

The Materials Genome Initiative and Materials Innovation Infrastructure

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Outline

- Materials Genome Initiative
- Materials Innovation Infrastructure
- MGI Culture
- Data and Software Infrastructure Needs











THE 21-LAYER SPACE SUIT



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- 2 VINYL TUBING
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- 4 NOMEX
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Nature designed man to inhabit the earth, but he will be brave to leave his home to explore other environments, such as the moon. The lunar environment is a hostile one, and in order to survive there, man requires special protective clothing. Science and technology have worked together to develop a suit (space technology) as the Lunar Extravehicular Mobility Unit which enables man to walk about the moon. This poster explains the complex layers of material from which the space suit is made.

At Du Pont, the world's largest chemical corporation, developed materials used in 20 of the 21 layers in the space suit, although it did not make the suit itself. (D.C. Industries makes the suits.) But some of these materials were developed with the moon in mind. Some were new materials, like "Kapton" film. Others, such as nylon, were discovered more than thirty years ago by scientists who had no idea of the distance the results of their research would travel some day. But achievements in science are often put to use in unexpected places. In the case of the space suit, materials which Du Pont had developed for use on earth ultimately found a place on the moon. We can expect to see them used, too, in man's strikes out for outer space and farther planets.

DuPont materials in Apollo moon suits were originally developed for earthbound use . . .

NYLON

LAYER 1

Soft fibers, there were only natural fibers—cotton, wool, and man-made fibers extracted from wood pulp. But nylon, announced in 1935, was an original accomplishment—of fiber made by man, not merely from chemicals. It combines two very desirable properties—strength and durability—even when made into the chemical of stockings. It is used in the first layer of the space suit, next to the astronaut, in a lightweight "sweater knit."



VINYL TUBING

LAYER 2

This layer of the space suit is designed to help keep the astronaut cool. Water is circulated through a network of slender vinyl tubes, much as blood is pumped through your body's veins and capillaries. Slender kinds of vinyl tubing are used in laboratories to transfer fluids from one container to another.



LYCRA

LAYER 3

"LYCRA" SPANDEX FIBER

"Lyra," invented by Du Pont, is a man-made fiber that has all the elastic qualities of natural rubber. It is stronger than natural elastic thread, but weighs one-third less and wears much longer. "Lyra's" flexibility and strength make it a good choice for a material to hold the cooling tubes close to the astronaut's body. The suit had to meet often in woman's work suits and undergarments.



NOMEX

LAYER 4

"NOMEX" NYLON FIBERS

The Du Pont scientists learned to make many types of nylon. "Nomex" is a high temperature resistant nylon. It cannot be melted or ignited even by burning gasoline. Its most useful use is for making a suit for the fire staff and will not wear out or melt out. "Nomex" nylon is also used in making driver's seats. In clothing for people who may not be able to protect themselves in case of fire (such as children and mental patients), and in aircraft seating (seat covers).



NYLON COIL

LAYER 5

Chased off from the vacuum of space by their protective suits, the astronauts must breathe. A network of ducts carries oxygen to the astronaut from his back pack. These ducts are kept open and clear by spring-like coils made of a "Dyne" nylon resin. The type of nylon used is used in gunnery aiming devices at 5000 ft. altitudes, to assure unobstructed flow of hot from pump to gun tank.



NEOPRENE-COATED NYLON

LAYERS 6, 8

Neoprene is a very special kind of synthetic rubber. It is not affected by heat, cold, oils, grease, vapors, or acids—and is liquid car soap or tank through it. In the space suit, it is used as a barrier layer to help keep oxygen lines for a minimum. The more common use of this fabric on earth is for tarpaulins that protect livestock and boat hulls, and for large inflatable shelters.



NYLON

LAYER 7

As we have indicated, nylon can be produced in a variety of forms. In Layer 7, because weight for weight it is stronger than steel wire, it is used as a resistant layer. In fact, the most famous example of it is steel. The same kind of nylon is used for seat belts in cars and airplanes.



MYLAR

LAYERS 9, 11, 12, 13, 14, 17
"MYLAR" POLYESTER FILM

Dr. Peter S. Plesch, producing super-strong "Mylar" in 1938, is taken a honor of 75,000 lbs. per square inch to just about a sheet of "Mylar" only one one-hundredth of an inch thick. It is used as the base material in membranes for packaging such things as poultry and frozen "back-to-the-land" foods, and as electric motor insulation. In the space suit, the layers of aluminum-coated "Mylar" help to block off radiant heat from the sun, and help body heat to be perfect against the suit of space.



