The Materials Genome Initiative and Materials Innovation Infrastructure

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White House Office of Science and Technology Policy

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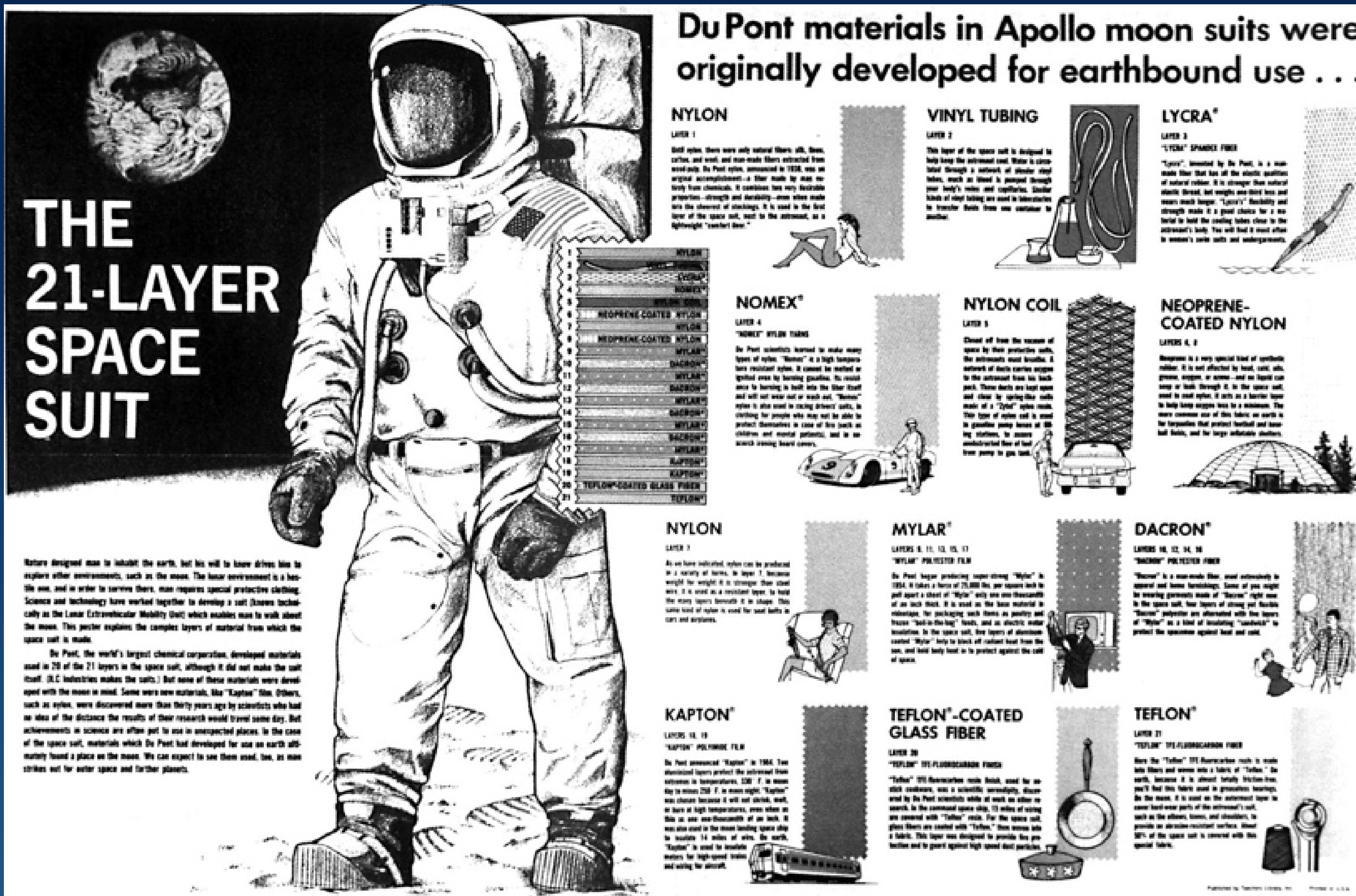
Outline

