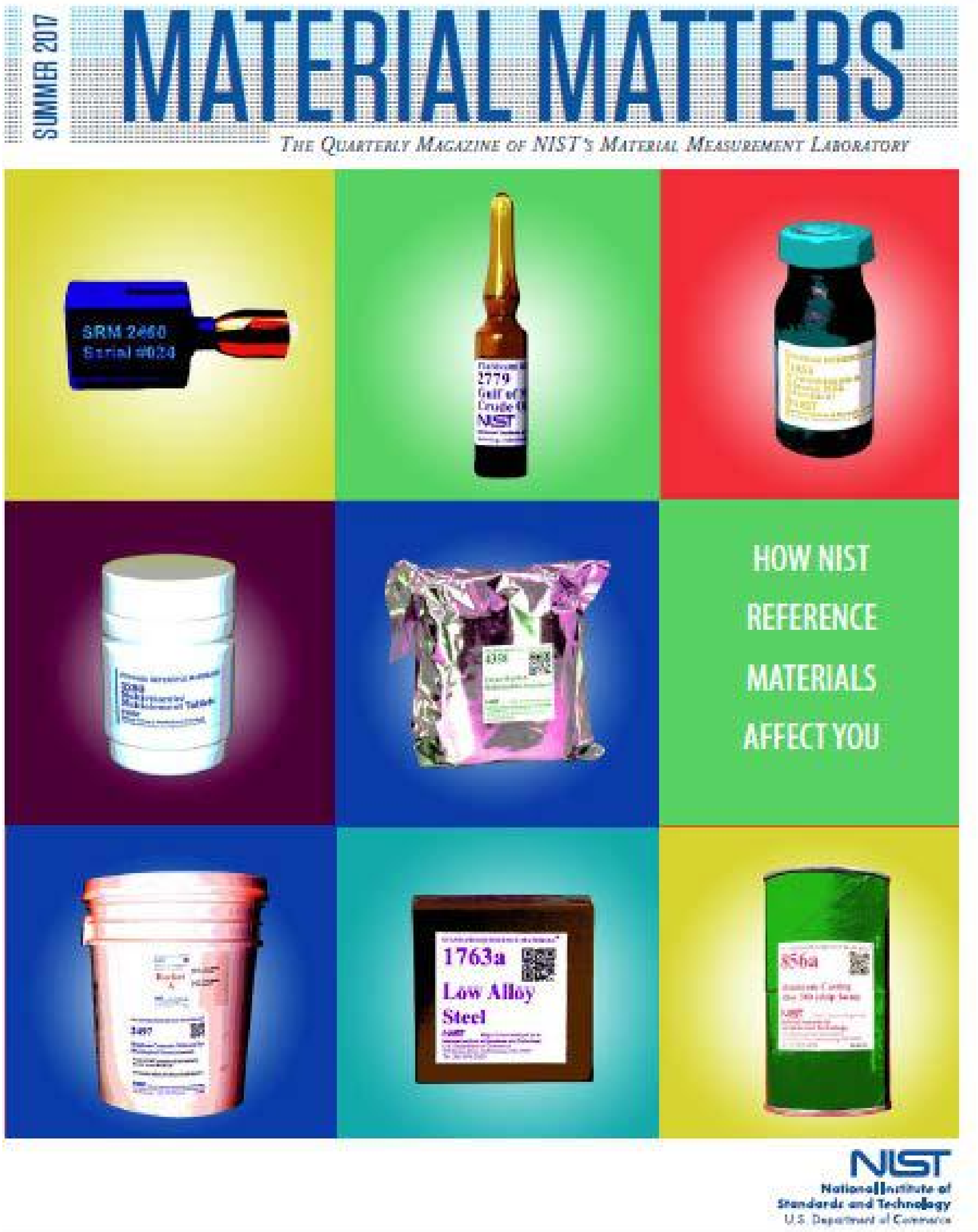
Launched in 2011, the MGI is a “multi-stakeholder effort to develop infrastructure to accelerate advanced materials discovery and development in the United States . . . through the use of computational capabilities, data management, and an integrated approach to materials science and engineering.”

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

Leading the MGI are the DOD, DOE, NSF, and NIST. Other agency partners include NASA, NIH, and U.S. Geol. Survey.



NIST is supporting the MGI through efforts to establish

- materials data-exchange and model-exchange protocols;
- means to ensure the quality of materials data and models;
- new methods, metrologies, and capabilities needed for accelerated materials development.

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.

Estimated economic impact of Materials Innovation Infrastructure within the U.S.

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.

Contextualizing these benefits:

- To fully fund physical U.S. infrastructure over the next 10 years, the annual cost is about $400 billion
- Germany's Fraunhofer Institutes receive about $800 million in government funding, annually
- Manufacturing USA institutes receive between $70 million and $110 million, annually

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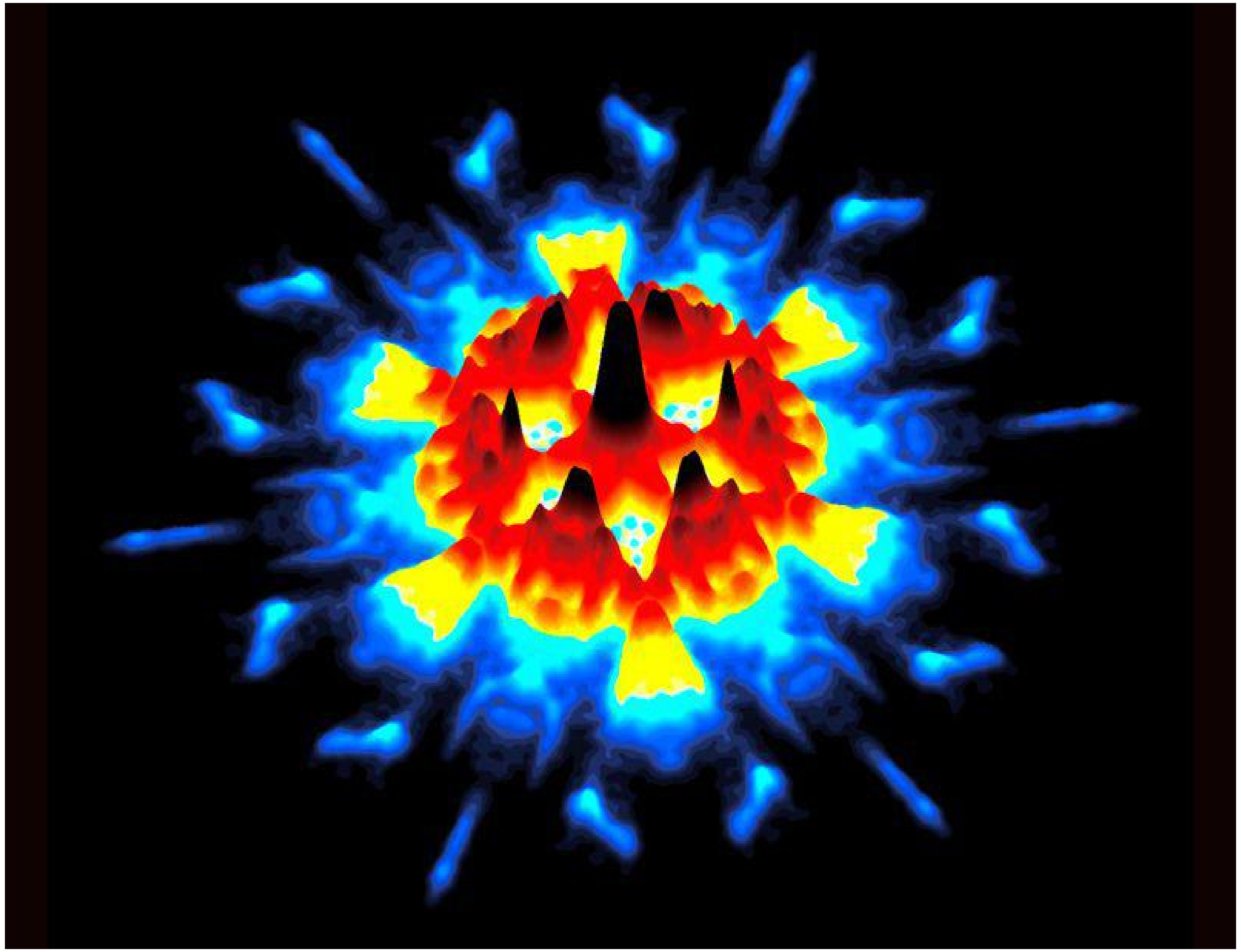
Areas of Industry Need