DACRON

LAYERS 10, 12, 14, 16
"DACRON" POLYESTER FIBER

"Dacron" is a man-made fiber used extensively in apparel and home furnishings. Some of you might be wearing garments made of "Dacron" right now. In the space suit, four layers of strong wet "Dacron" "Dacron" polyester are alternated with five layers of "Mylar" as a kind of "sandwich" to protect the astronaut against heat and cold.



KAPTON

LAYER 18, 19

"KAPTON" POLYIMIDE FILM

Dr. Paul announced "Kapton" in 1954. Two aluminum layers protect the astronaut from extremely high temperatures, 1200° F. in many places to more than 2500° F. in some spots. "Kapton" was chosen because it will not char, melt, or burn at high temperatures, even when as thin as one one-thousandth of an inch. It was also used in the moon landing space ship to insulate 14 miles of wire on earth. "Kapton" is used to insulate wires for high speed trains and wiring for aircraft.



TEFLON-COATED GLASS FIBER

LAYER 20

"TEFLON" TFE-FLUOROCARBON FIBER

"Teflon" TFE-fluorocarbon resin, used for aircraft components, was a scientific breakthrough, discovered by Du Pont scientists while at work on other research. In the combined space ship, 15 miles of wiring are covered with "Teflon" resin. For the space suit, glass fibers are coated with "Teflon." This resin also fills a fabric. This layer was designed to provide the protection and to guard against high speed dust particles.



TEFLON

LAYER 21

"TEFLON" TFE-FLUOROCARBON FIBER

Now the "Teflon" TFE-fluorocarbon resin is made into fibers and woven into a fabric of "Teflon." On earth, because it is almost totally friction-free, you'll find this fabric used in precision bearings. In the moon, it is used as the astronaut's outer cover for the parts of the astronaut's suit, such as the gloves, boots, and shoelaces, to provide an abrasion-resistant surface. About 50% of the space suit is covered with this special fabric.



