Summary of Findings: 2018 NIST Workshop on High-Throughput Experimental Materials Collaboratory (HTE-MC)

https://mgi.nist.gov/htemc

Martin L. Green, NIST

martin.green@nist.gov

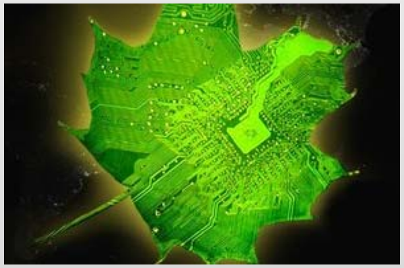
Materials are Technology Enablers

There would be no:

- Skyscrapers without **steel** girders
- Commercial aviation industry without **high-strength aluminum alloys and polymer composites**
- Information age without **silicon**
- Mobile phones without **functional ceramics**
- Solar electricity without **photovoltaic materials**
- Modern medicine without **biocompatible soft materials**

New Technologies Await Materials Solutions

Solar Fuels



- Platinum Group Metal (PGM) Free
- Higher efficiency

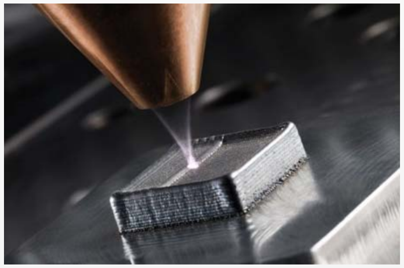
Gas/Steam Turbines

- “The hotter the engine, the better”
- New higher temp alloys

Corrosion Resistant Materials

- 3% of US GDP
- Broad applications
- Impact **health** and **safety**

Additive Manufacturing



- AM – Inconel 718 is not Inconel 718
- Difficult to process

The Materials Genome Initiative (MGI)

*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.*

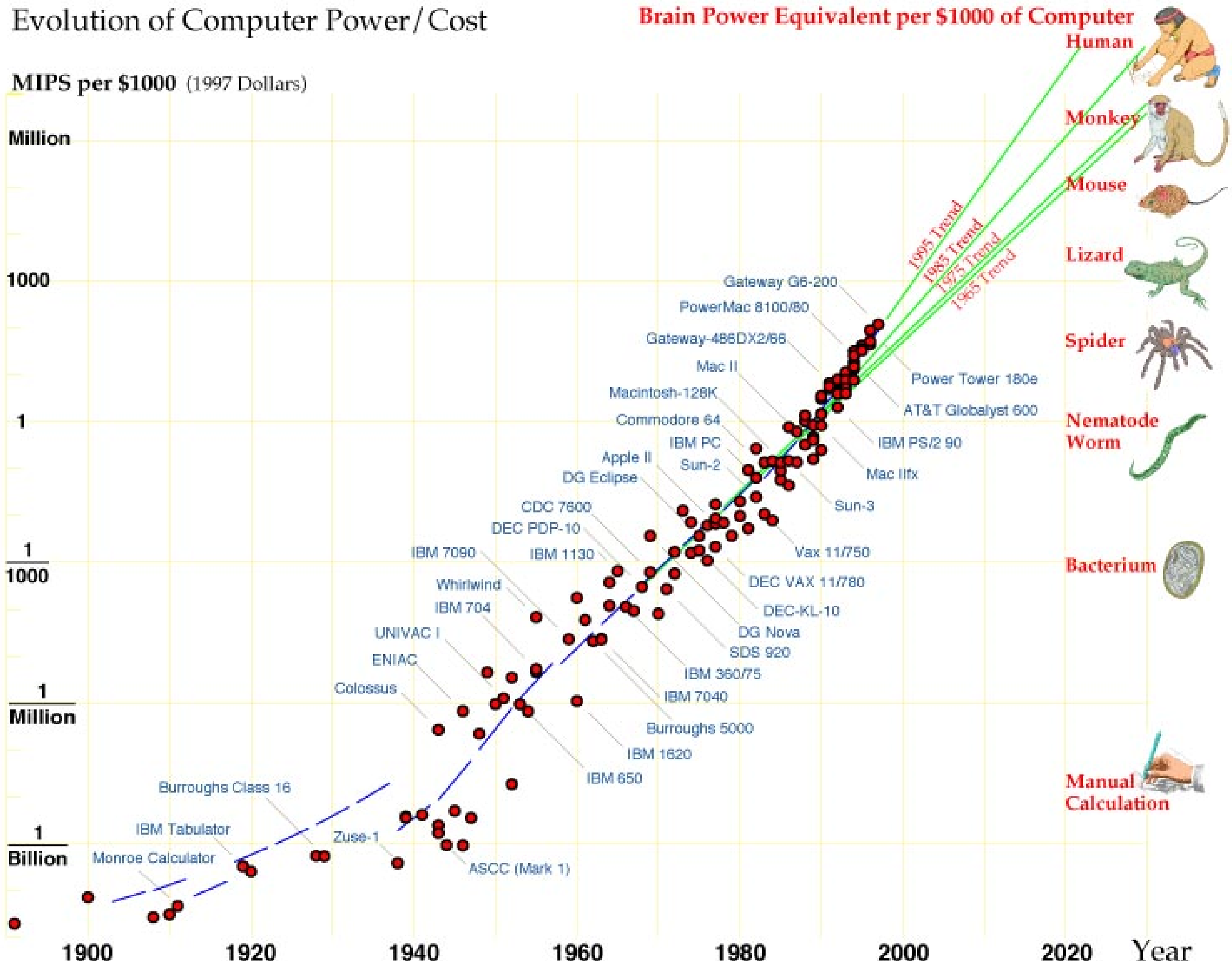
President Obama, Carnegie Mellon University, June 2011