1. Access to high-quality data
2. Collaborative networks
3. Material design methods
4. Production and scale-up
5. Quality assurance, quality control, and component certification
6. Model validation and uncertainty quantification



The interference patterns, modelled by a computer, formed by quantum waves in a material known as a topological insulator. Credit: A. Yazdani/SPL

Areas of Industry Need

1. **Access to high-quality data**
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Example of infrastructure technology to address need:

- Models underpinning accurate and repeatable material measurement

Potential Impacts:

- Enable greater reliance on more efficient computational approaches
- Multiply the value of every other element of a Materials Innovation Infrastructure

Areas of Industry Need

1. Access to high-quality data
2. **Collaborative networks**
3. Material design methods
4. Production and scale-up
5. Quality assurance, quality control, and component certification
6. Model validation and uncertainty quantification

Example of infrastructure technology to address need:

- Communication standards and translators (e.g. MT Connect for material measurement equipment)

Potential Impacts:

- Integrate experimental measurement and computational modeling to improve model fidelity and overall utility
- Realize network externalities

Areas of Industry Need

1. Access to high-quality data
2. Collaborative networks
3. **Material design methods**
4. Production and scale-up
5. Quality assurance, quality control, and component certification
6. Model validation and uncertainty quantification

Example of infrastructure technology to address need:

- Models, simulations, metrologies, and machine learning tools for advanced materials design and means of integrating tools with one another

Potential Impacts:

- Enable more targeted searches of design space for more promising candidate materials
- Enable purposeful design of materials to meet specific performance requirements

Areas of Industry Need

1. Access to high-quality data
2. Collaborative networks
3. Material design methods
4. **Production and scale-up**
5. Quality assurance, quality control, and component certification
6. Model validation and uncertainty quantification

Example of infrastructure technology to address need:

- Multiscale modeling frameworks (e.g. integrating macroscopic process models with microscopic materials simulation)

Potential Impacts:

- Reduce trial and error when scaling up
- Allow consideration of the production-scale processes to be integrated into the initial design process

Areas of Industry Need

1. Access to high-quality data
2. Collaborative networks
3. Material design methods
4. Production and scale-up
5. **Quality assurance, quality control, and component certification**
6. Model validation and uncertainty quantification

Example of infrastructure technology to address need:

- Process control tools (test protocols; reference databases)

Potential Impacts:

- Reduce cost of controlling and verifying the performance attributes of materials, and components and products embodying those materials
- Reduce risk of large costs incurred if defects are not detected and lead to product failures in use

Areas of Industry Need

1. Access to high-quality data
2. Collaborative networks
3. Material design methods
4. Production and scale-up
5. Quality assurance, quality control, and component certification
6. **Model validation and uncertainty quantification**

Example of infrastructure technology to address need:

- Validation of analytical methods and procedures, emphasizing industrially relevant systems, comparing predicted and measured properties from multiple sources

Potential Impacts:

- Enhance the utility of computational approaches from both engineering and business perspectives
- Advance reliance on computational approaches in situations where they can save cost and add value

Examples of Materials Innovation Infrastructure in Action (1/3)

Ford Motor Company developed the Virtual Aluminum Castings (VAC) software

- Integrated commercial software and Ford's proprietary data and original code
- 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
- VAC tools "bridge the many key dimensional scales from the atomistic level to the component level"[1]
- "accomplished by a combination of theoretical, experimental, and computational technologies and . . . the development of a deep, fundamental understanding of dozens of separate phenomena" [1]
- 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" [1]

[1] Allison, Li, Wolverton, and Su, 2006, pp. 28; 35

Examples of Materials Innovation Infrastructure in Action (2/3)

Rapid Qualification of New Structural Alloys in Aerospace

- QuesTek Innovations LLC has applied a collection of computational models to the design, development, and aerospace certification and flight qualification of advanced metal alloys
- Trademarked the suite of tools *Materials by Design*, integrating different models and data sources
- QuesTek credits these modeling tools with accelerating the development of several advanced alloys [2]
- 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[3]

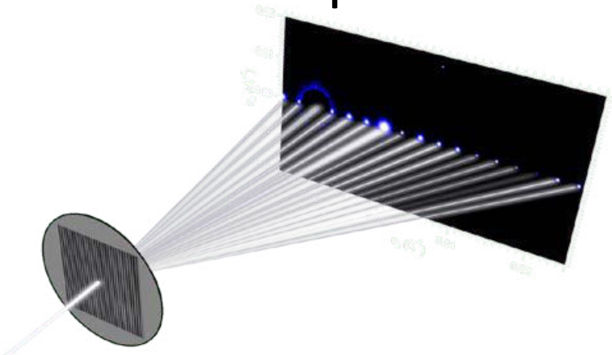
[2] Sebastian and Olson, 2014

[3] Materials Innovation Case Study, 2016a

Examples of Materials Innovation Infrastructure in Action (3/3)

Directed Self-Assembly (DSA) of Block Copolymers

- DSA of block copolymers is a leading candidate to replace conventional optical lithography [4, 5]
- This nanoscale patterning technique rests on decades of research that has provided the necessary knowledge base and well integrates theory, computation, and experimentation by research teams at universities and in industry [6]
- “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.” [6]



[4] Laachi, Shykind, and Fredrickson, 2014
[5] Laachi et al., 2015
[6] de Pablo et al., 2014, p. 112

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3. **Interview methodology**