The Age of Computational Materials Design



• Stone Age

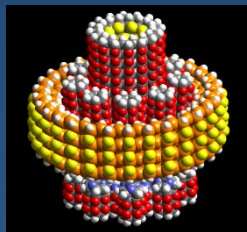
• Bronze Age



• Plastic Age



• Computational
Materials by
Design Age



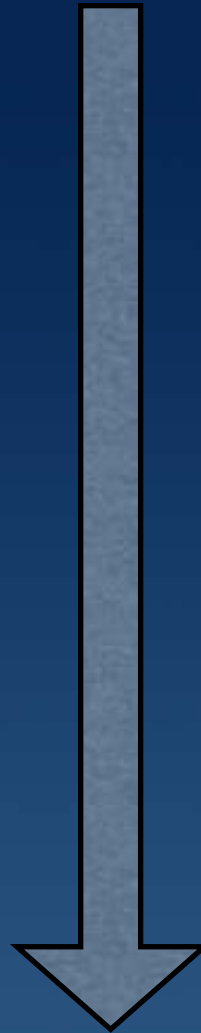
• Iron Age



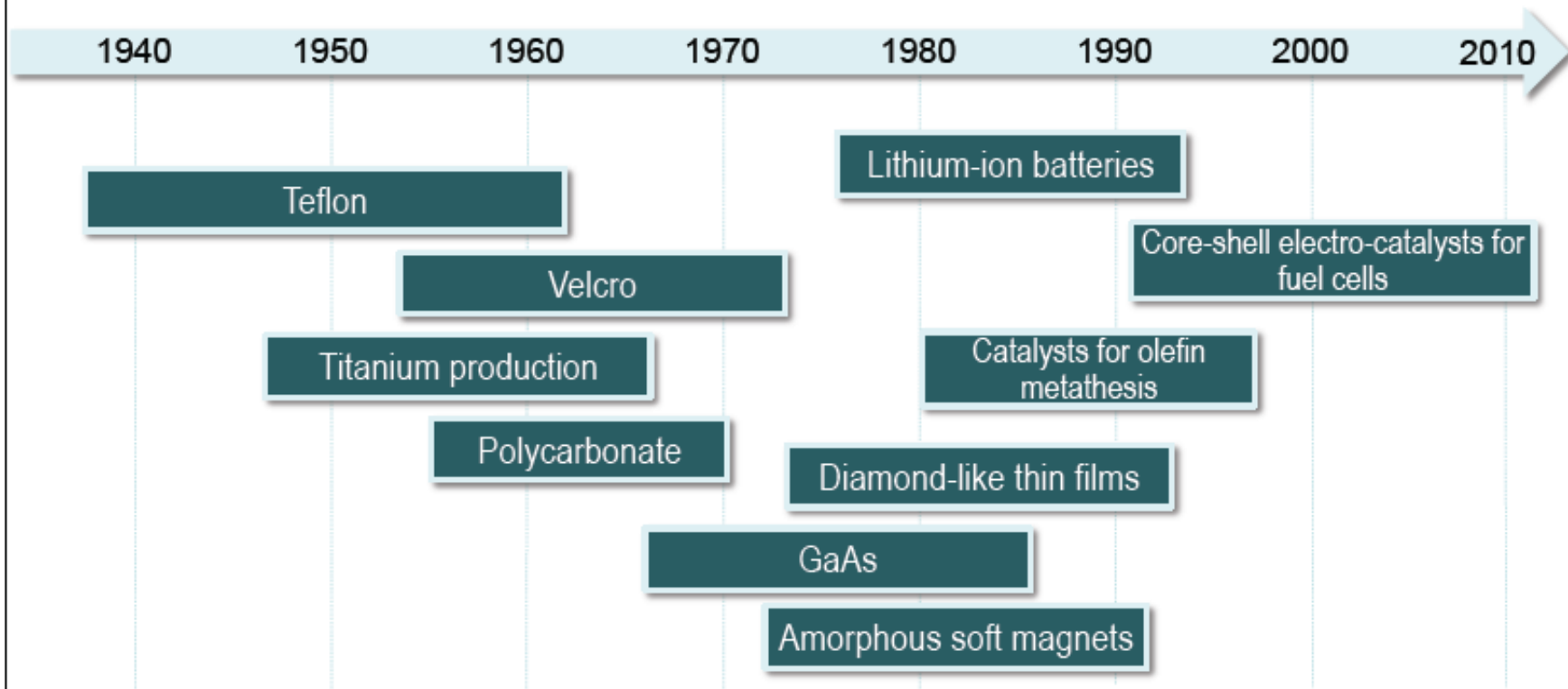
• Industrial
Age



• Silicon Age

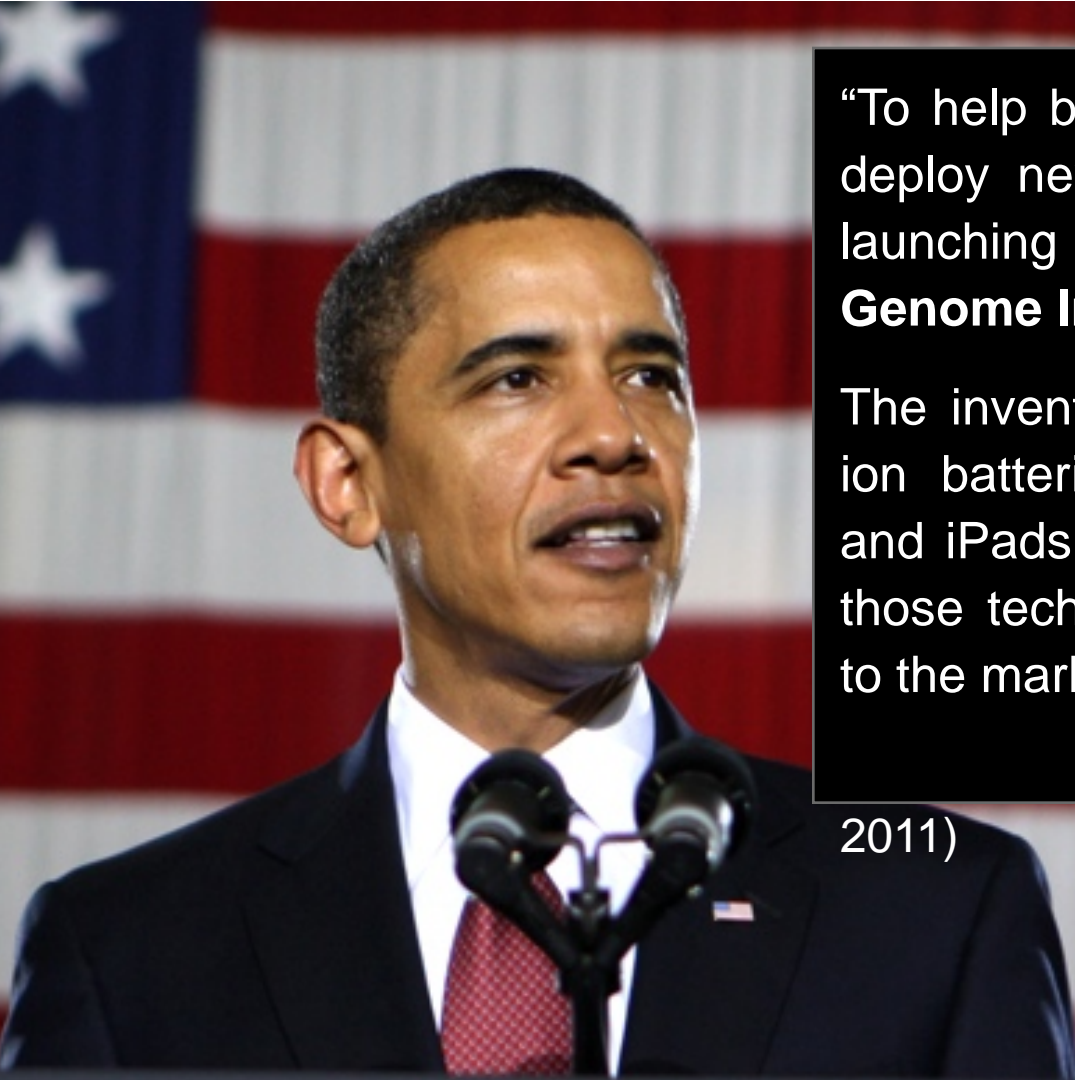


20+ Years to Market



After Gerd Ceder (MIT); materials information from T. W. Eagar and M. King, *Technology Review* 98 (2), 42 (1995).
