

# The Materials Genome Initiative: Opportunities for Materials Research to Accelerate Discovery

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[http://www.whitehouse.gov/sites/default/files/microsites/ostp/materials\\_genome\\_initiative-final.pdf](http://www.whitehouse.gov/sites/default/files/microsites/ostp/materials_genome_initiative-final.pdf)





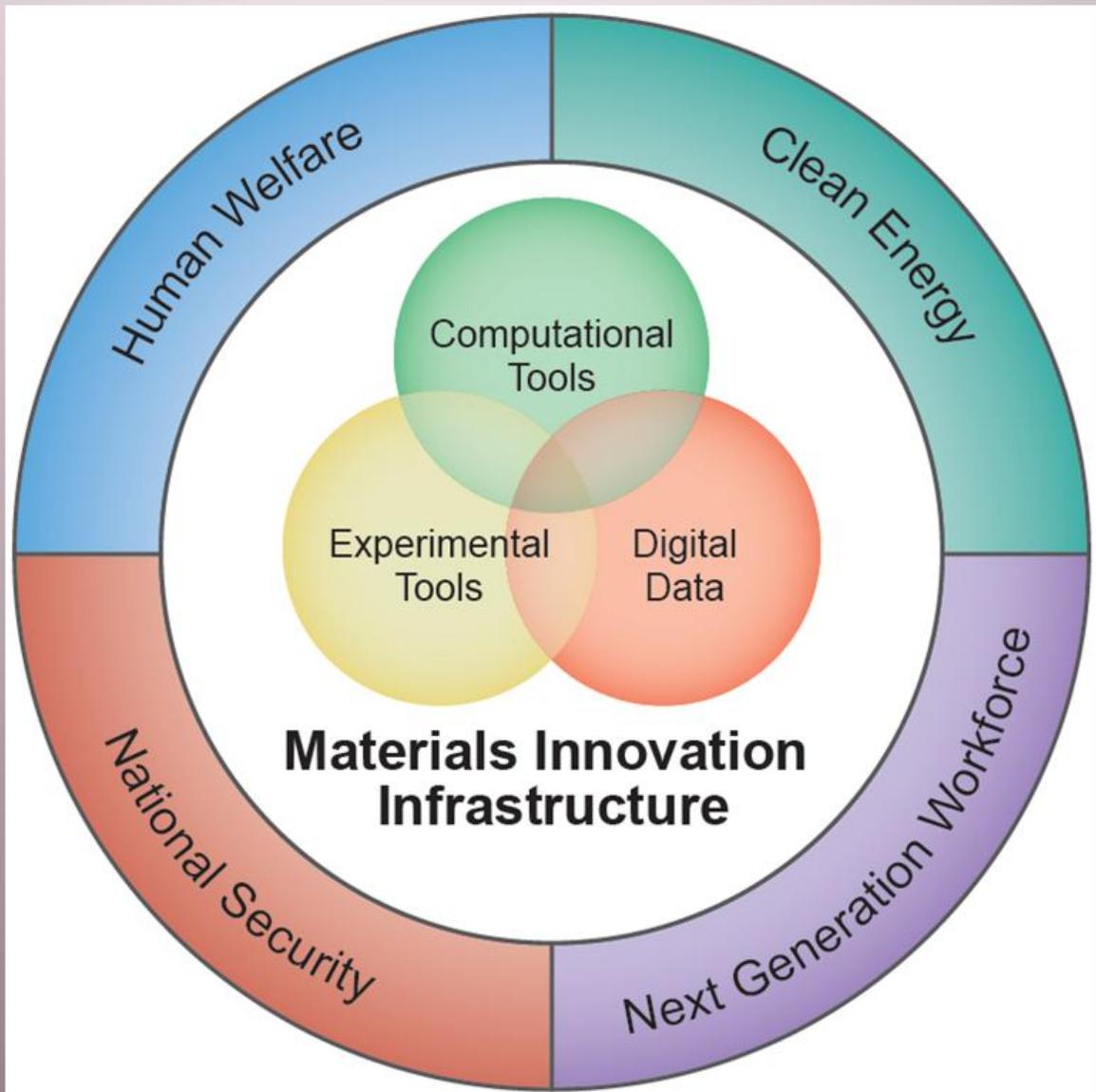
*To help businesses discover, develop, and deploy new materials twice as fast, we're launching what we call **the Materials Genome Initiative**. The invention of silicon circuits and lithium ion batteries made computers and iPods and iPads possible, but it took years to get those technologies from the drawing board to the market place. We can do it faster.*