4. Potential impact estimates if needs are met

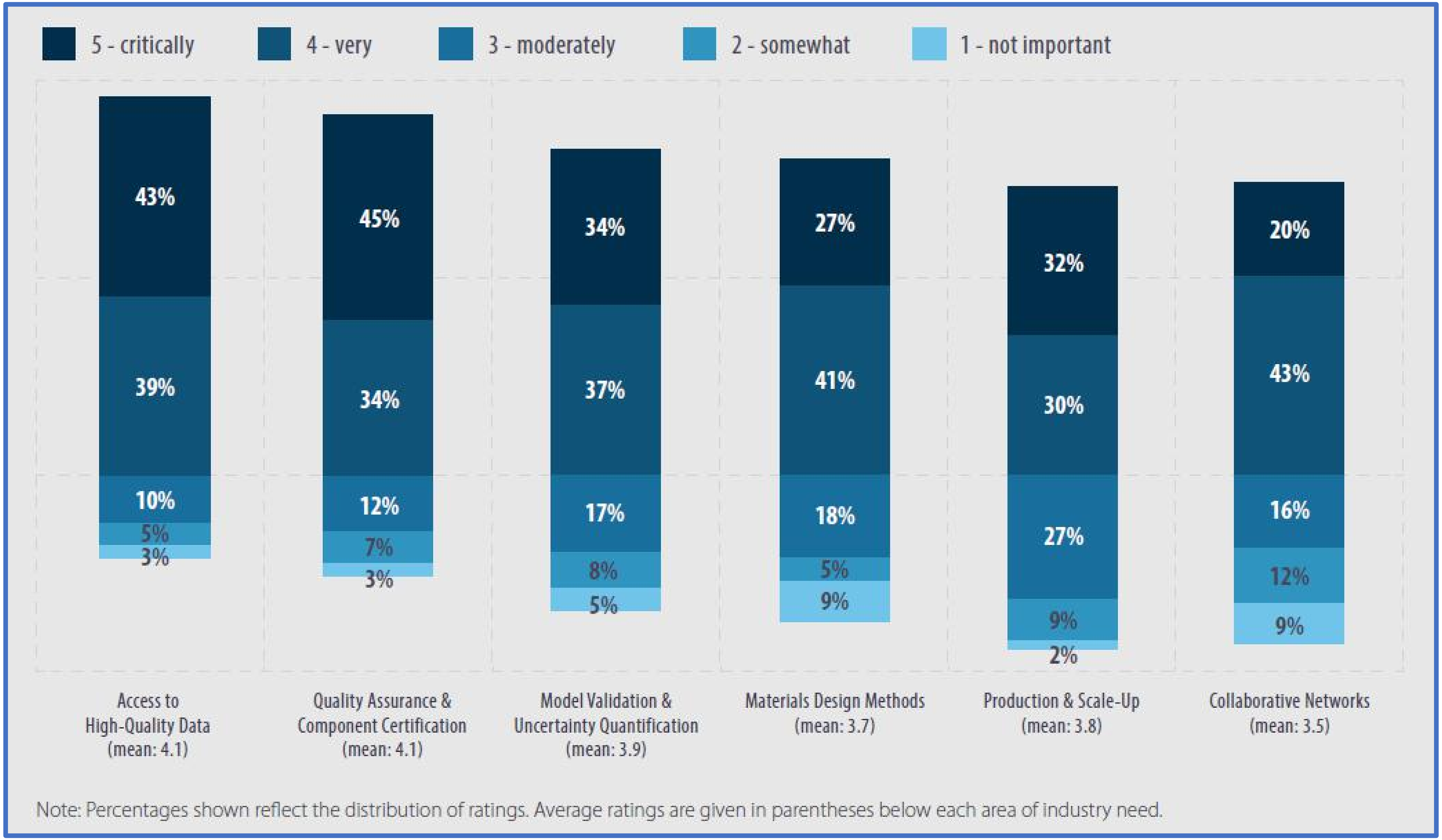
Data Collection and Interview Methodology

1. Interviews were conducted with industry experts
2. Sampling covered a diversity of
   - Industries using advanced materials
   - Company sizes
   - Points along various supply chains
   - Materials classes
   - Individual backgrounds (computationalists vs. experimentalists; R&D directors, managers, and scientists)
3. Perspective and questions covered all stages of the R&D process
4. Responses were weighted in proportion to industry composition in the U.S. economy

R&D Stages Covered by Interviews

Discovery/Design (lab scale)	Development (pilot scale)	Manufacturing (production scale)	Deployment
Experimentation and modeling at bench or lab scale	*Pilot-scale synthesis, processing, and evaluation*	*Production-scale product and process evaluation*	*Application-specific tailoring; supporting technology development*
Start: Intent to seek new material for a given application or end use articulated	Start: Synthesis of candidate material compositions for application/end-use testing	Start: Production-scale trials begin	Start: New material is available as a commercial product
End: Candidate compositions and processing methods identified	End: Composition and synthesis/processing approach identified for transition to production scale	End: Production-scale process and resulting product finalized; standards established	End: New material is used in a commercial application

Interviewees' Rating of the Importance of Technology Infrastructure Needs



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Interviewees' Rating of the 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.

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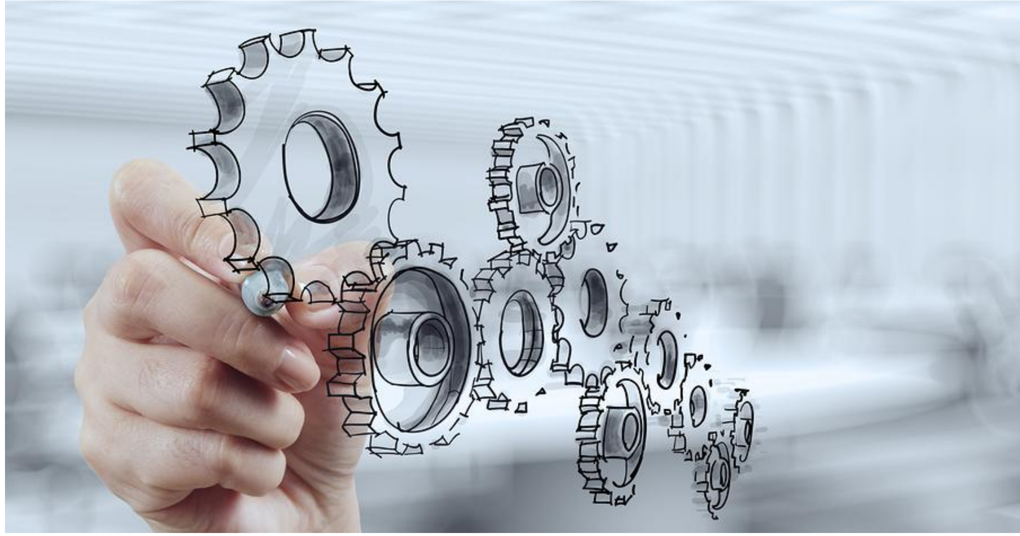
Two types of Potential Economic Impacts:

1. Efficiency of R&D
    - Improved probabilities of successful projects
    - Improved cycle times (speed of project advancement)
    - Cost reductions (annualized; time-fixed)



2. Improved R&D outcomes (greater innovation)
    - Superior products emerging from R&D and ability to reach new markets
    - Increased allocation of efforts toward R&D (due to increases in the marginal product of R&D effort)