Catalysis information from R. Schrock et al. and R. Adzic et al.





“To help businesses discover, develop, and deploy new materials twice as fast, we’re launching what we call **the Materials Genome Initiative**.

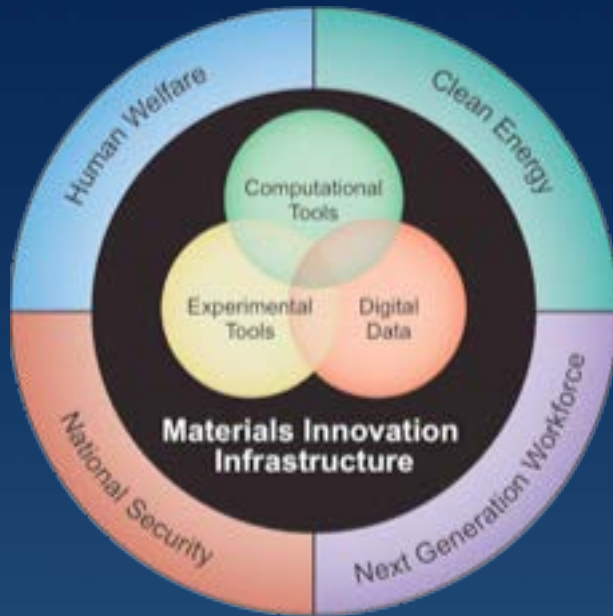
The invention of silicon circuits and lithium ion batteries made computers and iPods and iPads possible, but it took years to get those technologies from the drawing board to the market place. **We can do it faster.**”

-President Obama (June

2011)