-President Obama

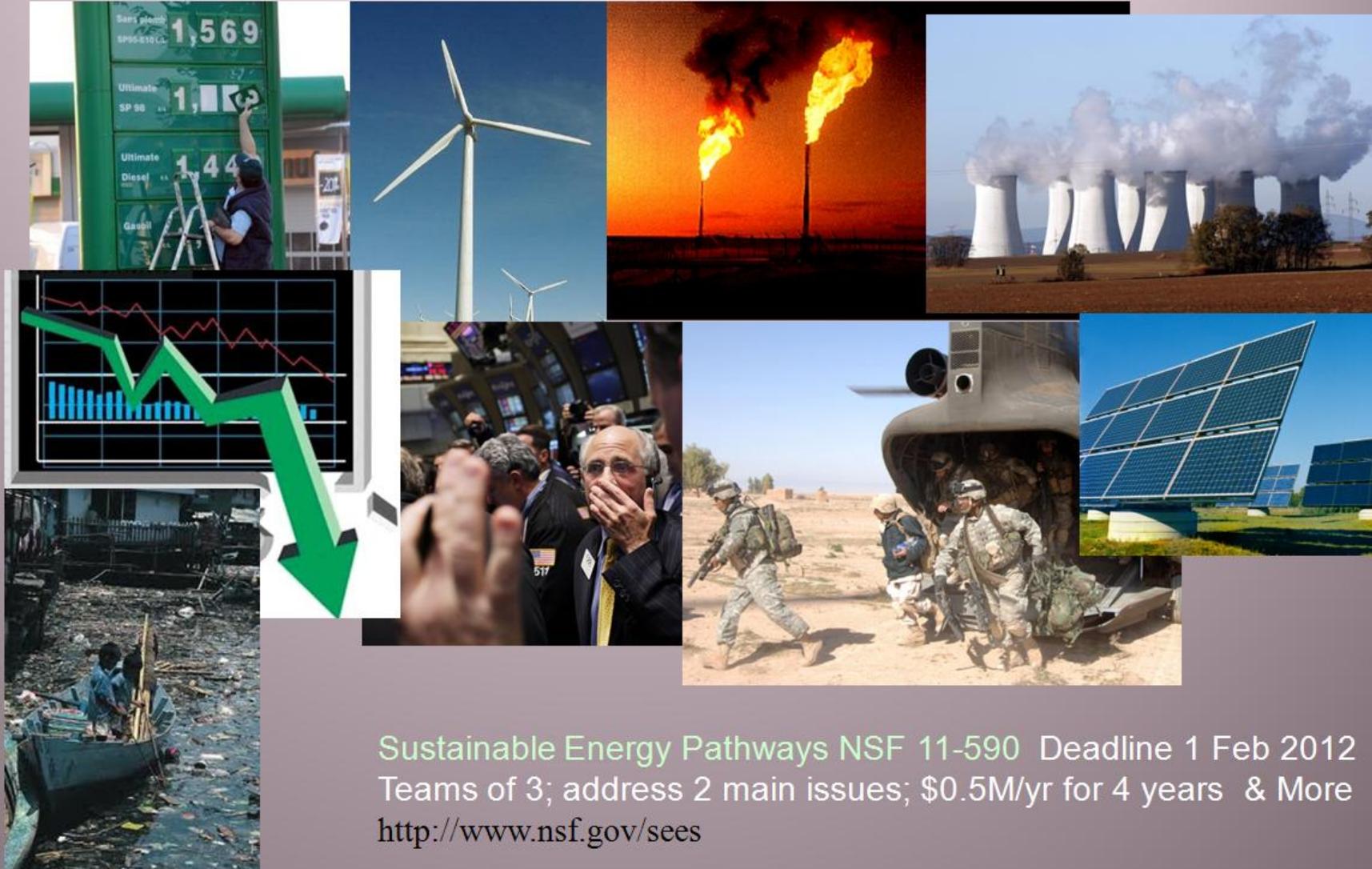
Carnegie Mellon University, June 2011

# The Materials Innovation Infrastructure

Goal: *decrease the time-to-market by over 50%*



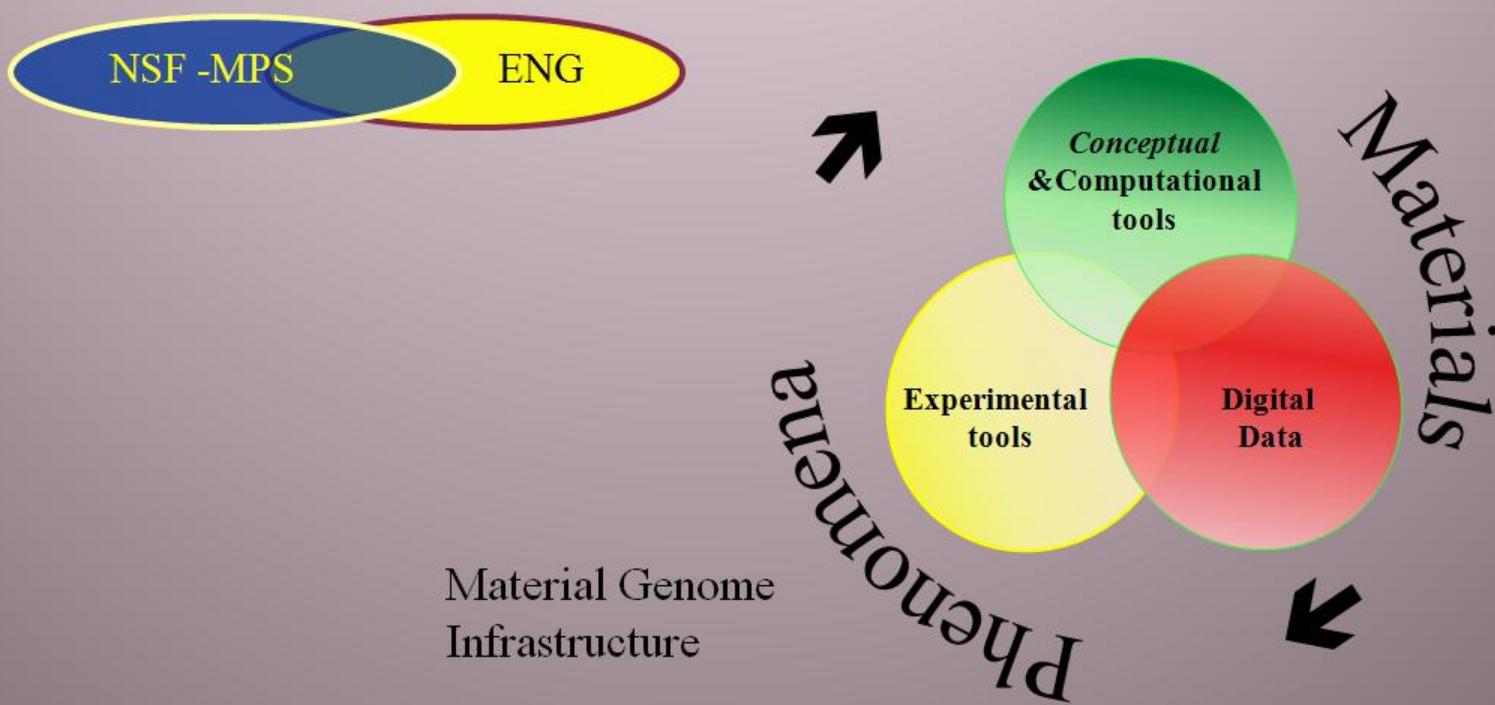
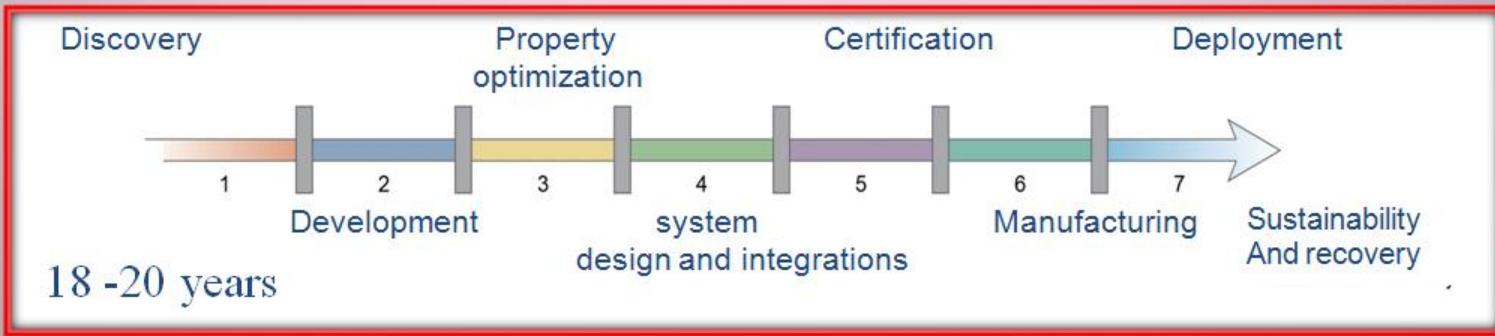
# We live in interesting times ...