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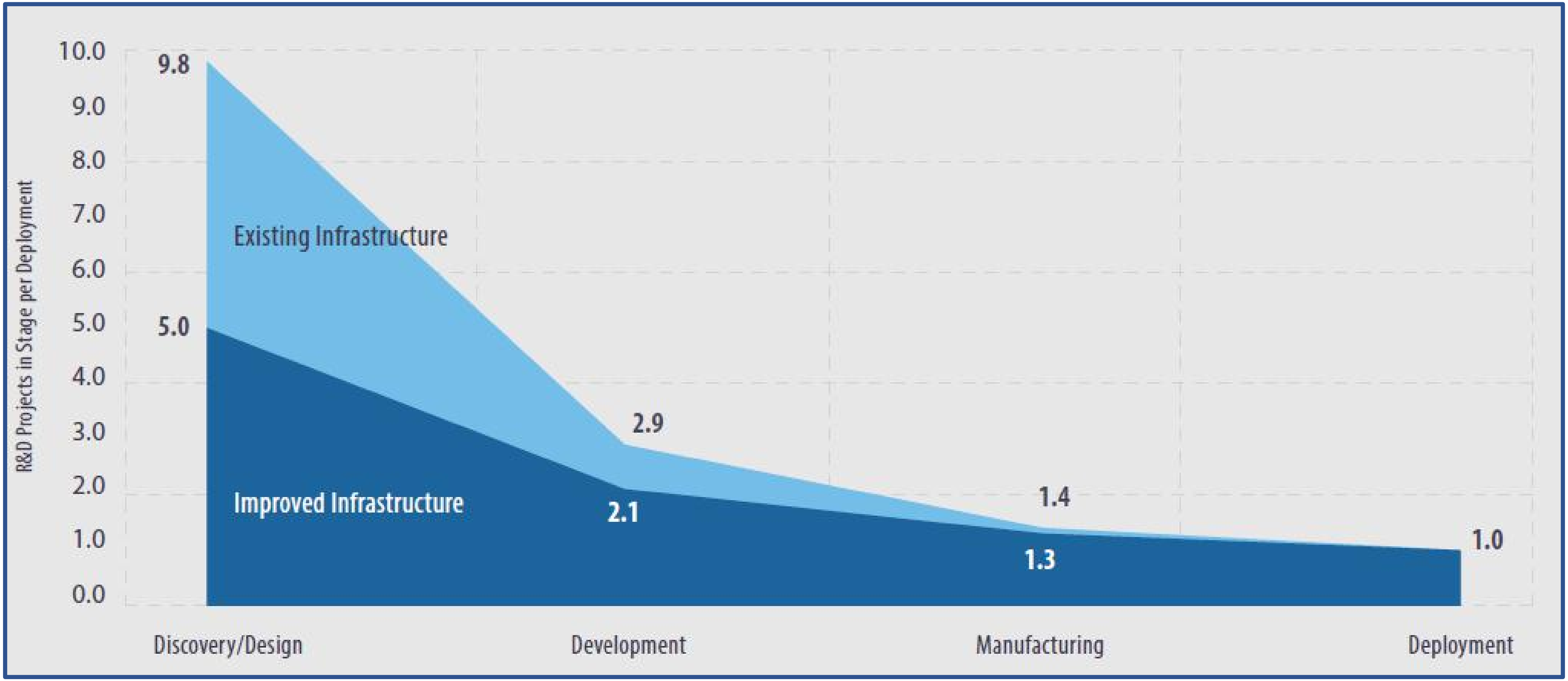
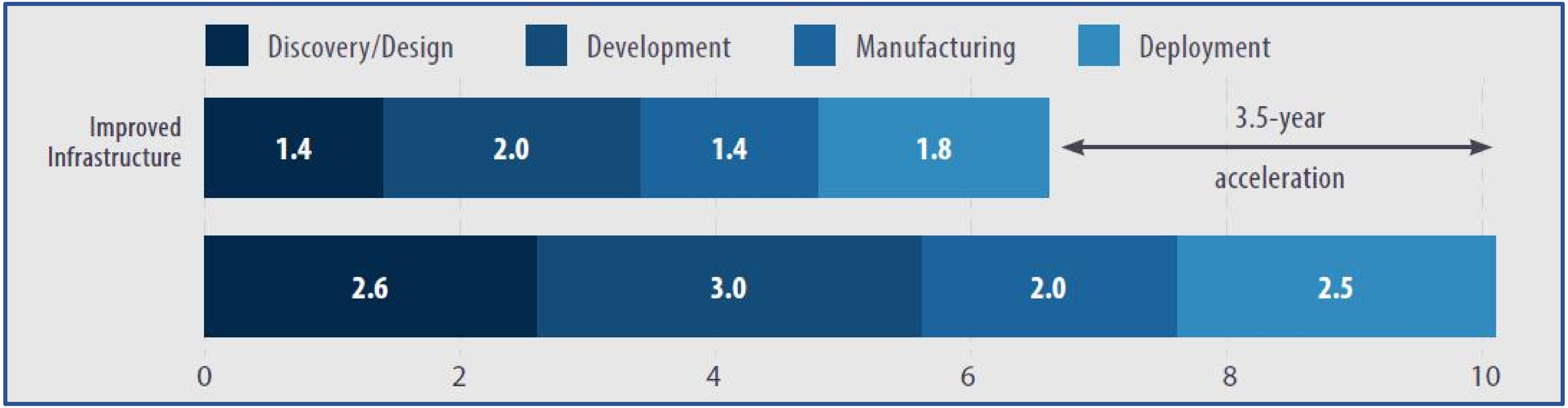
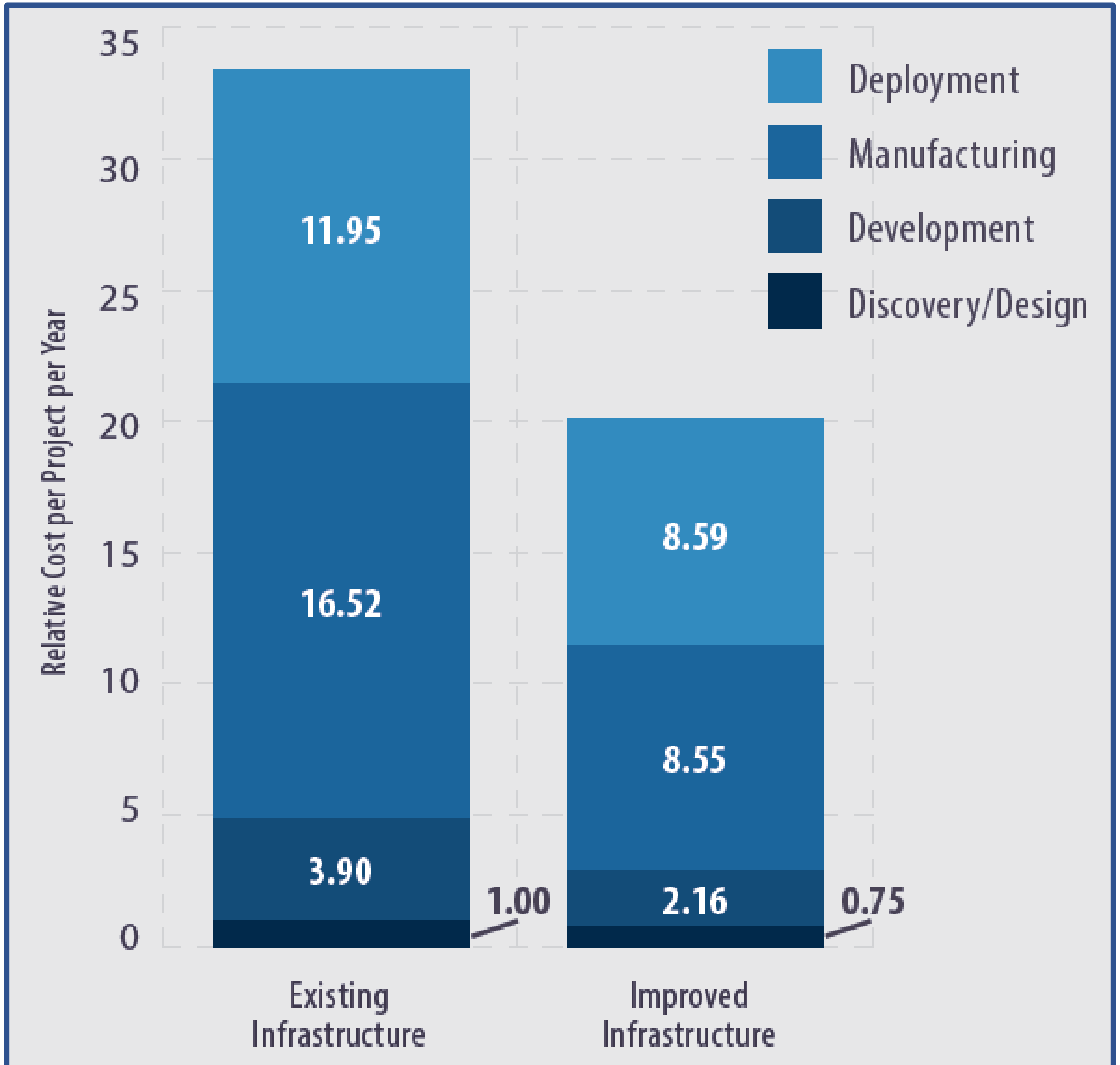
Potential Impact on Risk: Number of R&D Projects in Stage per Deployment