- Part of a larger program to enhance manufacturing in the US
- Goal: cut the time between discovery and commercialization of advanced materials *in half* (from 10–20 to 5–10 years), and do so at *lower cost*
- Will integrate experiments, computation, and theory
- Must facilitate access to materials data

A genome is a set of information encoded in the language of DNA that serves as a blueprint for an organism's growth and development. The word genome, when applied in non-biological contexts, connotes a fundamental building block toward a larger purpose.

Computing Power Has Increased By A Factor of 10^7 Since 1970

Computation is
<u>faster</u> and
<u>less expensive</u>
than
experimentation!



MGI Directions To Date

Materials by Design projects:

DOE EFRCs, EMNs

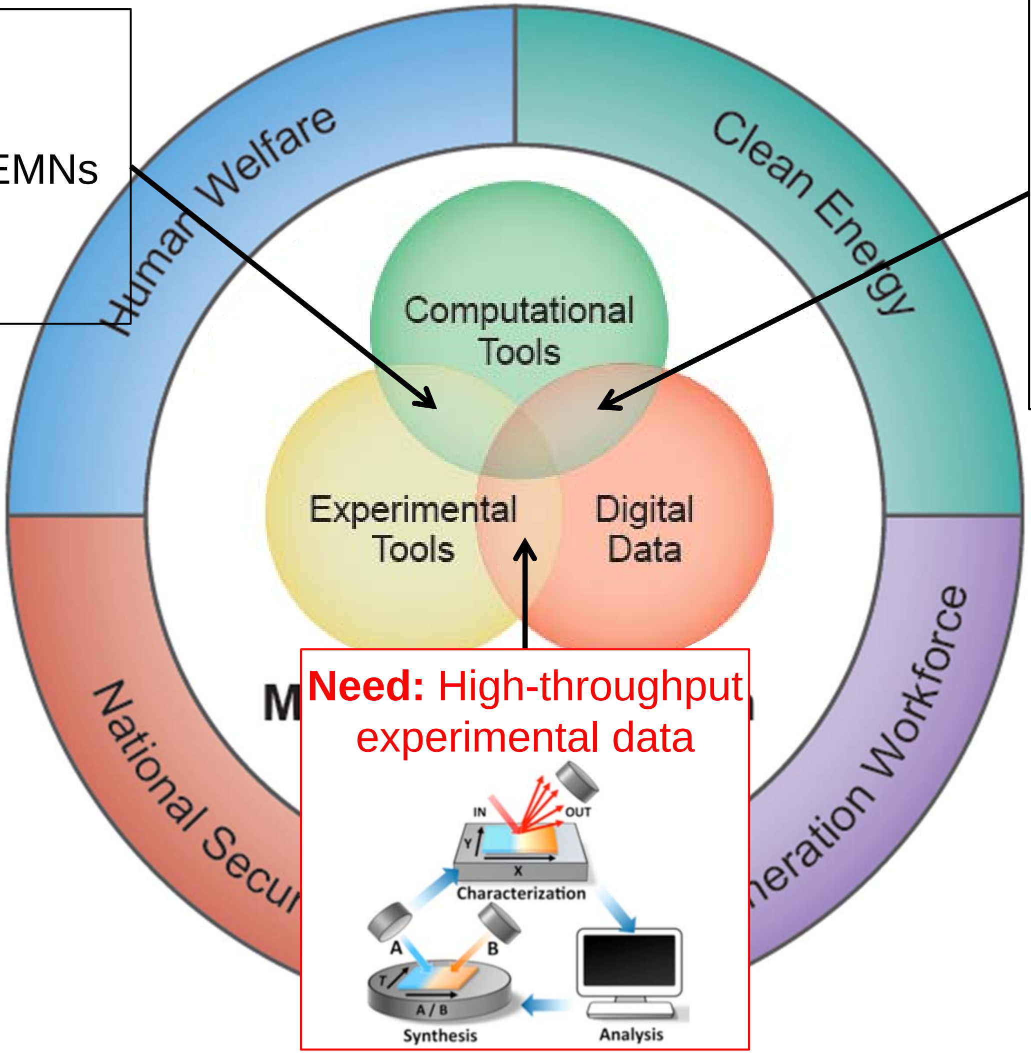
NSF DMREFs

HT computational databases:

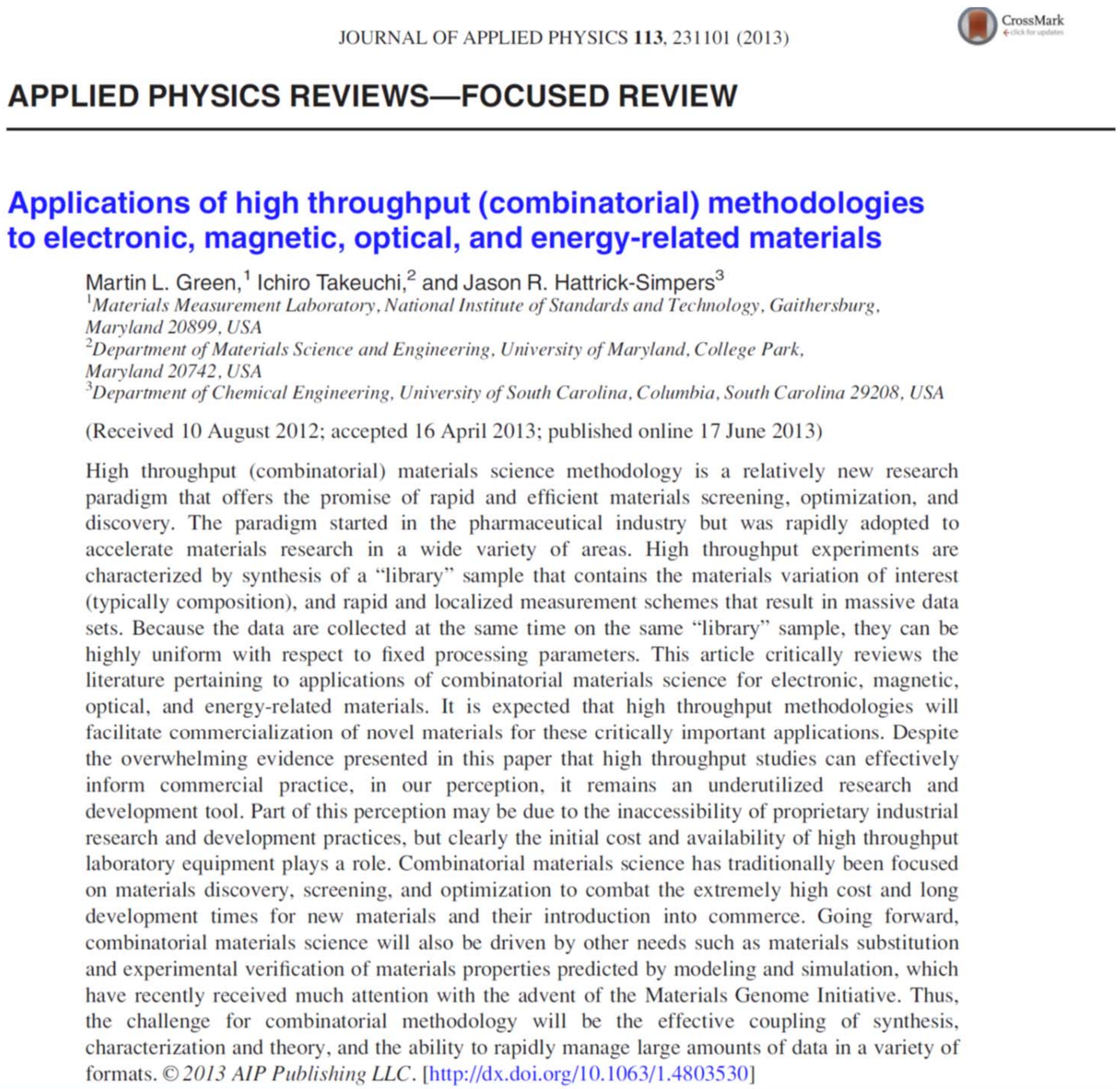
MATERIALS PROJECT

AFLOW
Automatic - FLOW for Materials Discovery

OQMD



Need: High-throughput experimental data



JOURNAL OF APPLIED PHYSICS **113**, 231101 (2013)

APPLIED PHYSICS REVIEWS—FOCUSED REVIEW

Applications of high throughput (combinatorial) methodologies to electronic, magnetic, optical, and energy-related materials

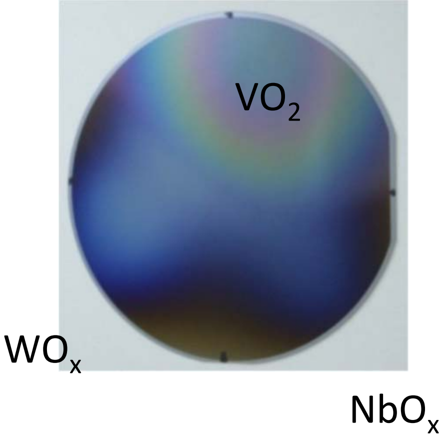
Martin L. Green,[1] Ichiro Takeuchi,[2] and Jason R. Hattrick-Simpers[3]
[1]*Materials Measurement Laboratory, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA*
[2]*Department of Materials Science and Engineering, University of Maryland, College Park, Maryland 20742, USA*
[3]*Department of Chemical Engineering, University of South Carolina, Columbia, South Carolina 29208, USA*

(Received 10 August 2012; accepted 16 April 2013; published online 17 June 2013)