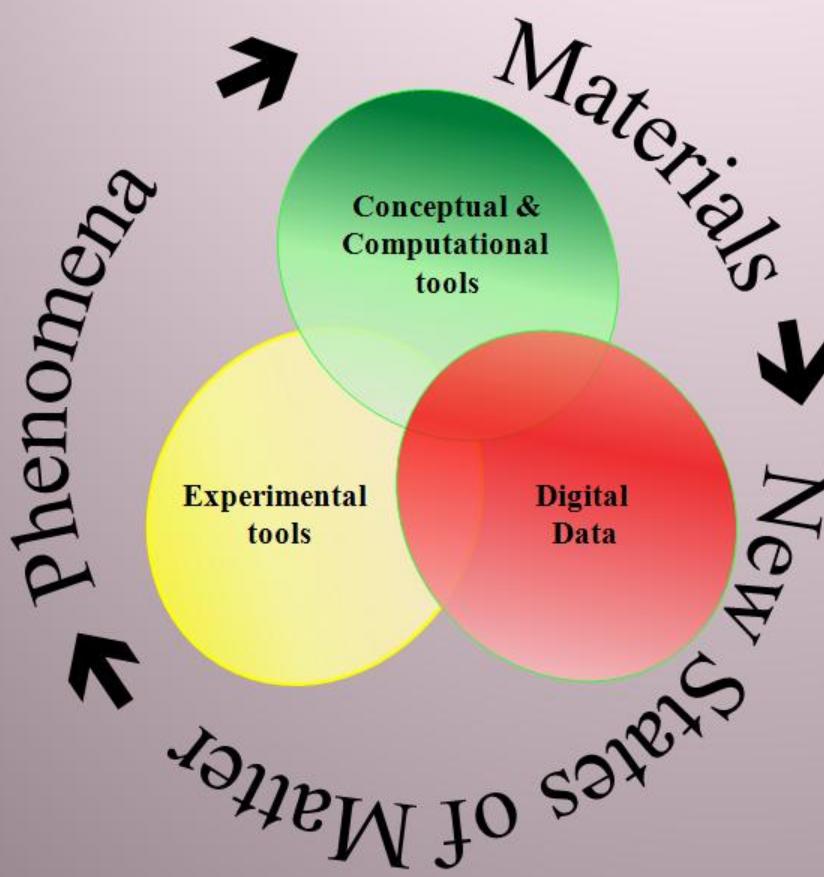




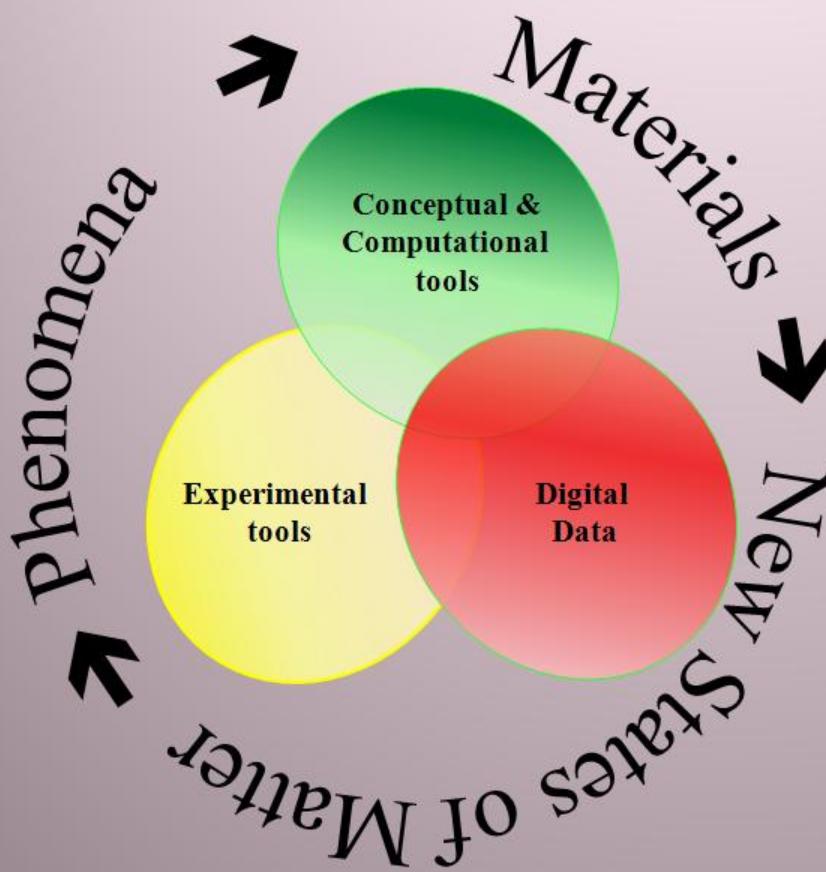
# Materials Genome Initiative

## New paradigm: “twice as fast, at a fraction of the cost”

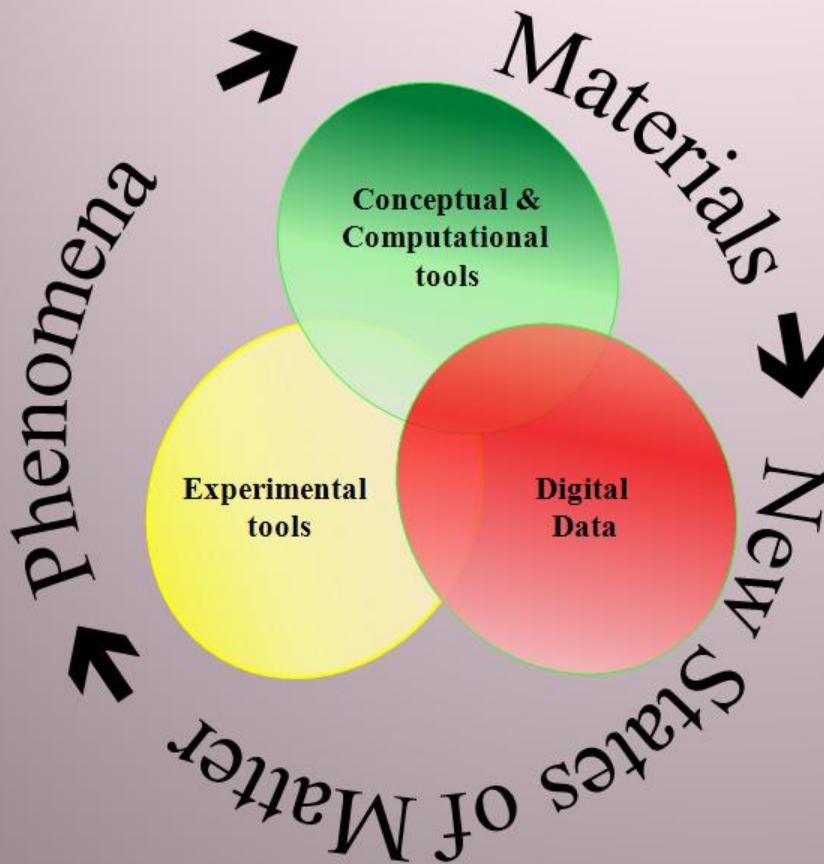




# Materials Genome Initiative

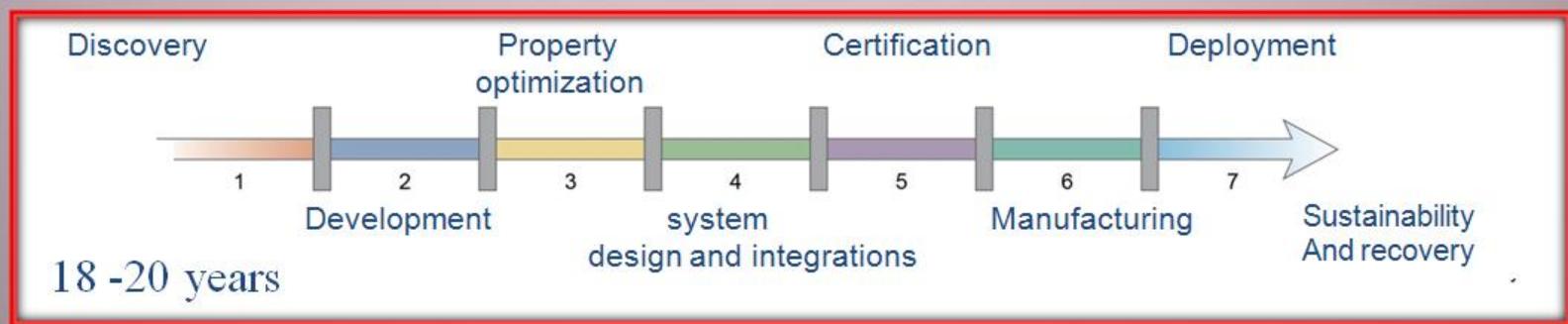