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


THE 21-LAYER SPACE SUIT
Du Pont materials in Apollo moon suits were originally developed for earthbound use . . .
NYLON
VINYL TUBING
LYCRA®
NOMEX®
NYLON COIL
NEOPRENE-COATED NYLON
NYLON
MYLAR®
DACRON®
KAPTON®
TEFLON®-COATED GLASS FIBER
TEFLON®

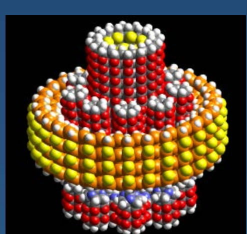
The Age of Computational Materials Design

•Stone Age

•Bronze Age

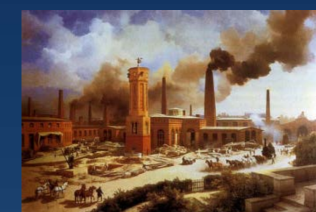
•Plastic Age

•Computational Materials by Design Age



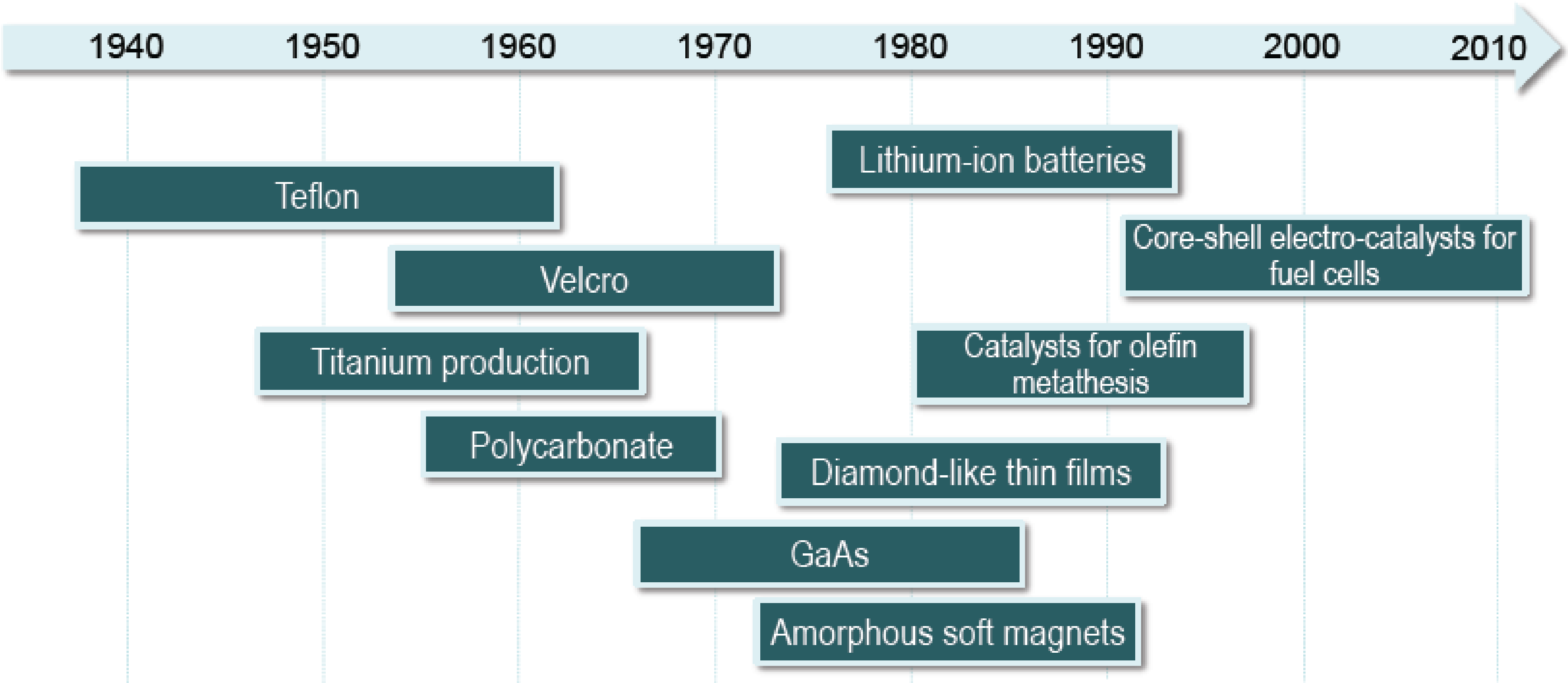
•Iron Age

•Industrial Age



•Silicon Age

20+ Years to Market



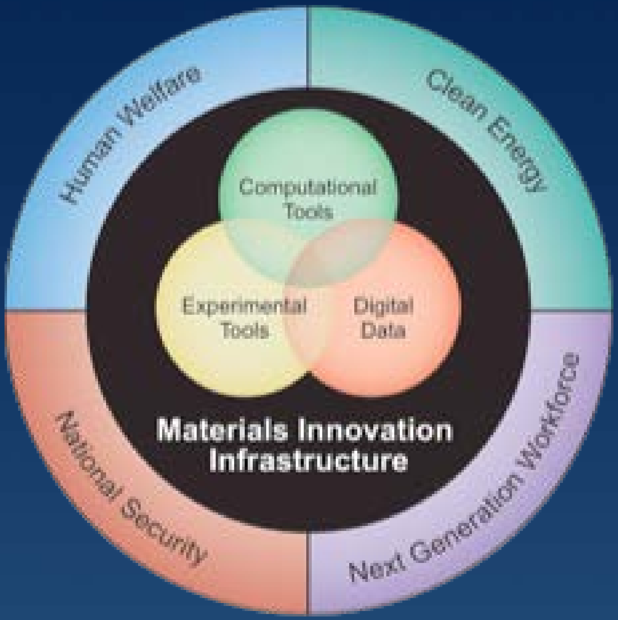
After Gerd Ceder (MIT); materials information from T. W. Eagar and M. King, Technology Review 98 (2), 42 (1995).
Catalysis information from R. Schrock et al. and R. Adzic et al.

"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)