Potential Impact on Time to Market: Average Time in Each Stage per R&D Project



Potential Impact on Relative Costs: Relative Cost per R&D Project per Year



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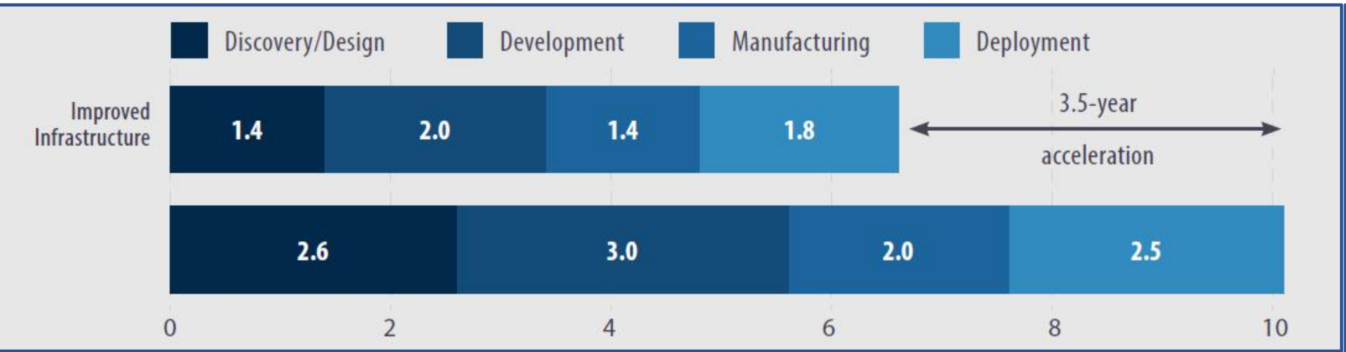
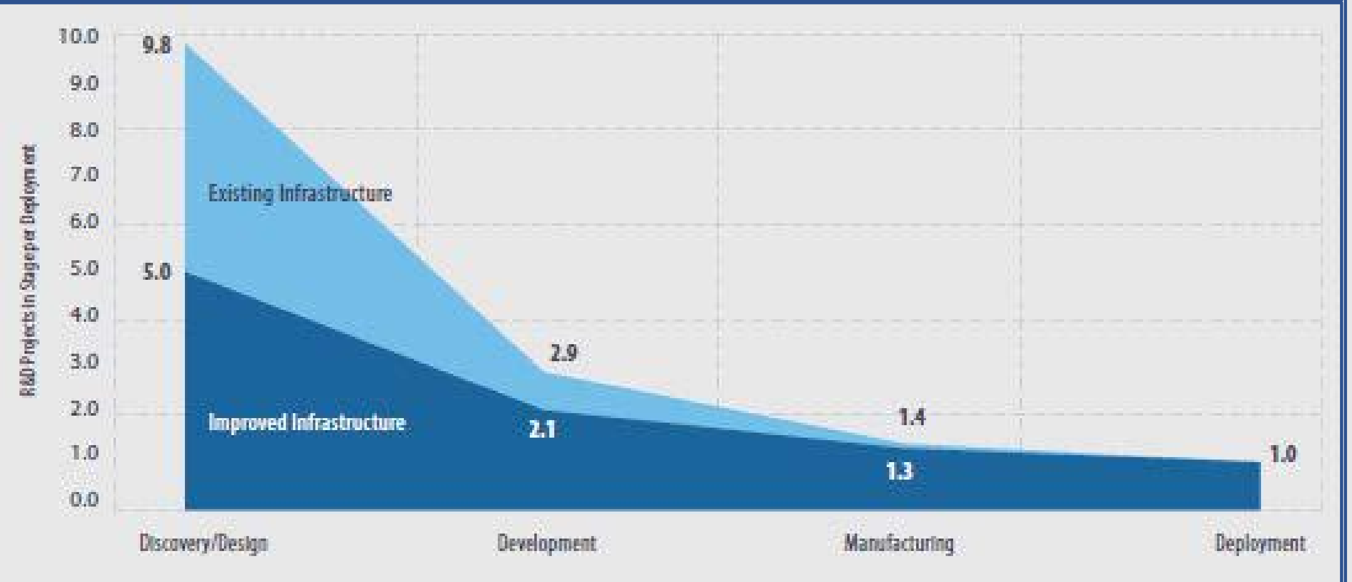
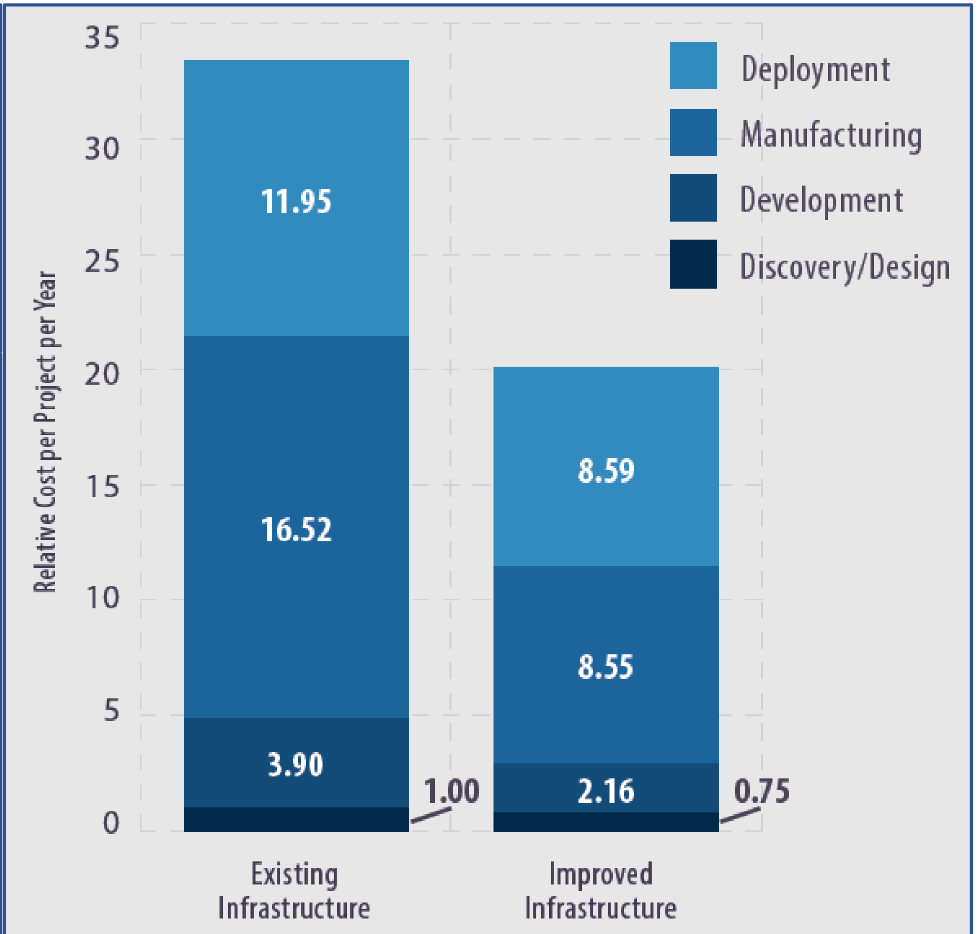
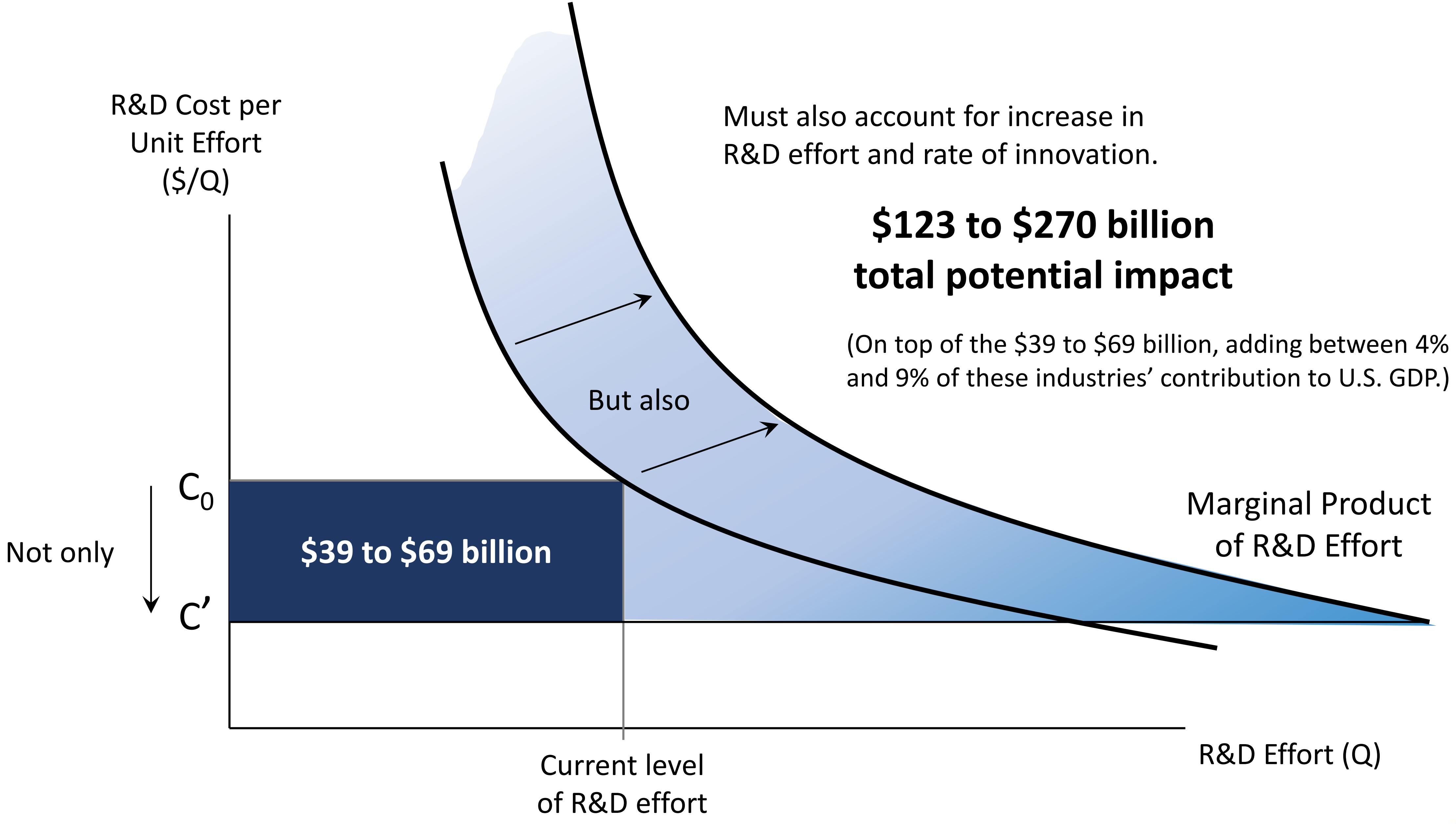
Overall, estimated potential impacts of an improved Materials Innovation Infrastructure achieve a 71% improvement in R&D efficiency, worth an estimated **$39 billion to $69 billion** per year to U.S. companies that comprise the new materials supply chain (between 15% and 25% of all R&D expenditure in these industries).