MGI - Two Core Objectives



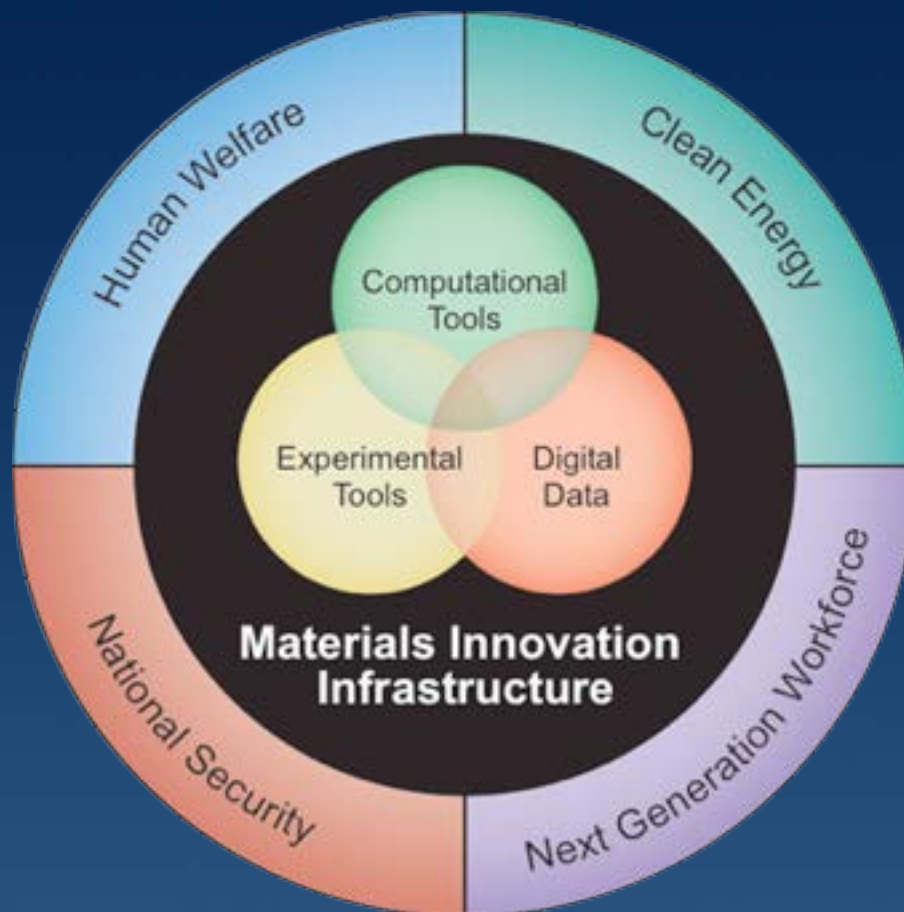
1. INFRASTRUCTURE

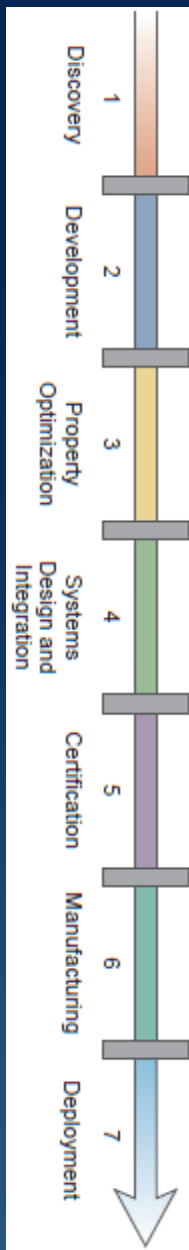


2. CULTURE



Materials Innovation Infrastructure





1

Discovery

2

Development

3

Property Optimization

4

Systems Design/ Integration

5

Certification

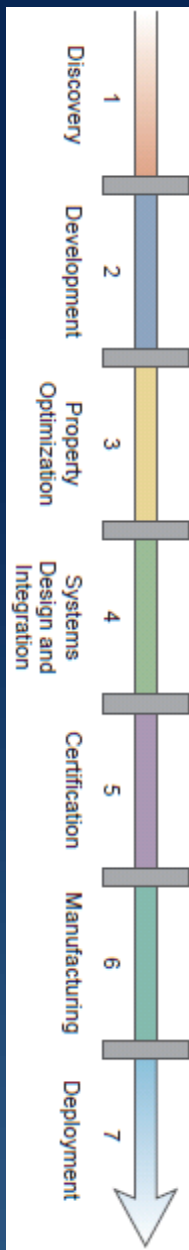
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Manufacturing