# Materials Genome Initiative

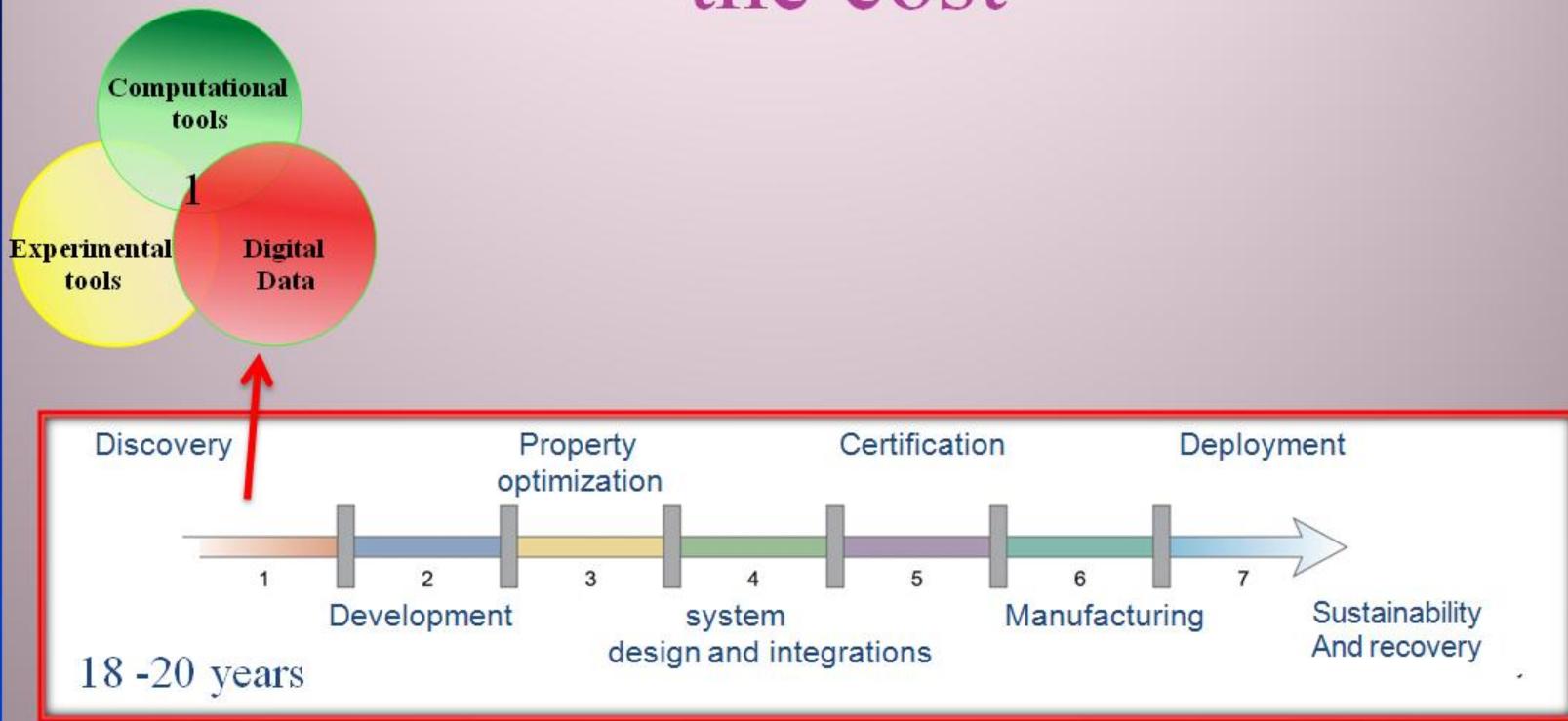


*Can we accelerate and amplify discovery?*

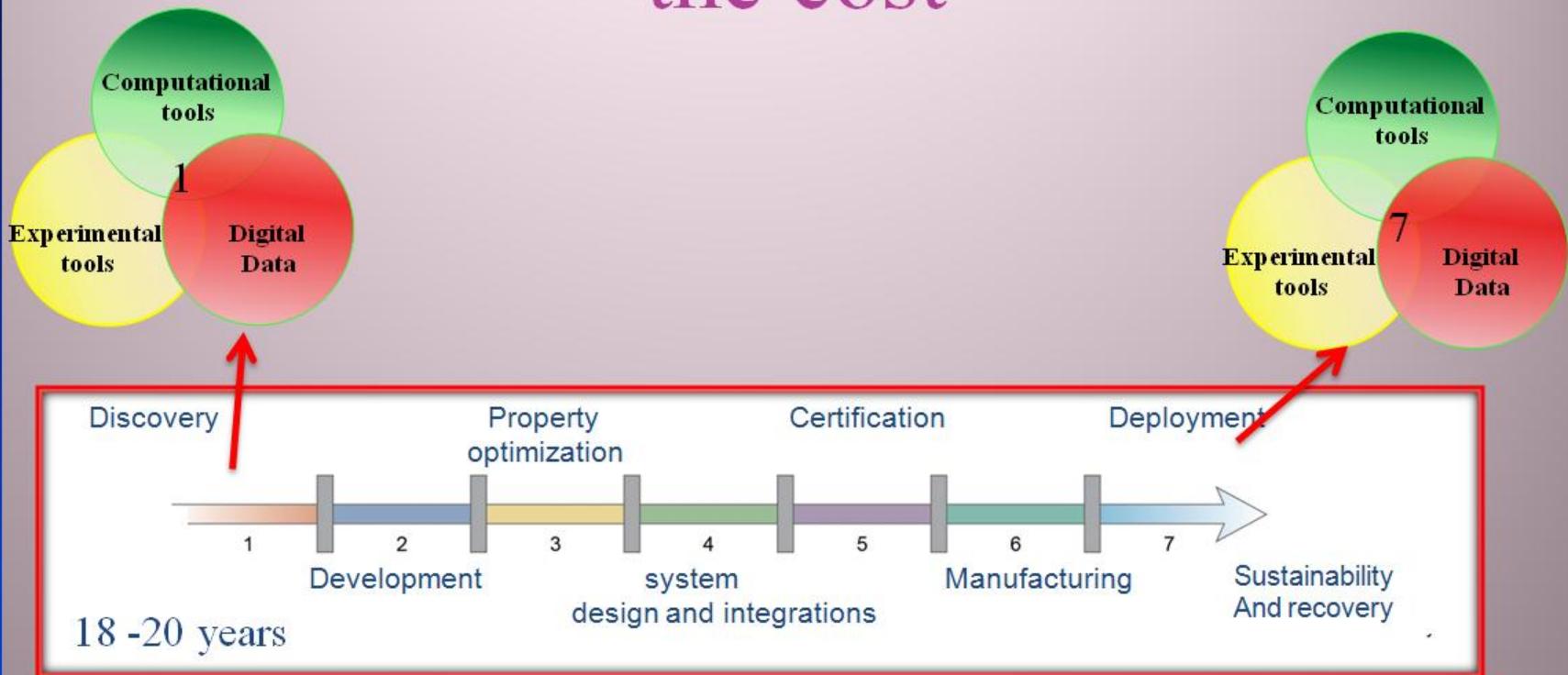
# MGI: “twice as fast, at a fraction of the cost



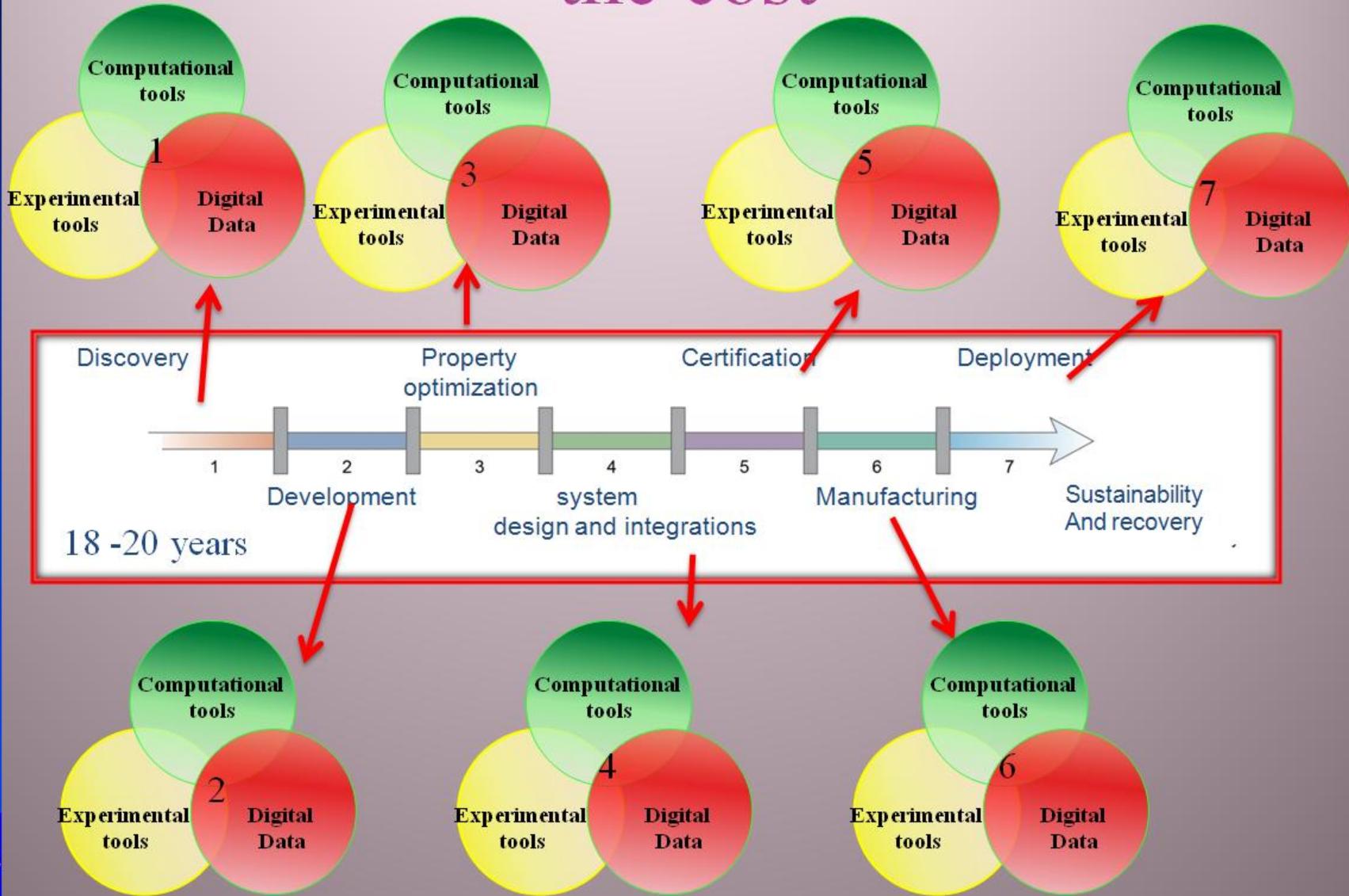
# MBI: “twice as fast, at a fraction of the cost