R&D Cost per Unit Effort ($/Q)
Must also account for increase in R&D effort and rate of innovation.
$123 to $270 billion total potential impact
(On top of the $39 to $69 billion, adding between 4% and 9% of these industries' contribution to U.S. GDP.)
But also
C_0
Not only
C'
$39 to $69 billion
Marginal Product of R&D Effort
R&D Effort (Q)
Current level of R&D effort
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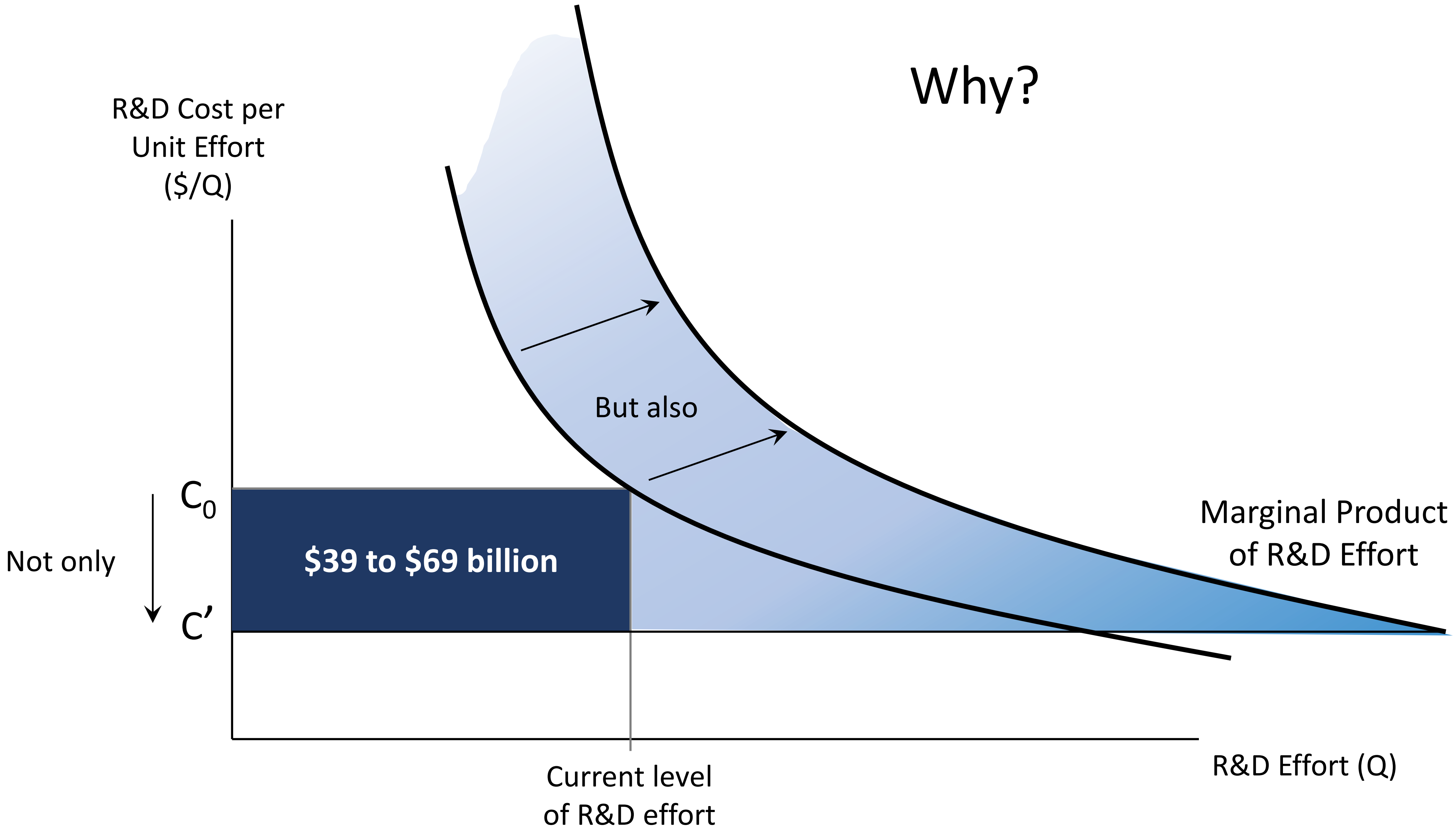
Why?
R&D Cost per
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C_0
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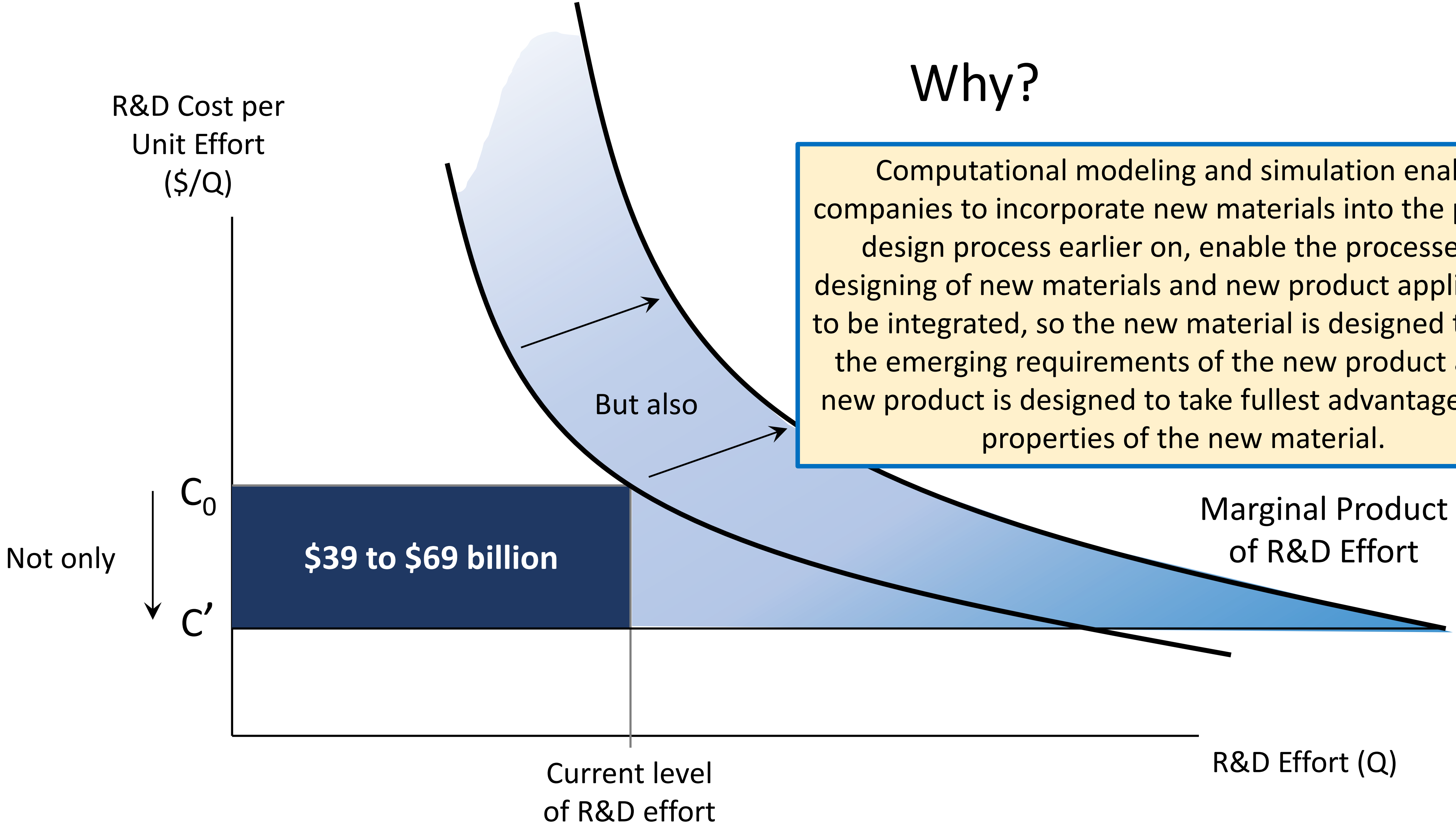
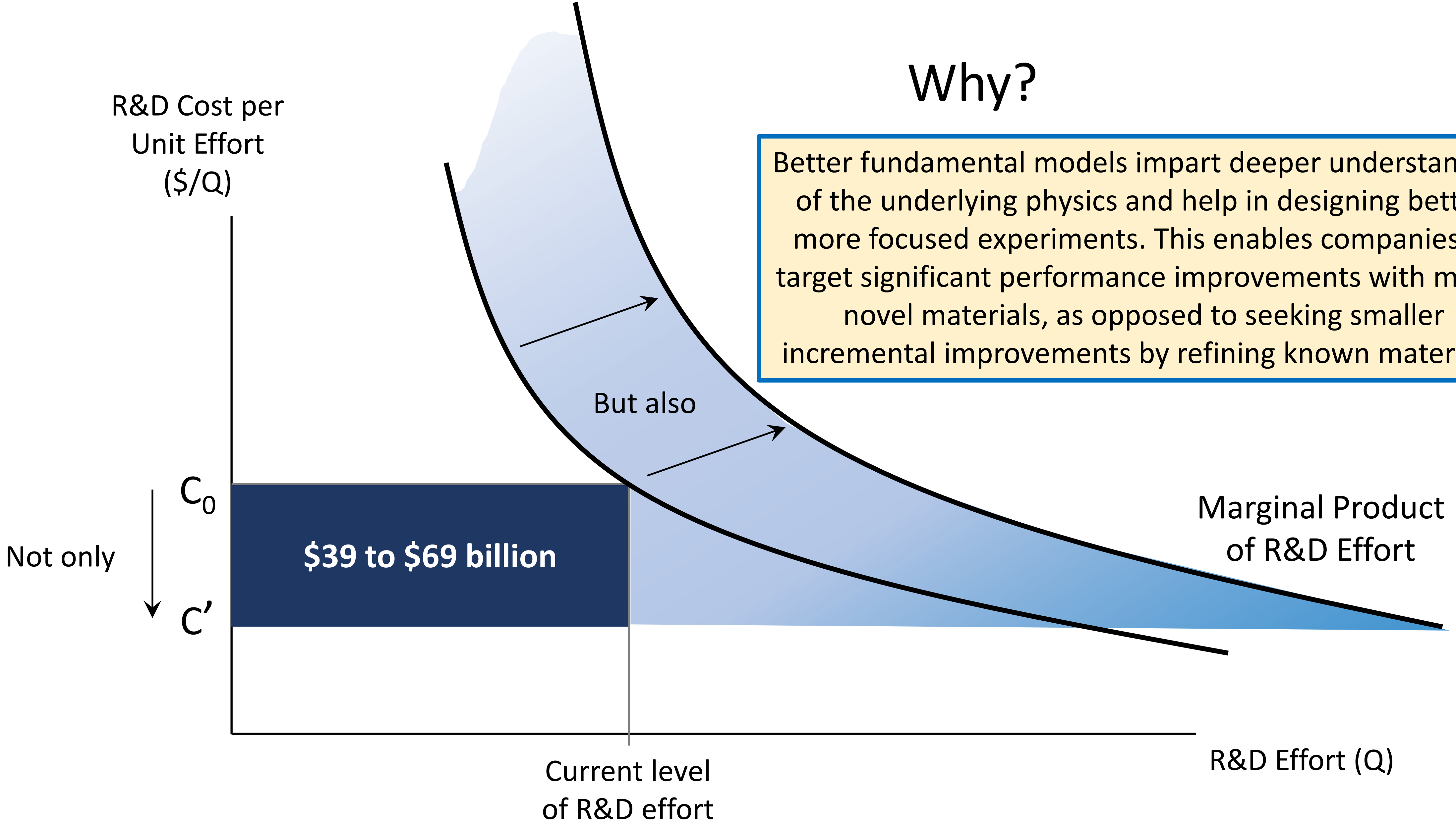
Why?