7

Deployment





1

Discovery

2

Development

3

Property Optimization

4

Systems Design/ Integration

5

Certification

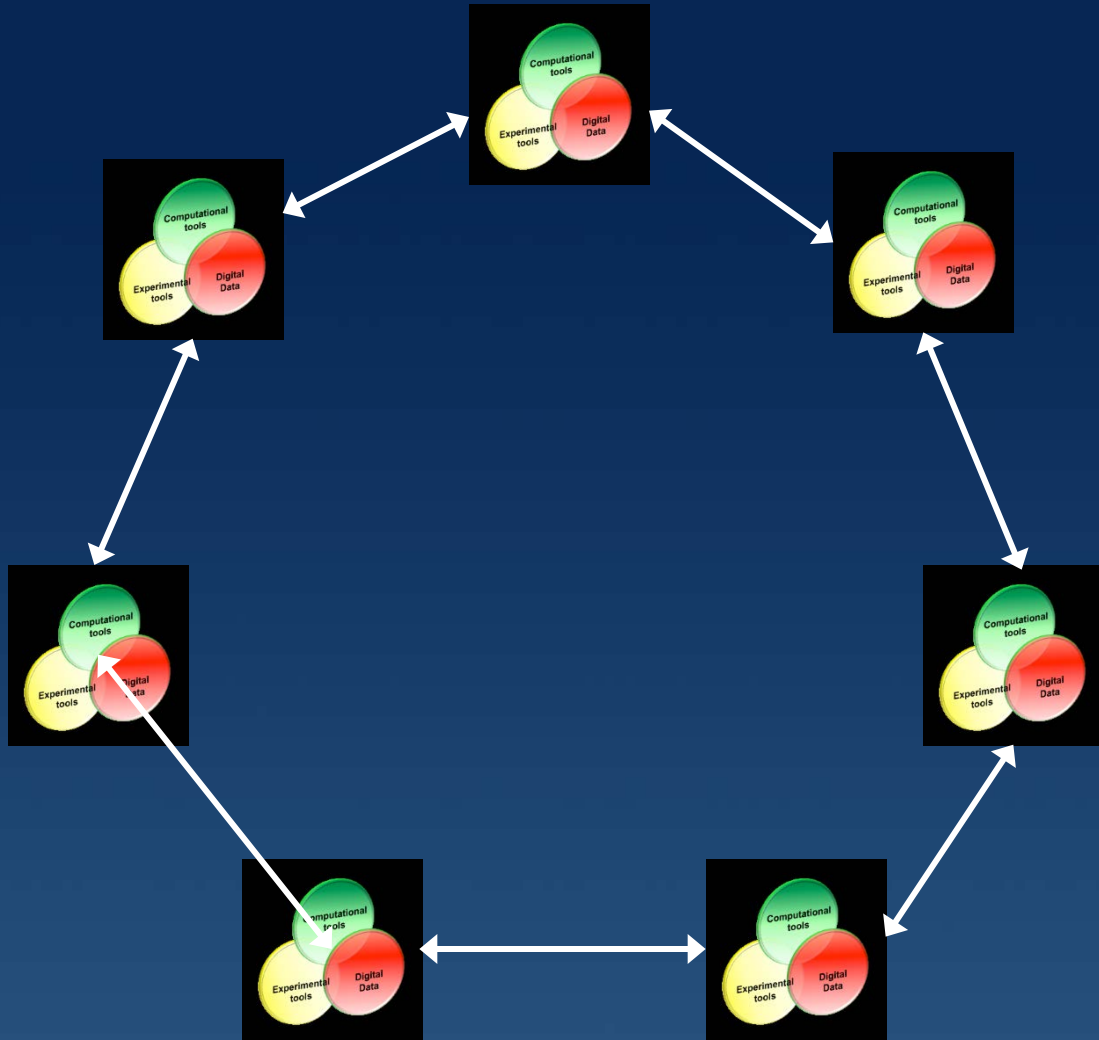
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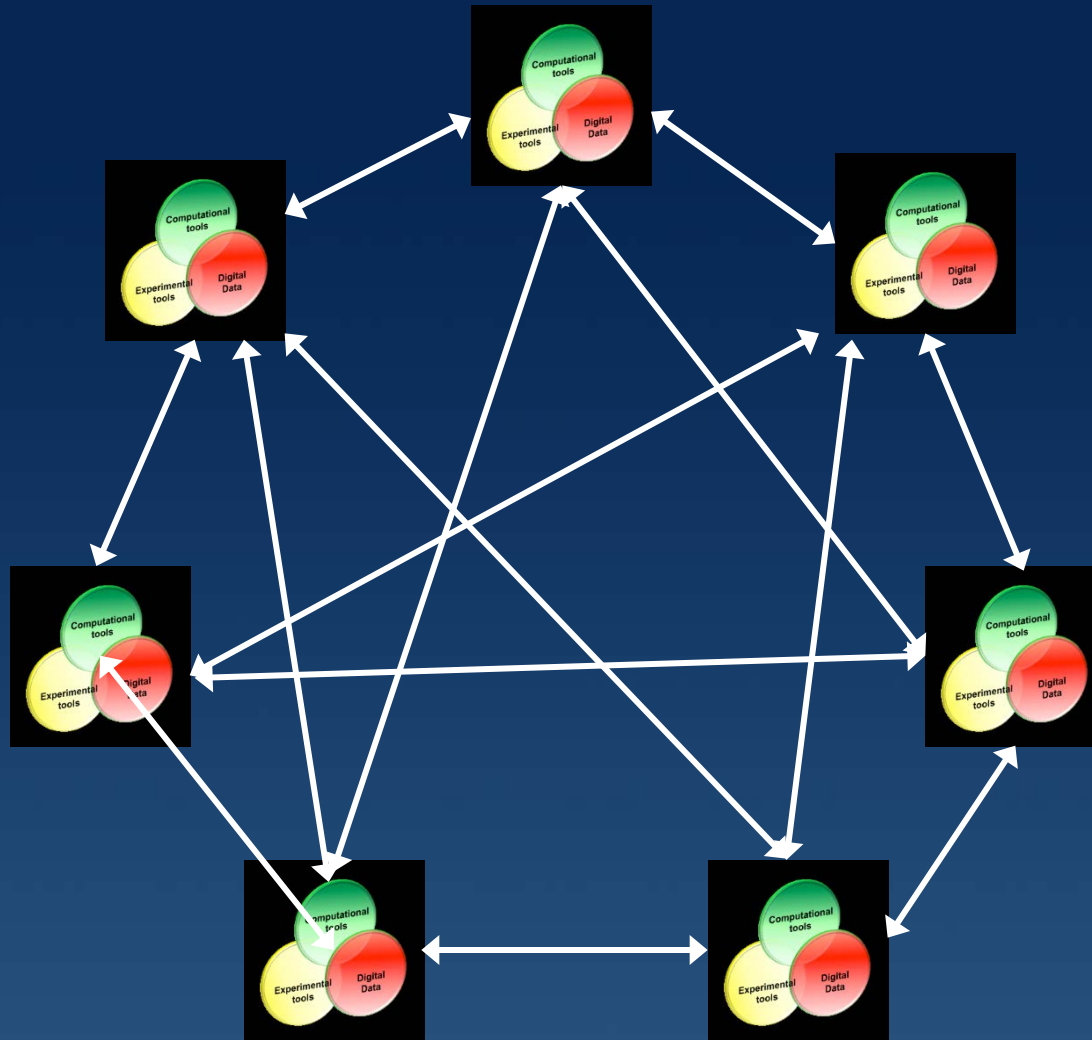
Manufacturing