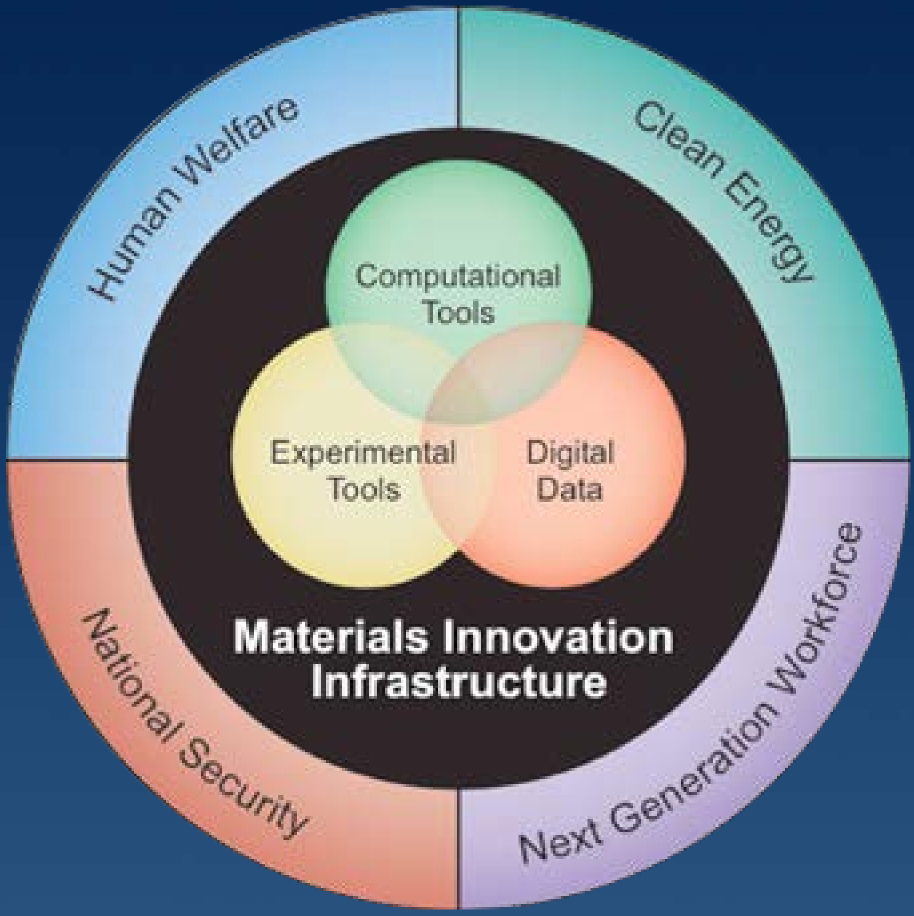
MGI - Two Core Objectives

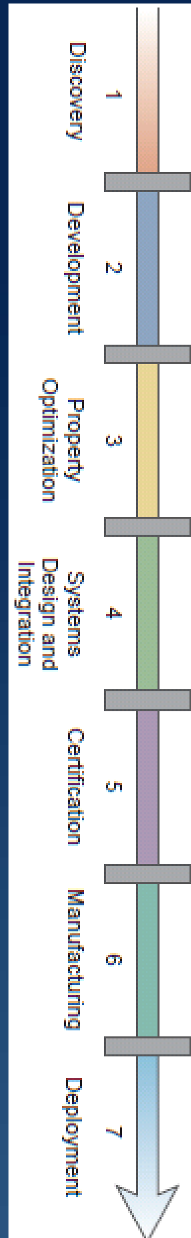


1. INFRASTRUCTURE

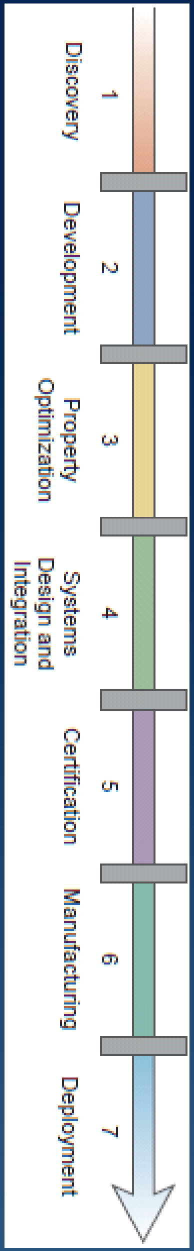
2. CULTURE

Materials Innovation Infrastructure





1. Discovery
2. Development
3. Property Optimization
4. Systems Design/ Integration
5. Certification
6. Manufacturing
7. Deployment