Computational modeling and simulation enable companies to incorporate new materials into the product design process earlier on, 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.

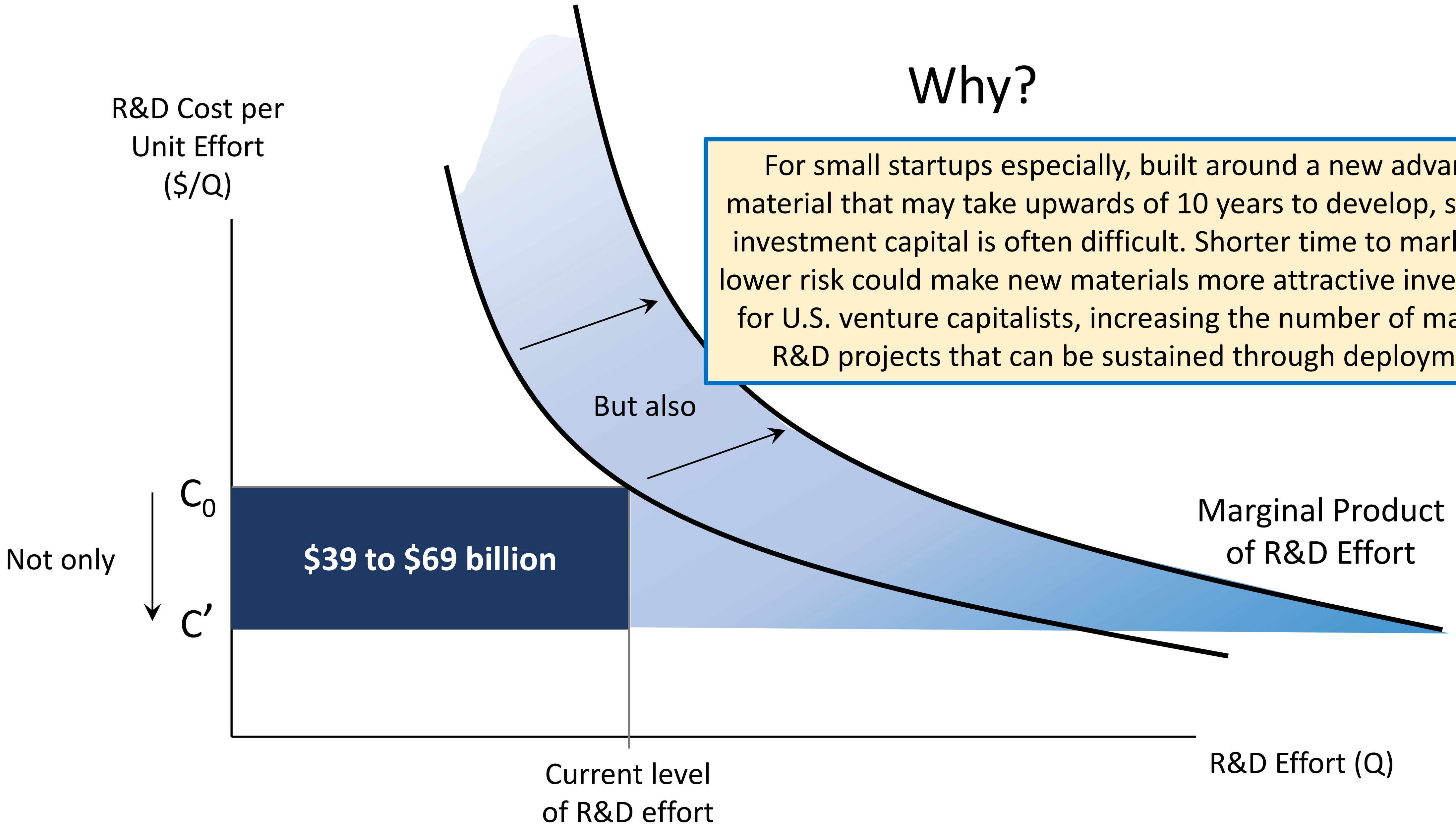


Why?

Better fundamental models impart deeper understanding of the underlying physics and help in designing better, more focused experiments. This enables companies to target significant performance improvements with more-novel materials, as opposed to seeking smaller incremental improvements by refining known materials.

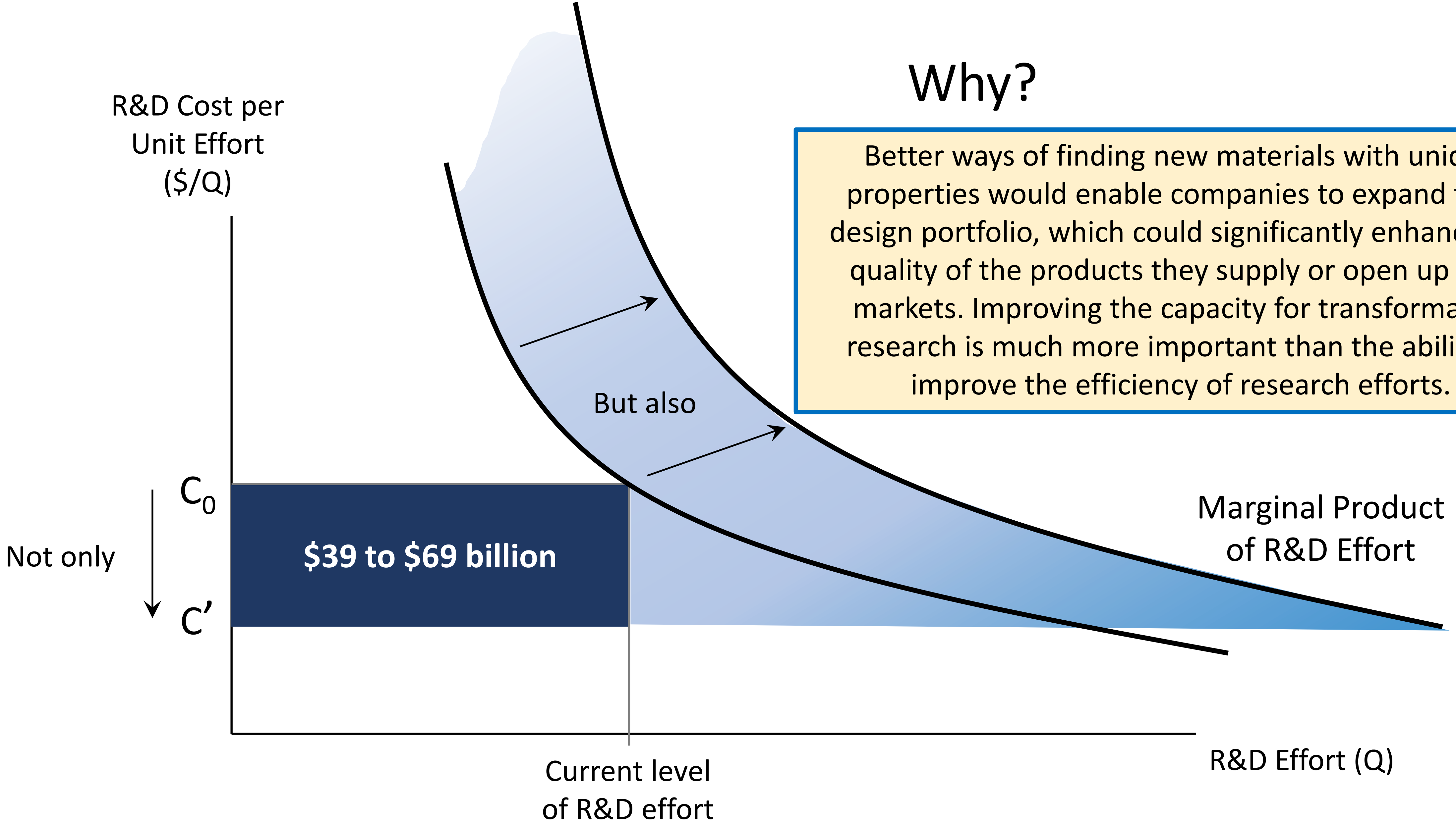
Why?

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 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.



Why?

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. Improving the capacity for transformative research is much more important than the ability to improve the efficiency of research efforts.



Summary of Potential Economic Impact Estimates by Type of Impact
(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)**

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Full report and analysis brief at **nist.gov/mgi/mgi-reports**

April 2018

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

Final Report

Prepared for

Technology Partnerships Office, Office of Innovation and Industry
National Institute of Standards and Technology
U.S. Department of Commerce
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Thank you!

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Supplementary slides

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

INDUSTRY NEED	EXAMPLES OF INFRASTRUCTURE TECHNOLOGY TO ADDRESS NEED	POTENTIAL IMPACTS
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
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

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