7

Deployment







MGI Culture

- Enable a paradigm shift in the materials R&D community
 - Emphasize collaboration, including experiment and computation
 - Engage not only the basic research community, but later stages in the development continuum including product design and manufacturing
 - Make this MGI workstyle the community standard through specialized undergraduate and graduate curricula



Highlights of Activities

- \$63M in FY 2012 (DOE, NSF, DOD, NIST)
- Leveraging existing investments and building a strong tie-in to other Federal programs (National Nanotechnology Initiative, National Network for Manufacturing Innovation, open data)
- Over 60 institutions have pledged financial resources totaling a few hundred million dollars
- Commitments from more than 30 universities (curricula, degree programs, etc.)
- Chartered a formal NSTC Subcommittee for active interagency coordination
- Multiple stakeholder meetings on MGI (NSF, DOD, NIST, DOE, scientific societies)



June 24, 2013 – 2 Year Anniversary

- NIST announced \$25 million for new Center of Excellence
- Start of a Materials Innovation Accelerator Network
- Harvard/IBM Debut Database of 2.3 million new materials
- ASM/NIST partnership on open data repository pilot
- DARPA, US Army, NASA Partner on Data Repository
- Lawrence Berkeley National Laboratory/Intermolecular form Public-Private Collaboration
- 8 universities announce efforts to improve MGI education
- 5 universities commit to host regional meetings
- Strategic Plan & Community Input



Materials Innovation Infrastructure

- ***Vision*** - to enable researchers to easily incorporate their own data into models as well as incorporate each other's data
- MGI wants to create a data-sharing system to:
- Use a broader set of data to render more accurate models
- Facilitate multi-disciplinary communication between scientists and engineers working on different stages of the materials development continuum
- Enable searches for advanced materials with specific, desired properties
- Curate and share reliable computational code for modeling and simulation