# MGIs: “twice as fast, at a fraction of the cost

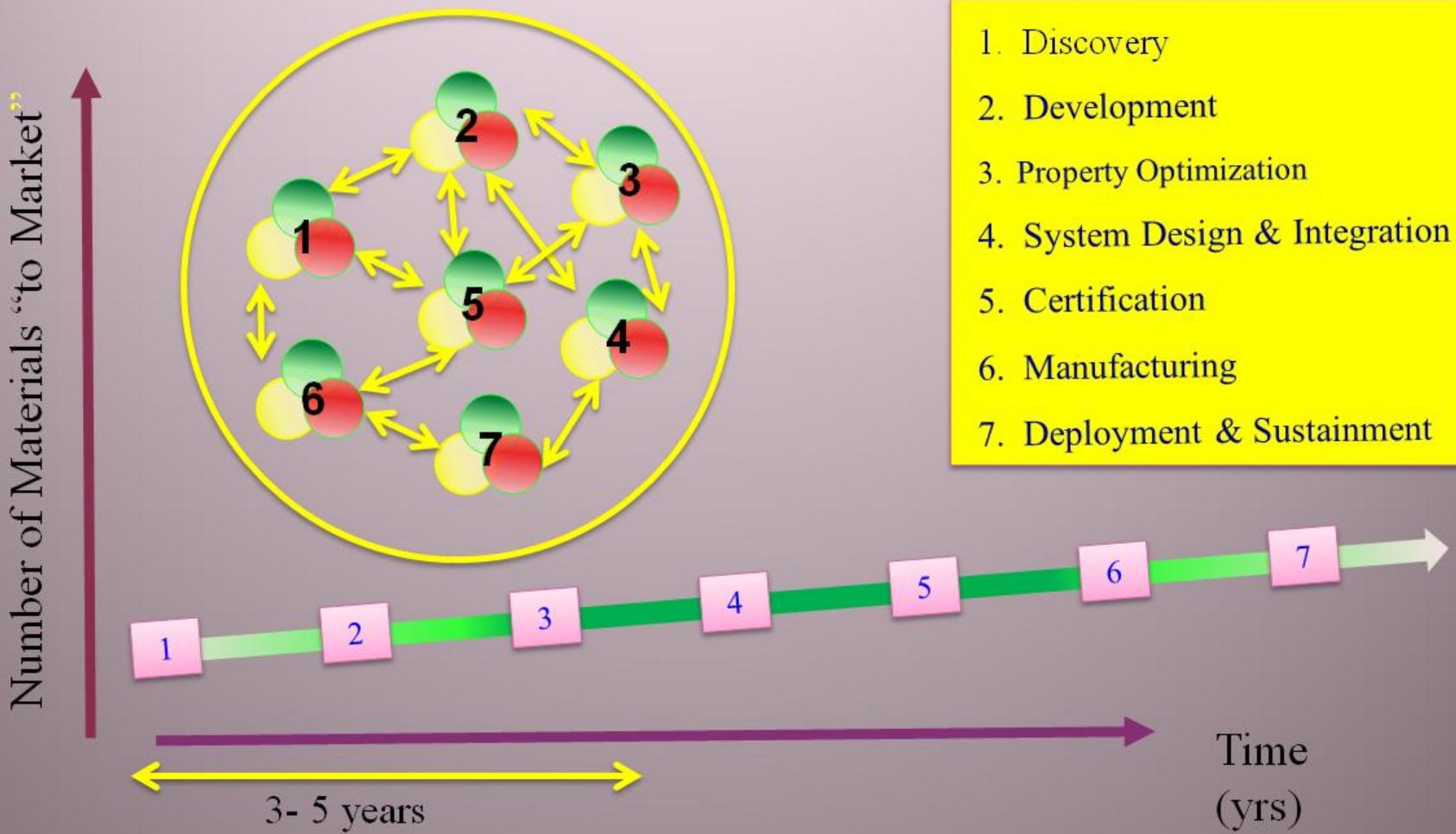


# MGIs: “twice as fast, at a fraction of the cost

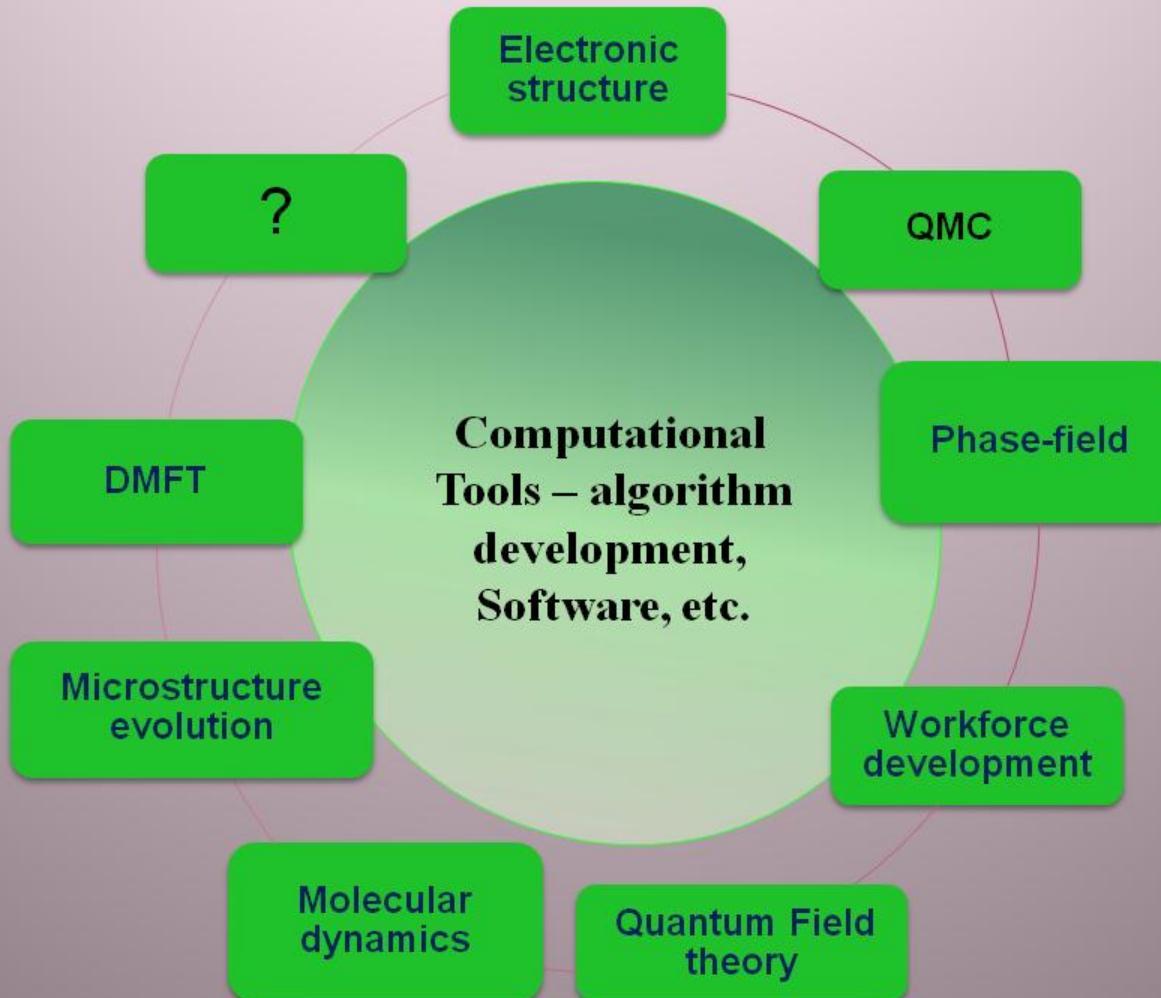


# MGCI for Global Competitiveness

## Materials Genome Initiative for Global Competitiveness



# Software and