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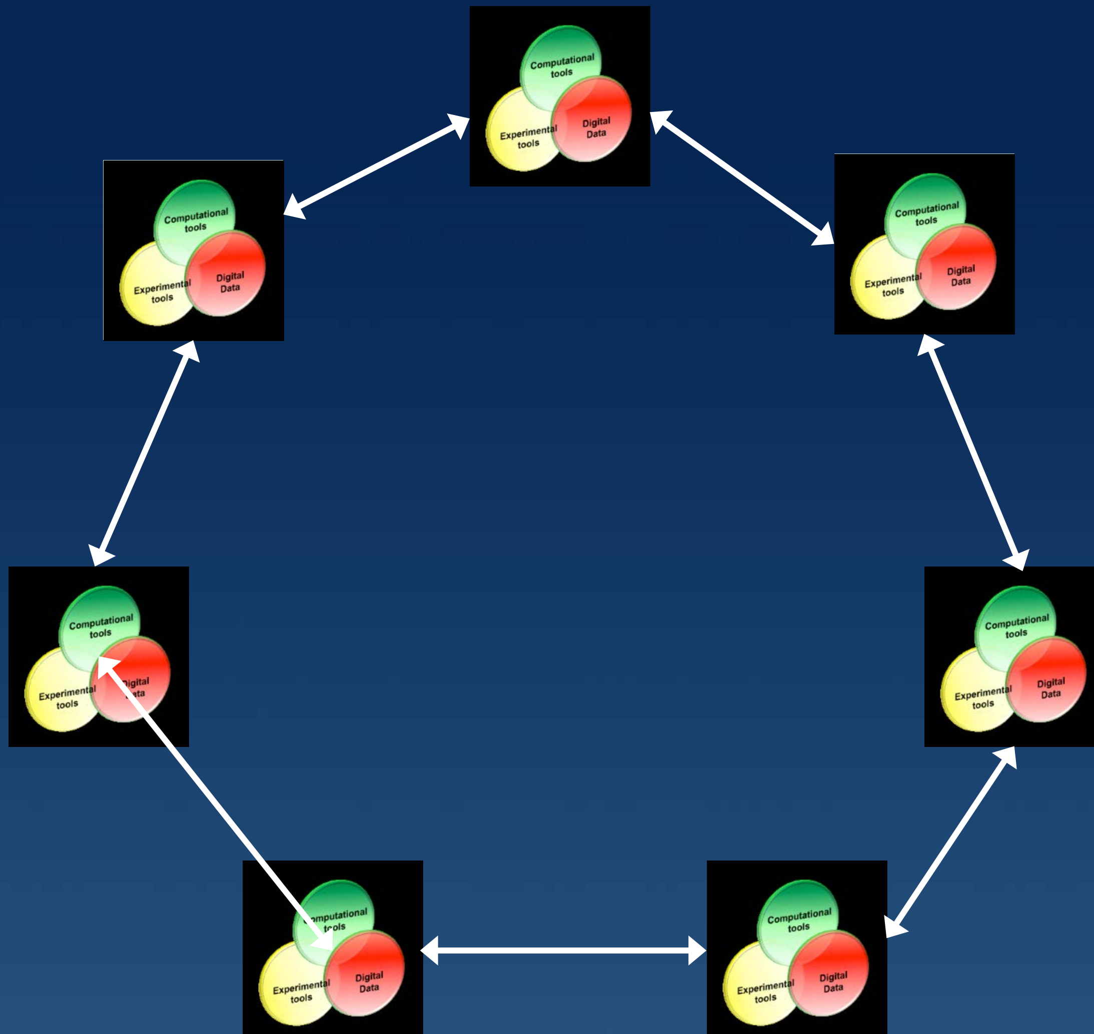
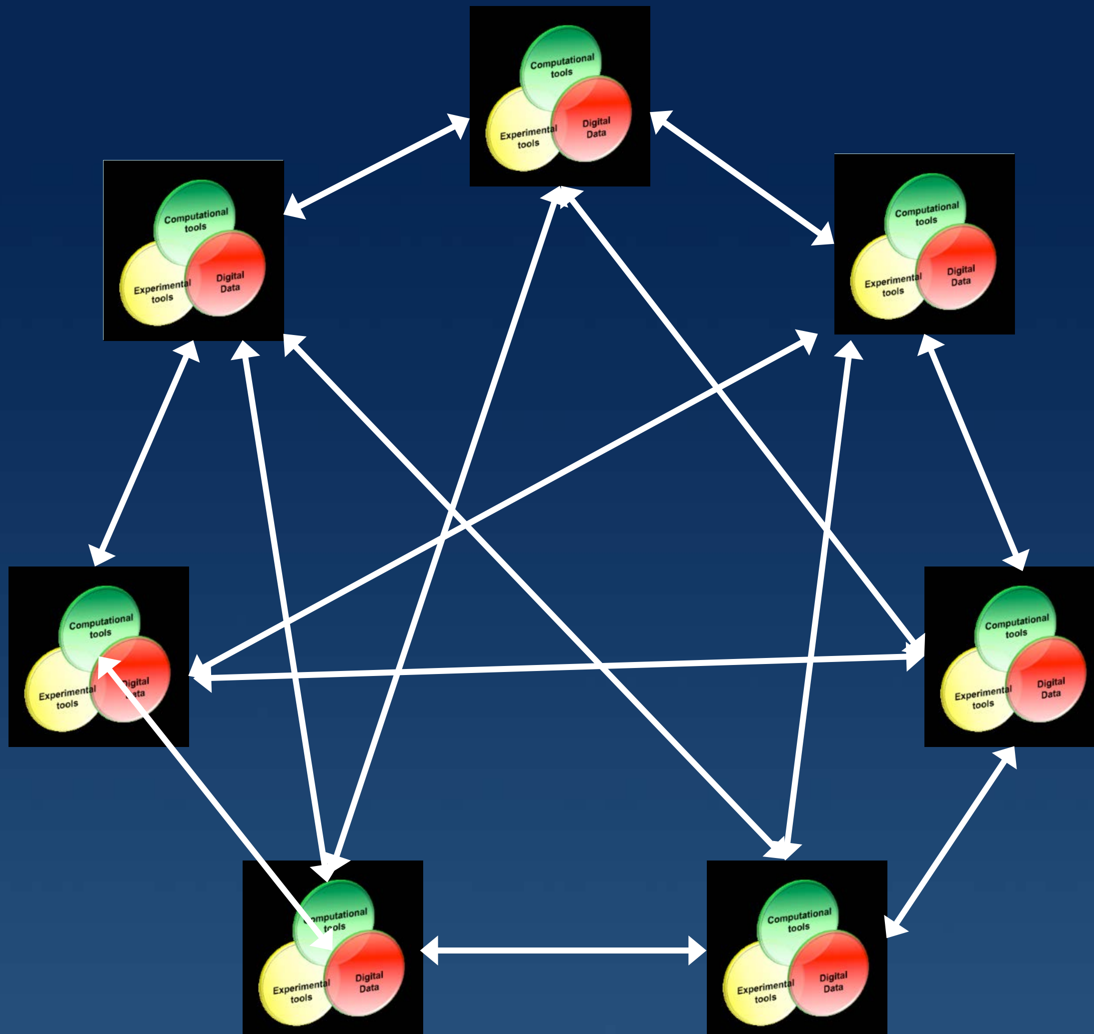