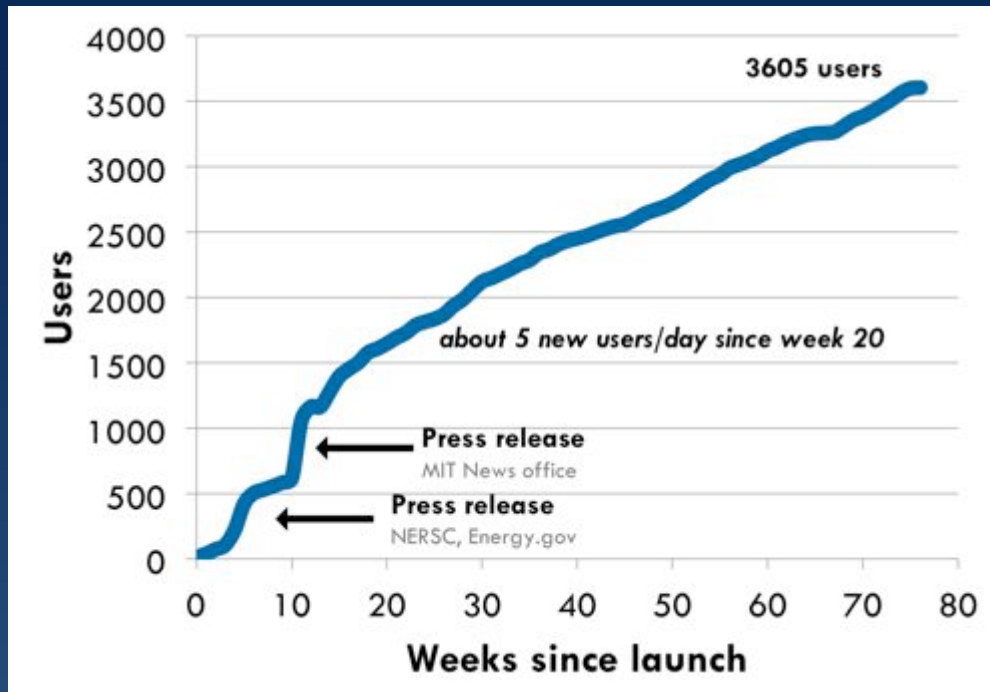


Goals for MGI Innovation Infrastructure

- Develop and deploy materials data and software repositories



Example: The Materials Project



- Launched Oct 2011
- initially included 15,000 compounds

Today's Status:

- > 33,000 compounds
- New data every month
- Multiple materials tools
- Crowd-sourcing
- API for data access

Figure by G. Ceder



Goals for MGI Innovation Infrastructure

- Develop and deploy materials data and software repositories
- Establish tools and practices for widespread use of repositories



Goals for MGI Innovation Infrastructure

- Develop and deploy materials data and software repositories
- Establish tools and practices for widespread use of repositories
 - Data and software standards
 - Minimum necessary metadata
 - Metrics of data quality
 - Protected Intellectual Property and non-public data



Goals for MGI Innovation Infrastructure

- Develop and deploy materials data and software repositories
- Establish tools and practices for widespread use of repositories
- Develop and adopt actions to support data attribution and citation



Key Questions

- An open collaboration platform is vital to the success of MGI – how should we approach this?
- What can we learn from HubZero?
- What considerations should MGI be thinking about to scale up from individual repositories or hubs to a national scale network?
- What unique considerations are there between computational code and data?



For more information:
www.whitehouse.gov/mgi

The screenshot shows a web browser window displaying the White House website for the Materials Genome Initiative. The browser's address bar shows the URL www.whitehouse.gov/mgi. The page header includes the White House logo and navigation links such as "BLOG", "PHOTOS & VIDEO", "BRIEFING ROOM", "ISSUES", "the ADMINISTRATION", "the WHITE HOUSE", and "our GOVERNMENT". The main content area features the title "Materials Genome Initiative" and a navigation menu with links for "About", "Goals", "Examples", "News & Announcements", "Federal Programs", "External Stakeholder Activities", and "Contact Us". A large text block on the left contains a quote from President Obama, and a photograph on the right shows President Obama in a factory setting.

the WHITE HOUSE PRESIDENT BARACK OBAMA

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BLOG PHOTOS & VIDEO BRIEFING ROOM ISSUES the ADMINISTRATION the WHITE HOUSE our GOVERNMENT

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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 marketplace. We can do it faster.

- President Obama, June 2011 at Carnegie Mellon University



About the Materials Genome Initiative

MATERIALS GENOME