algorithm development for acceleration at each stage of the continuum

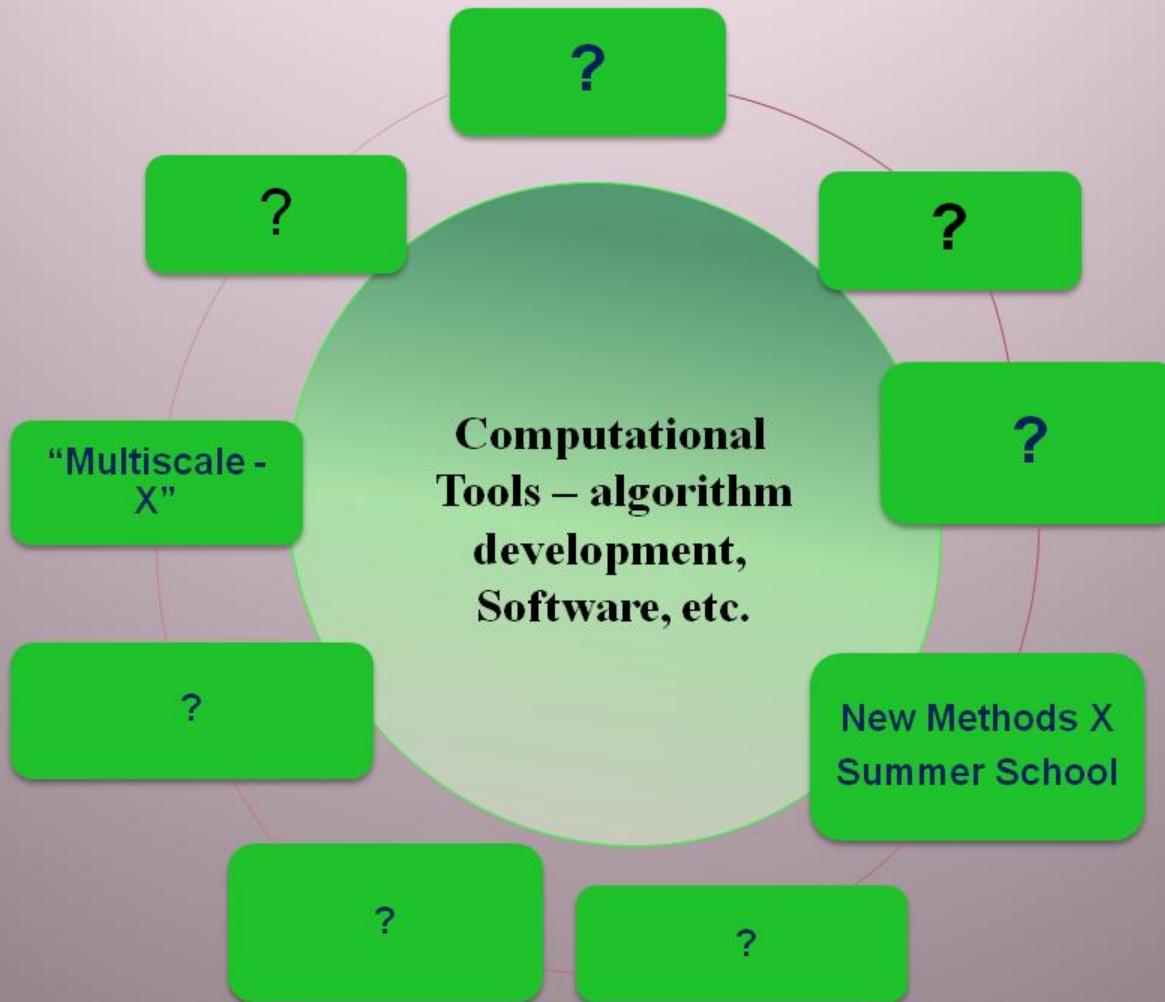


# Software and algorithm development

*What will be in your ‘toolbox’?*



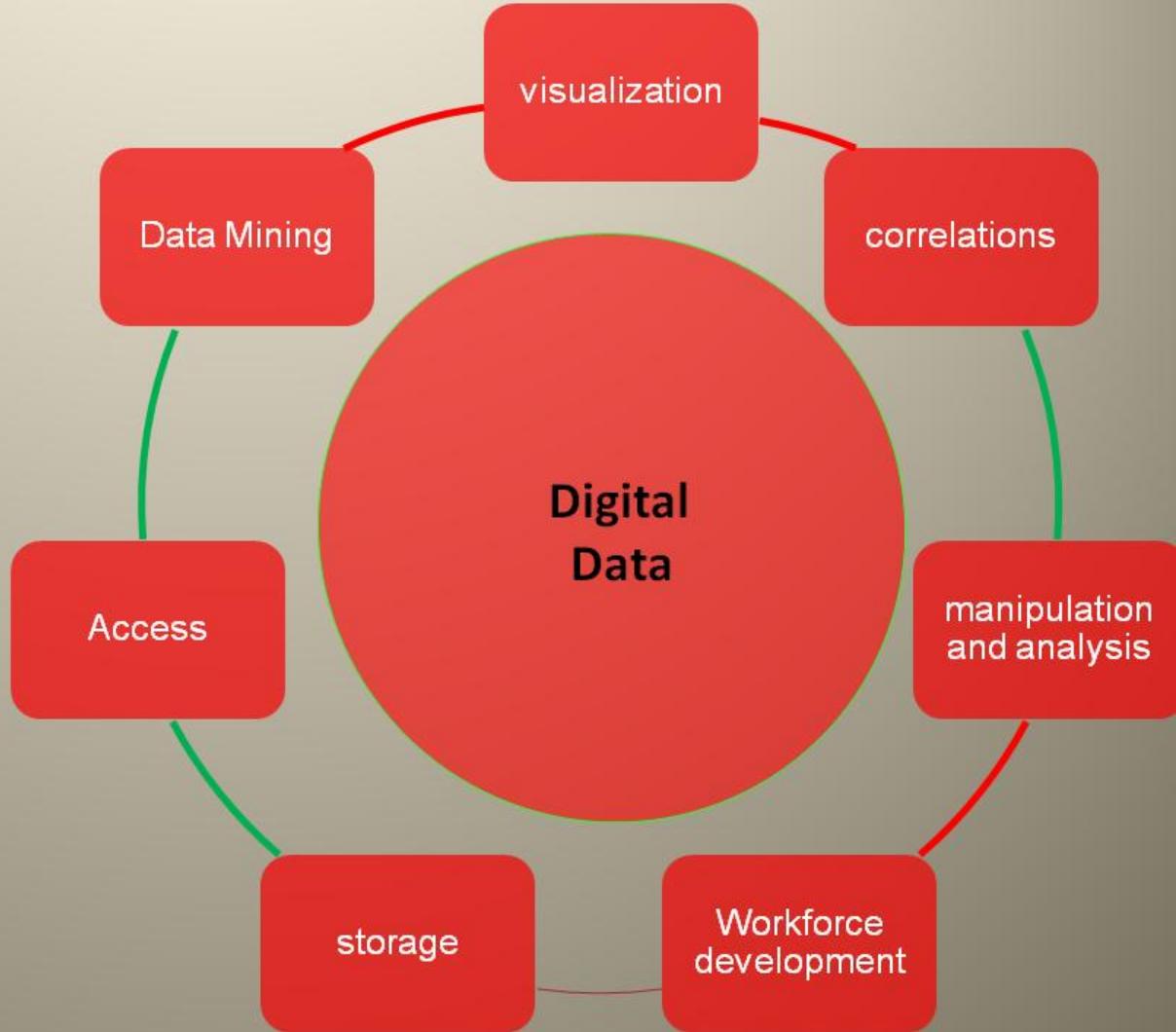
## *What will be in your ‘toolbox’?*



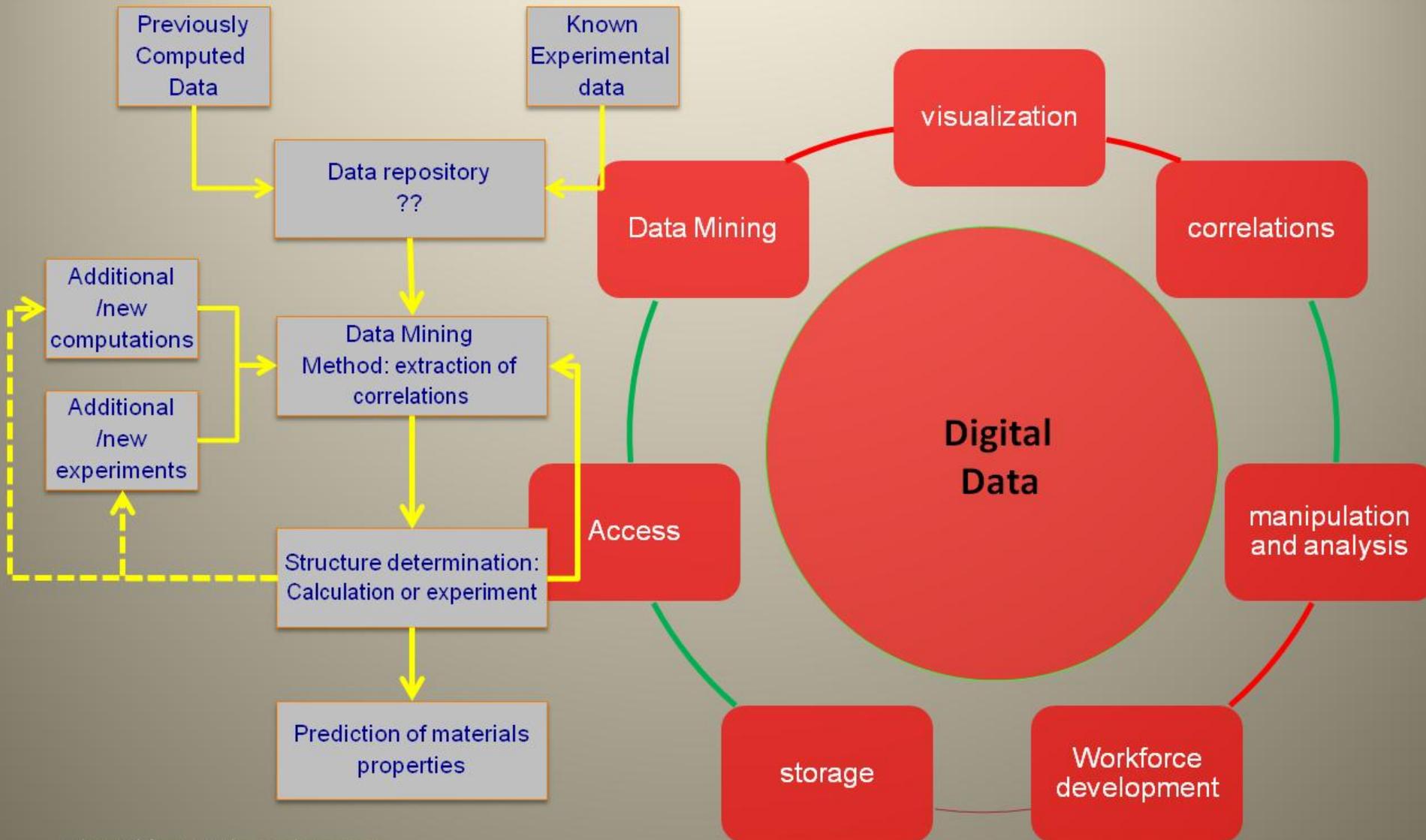