Computational tools
Experimental tools
Digital Data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MGI Culture

- 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 (curriculua, 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

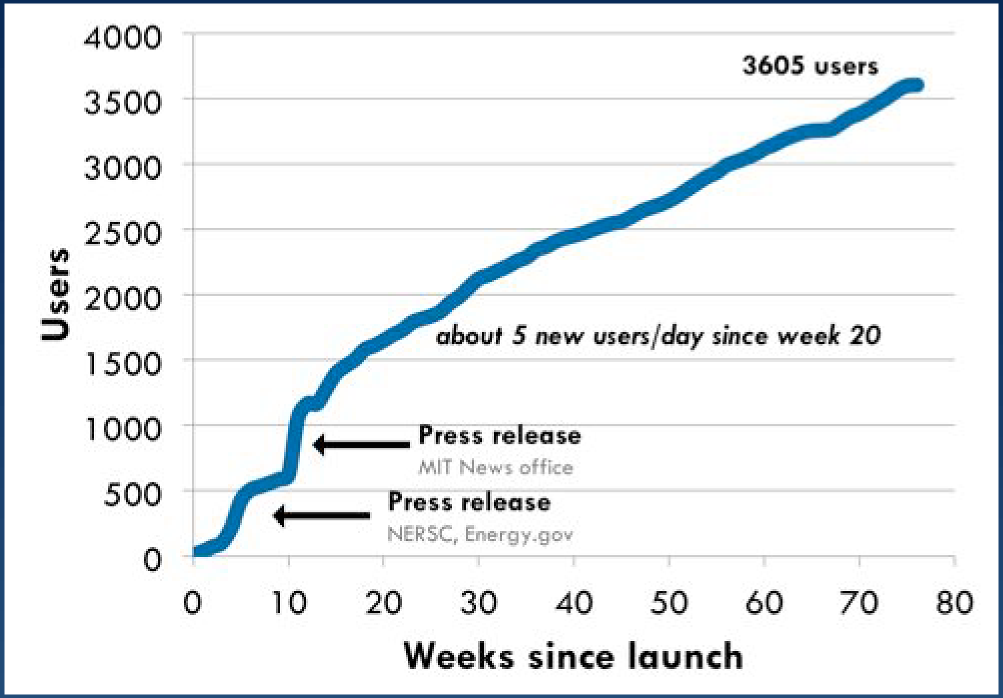

Figure by G. Ceder

- 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

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- 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