# Data for accelerated discovery of new materials and phenomena – new paradigms?

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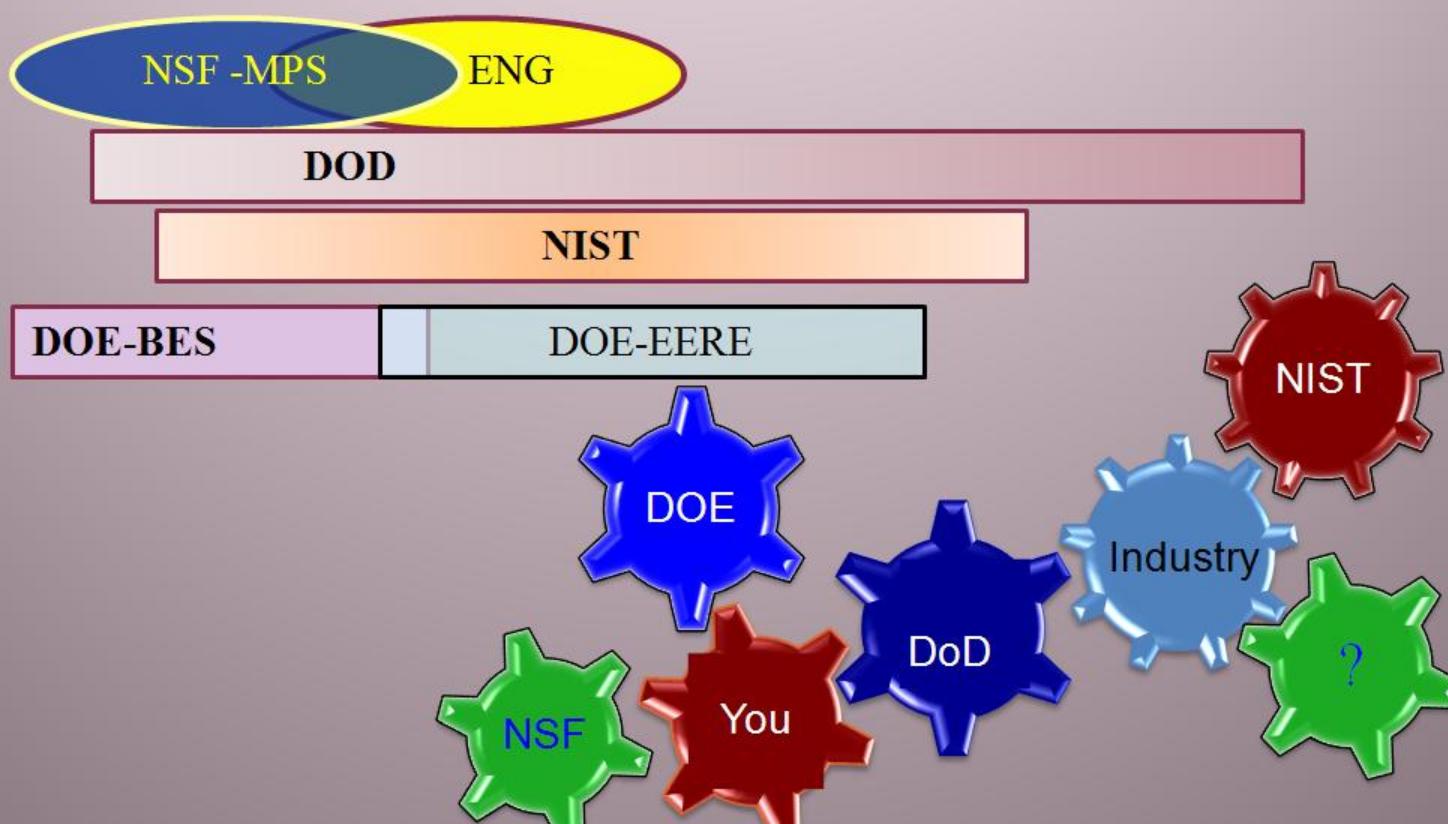
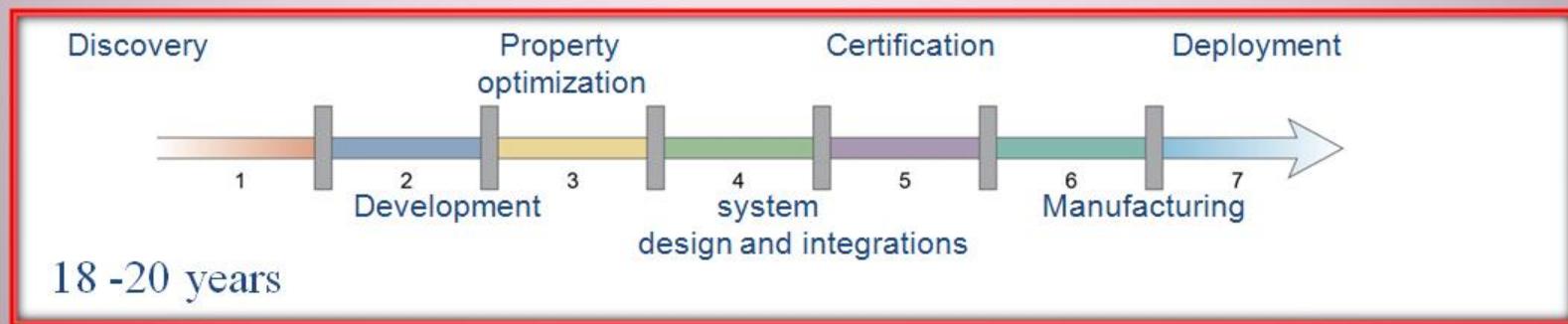
# Data for accelerated discovery of new materials and phenomena – new paradigms?



# Data for accelerated discovery of new materials and phenomena – new paradigms?



# A multi-agency partnership



# National Science Foundation

## Dear Colleague Letter – Submission Window: January 15 - February 15



The screenshot shows a Microsoft Internet Explorer window with the following details:

- Title Bar:** US NSF - Dear Colleague Letter: Designing Materials to Revolutionize and Engineer our Future (D - Microsoft Internet Explorer p)
- Address Bar:** http://www.nsf.gov/pubs/2011/nsf11089/nsf11089.jsp
- Toolbar:** File, Edit, View, Favorites, Tools, Help, Convert, Select, Live Search.
- Favorites Bar:** Department of Energy - Pho..., SC Homepage U.S. DOE Office..., U.S. Office of Personnel Ma..., 7-Day Forecast for Latitude..., Google.
- Page Title:** US NSF - Dear Colleague Letter: Designing Materials t...
- Header:** NSF Web Site, Search bar.
- Navigation:** Home, Funding, Awards, Discoveries, News, Publications, Statistics, About, FastLane.
- Section:** NSF 11-089, **Dear Colleague Letter: Designing Materials to Revolutionize and Engineer our Future (DMREF)**
- Text:** The National Science Foundation (NSF) through the Mathematical and Physical Sciences (MPS) and Engineering (ENG) Directorates, is excited to bring to your attention a new national materials initiative entitled *Materials Genome Initiative for Global Competitiveness*.<sup>1</sup> The Materials Genome Initiative (MGI) recognizes the importance of materials science to the well-being and advancement of society and aims to "deploy advanced materials at least twice as fast as possible today, at a fraction of the cost." The national initiative integrates all components in the materials continuum, including materials discovery, development, property optimization, systems design and optimization, certification, manufacturing and deployment, with each employing the toolset developed within the materials innovation infrastructure. The toolset integrates synergistically advanced computational methods with data-enabled scientific discovery and innovative experimental techniques in such a manner as to revolutionize our approach to materials research and engineering.
- Text:** NSF will support this initiative through well-coordinated activities spearheaded jointly by the Divisions of Materials Research (DMR) in MPS and Civil, Mechanical, Manufacturing Innovation (CMMI) and Chemical, Bioengineering, Environmental and Transport Systems (CBET) in ENG. Of interest to NSF are activities that accelerate materials discovery and development by building the fundamental knowledge base needed to progress towards designing and making a material with a specific and desired function or property from first principles. Also of interest to NSF are proposals that seek to advance fundamental materials understanding across length and time scales to elucidate the effects of microstructure, surfaces, and coatings on the properties and performance of engineering materials. The ultimate goal is to enable control of material properties through design via the establishment of the interrelationships between constitution, processing, structure, properties, performance and process control. It is anticipated that many proposed efforts will bridge program and divisional interests and that these will be coordinated, co-reviewed and funded by the programs and divisions as appropriate. The proposed research must be a collaborative and iterative process where computation guides experiments and theory, while experiments and theory advance computation. Designs should include consideration of recyclability and sustainability of materials. While not required, ties with industry, national laboratories, engineering partners or other organizations are encouraged. If there are strong collaborations with industry, please see the Grant Opportunities for Academic Liaison with Industry (GOALI) program solicitation, which can be used in conjunction with this effort.<sup>2</sup> Future funding opportunities within the Software Infrastructure for Sustained Innovation solicitation also may be of interest.<sup>3</sup> Because this MGI approach emphasizes a more integrated approach to materials research, cross-disciplinary educational activities are encouraged.
- Bottom:** Done, Internet, Microsoft Internet Explorer, 100%, Taskbar: Start, Microsoft Outlook, Microsoft PowerPoint, US NSF - Dear Colleague Letter: Designing Materials to Revolutionize and Engineer our Future (DMREF).



# National Science Foundation

## Dear Colleague Letter – Submission Window:

### January 15 - February 15

**FRG Interaction of synergistic Experiment! and**

US NSF - Dear Colleague Letter: Designing Materials to Revolutionize and Engineer our Future (D) - Microsoft Internet Explorer

File Edit View Favorites Tools Help

NSF Web Site

NSF 11-089  
**Dear Colleague Letter: Designing Materials to Revolutionize and Engineer our Future (D) (REF)**

The National Science Foundation (NSF) through the Mathematical and Physical Sciences (MPS) and Engineering (ENG) Directorates, is excited to bring to your attention a new national materials initiative, the *Materials Genome Initiative for Global Competitiveness*.<sup>1</sup> The Materials Genome Initiative (MGI) recognizes the importance of materials science to the well-being and advancement of society and aims to "deploy advanced materials at least three times faster than possible today, at a fraction of the cost." The national initiative integrates all components in the materials continuum, including materials discovery, development, property optimization, systems design and optimization, certification, manufacturing and deployment, with each employing the toolset developed within the materials innovation infrastructure. The toolset integrates synergistically advanced computational methods with data-enabled scientific discovery and innovative experimental techniques in such a manner as to revolutionize our approach to materials research and engineering.

NSF will support this initiative through well-coordinated activities spearheaded jointly by the Divisions of Materials Research (DMR) in MPS and Civil, Mechanical, Manufacturing Innovation (CMMI) and Chemical, Bioengineering, Environmental and Transport Systems (CBET) in ENG. Of interest to NSF are activities that accelerate materials discovery and development by building the fundamental knowledge base needed to progress towards designing and making a material with a specific and desired function or property from first principles. Also of interest to NSF are proposals that seek to advance fundamental materials understanding across length and time scales to elucidate the effects of microstructure, surfaces, and coatings on the properties and performance of engineering materials. The ultimate goal is to enable control of material properties through design via the establishment of the interrelationships between constitution, processing, structure, properties, performance and process control. It is anticipated that many proposed efforts will bridge program and divisional interests and that these will be coordinated, co-reviewed and funded by the programs and divisions as appropriate. The proposed research must be a collaborative and iterative process where computation guides experiments and theory, while experiments and theory advance computation. Designs should include consideration of recyclability and sustainability of materials. While not required, ties with industry, national laboratories, engineering partners or other organizations are encouraged. If there are strong collaborations with industry, please see the Grant Opportunities for Academic Liaison with Industry (GOALI) program solicitation, which can be used in conjunction with this effort.<sup>2</sup> Future funding opportunities within the Software Infrastructure for Sustained Innovation solicitation also may be of interest.<sup>3</sup> Because this MGI approach emphasizes a more integrated approach to materials research, cross-disciplinary educational activities are

Done

Start Inbox - Microsoft Outlook Q:\BES\_Briefings\MSR M... Microsoft PowerPoint - [...] US NSF - Dear Colleague Letter: Designing Materials to Revolutionize and Engineer our Future (D) (REF)

# Some Questions for Discussion

## *What will the MGI ‘materials discovery’ environment/infrastructure look like?*

- What are the scientific opportunities?
  - How do we find the next: TI? HTSC? *Surprise!?*
  - What are the conceptual gaps?
- How do we bridge the gaps in the discovery process?
  - *Concept → Cyber-realization → ‘I can hold it my hand!’*
- How can we build on what we know / have done?
  - *The role of data: What do we need? How do we access it? ...*
- What ‘tools’ are needed?
  - **Formal & computational methods, data repositories, materials discovery collaboration networks, ...**
- How do we give this to the next generation? *Progress ...*

# Some Questions for Discussion

*What will the MGI ‘materials discovery’ environment/infrastructure look like?*

- How will we use it?
- What will we do?
- What will we discover?
- ...

*It is up to You!*