High throughput (combinatorial) materials science methodology is a relatively new research paradigm that offers the promise of rapid and efficient materials screening, optimization, and discovery. The paradigm started in the pharmaceutical industry but was rapidly adopted to accelerate materials research in a wide variety of areas. High throughput experiments are characterized by synthesis of a "library" sample that contains the materials variation of interest (typically composition), and rapid and localized measurement schemes that result in massive data sets. Because the data are collected at the same time on the same "library" sample, they can be highly uniform with respect to fixed processing parameters. This article critically reviews the literature pertaining to applications of combinatorial materials science for electronic, magnetic, optical, and energy-related materials. It is expected that high throughput methodologies will facilitate commercialization of novel materials for these critically important applications. Despite the overwhelming evidence presented in this paper that high throughput studies can effectively inform commercial practice, in our perception, it remains an underutilized research and development tool. Part of this perception may be due to the inaccessibility of proprietary industrial research and development practices, but clearly the initial cost and availability of high throughput laboratory equipment plays a role. Combinatorial materials science has traditionally been focused on materials discovery, screening, and optimization to combat the extremely high cost and long development times for new materials and their introduction into commerce. Going forward, combinatorial materials science will also be driven by other needs such as materials substitution and experimental verification of materials properties predicted by modeling and simulation, which have recently received much attention with the advent of the Materials Genome Initiative. Thus, the challenge for combinatorial methodology will be the effective coupling of synthesis, characterization and theory, and the ability to rapidly manage large amounts of data in a variety of formats. © *2013 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4803530]

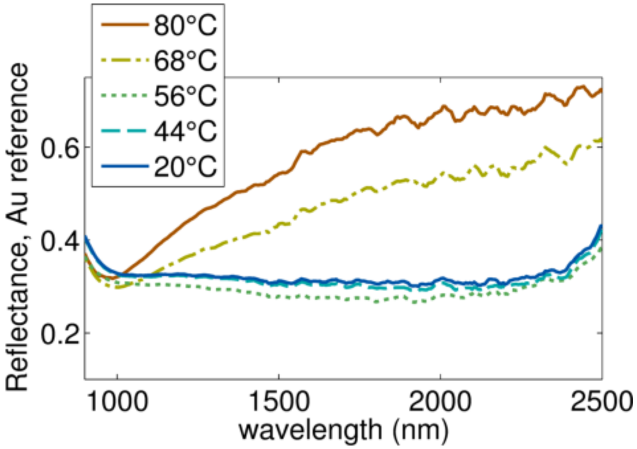
Three Components of High-Throughput Experimentation

Synthesis



Combinatorial library

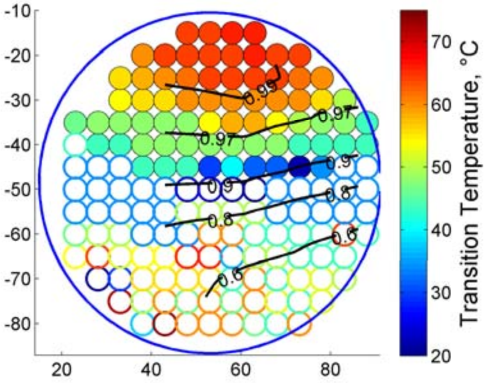
Measurement



Measure near-IR reflectance at many temperatures and locations (compositions)

5775 reflectance spectra: 165 locations and 35 temperatures

Data Analytics



Map of thermochromic transition temperatures

NIST/OSTP/AMAT Workshop Conclusions

- Prodigious amounts of experimental data will be required to *inform and validate* modeling and simulation, to "power the MGI computational engine."

- HTE can rapidly establish relationships between composition, structure, and properties for a wide variety of materials classes, and therefore is <u>uniquely suited to rapidly generate high quality, consistent data sets</u>

- Enable broad access to HTE methodologies and data

High Throughput Experimental Materials Collaboratory (HTE-MC)

Problem	Solution
• Experimental databases are not keeping pace with computational databases	• *Integrate HTE laboratories with materials cyberinfrastructure*
• HTE is out of reach to most researchers due to high startup and operating costs	• HTE as a shared resource; operate on demand by access fees and core funding
• Materials are diverse; no single institution can have all the necessary equipment	• HTE as a federated resource; enable connectivity via cyberinfrastructure

High Throughput Experimental Materials Collaboratory (HTE-MC)

- Necessary because even one “brick and mortar” HTE facility would be very costly, and multiple facilities dedicated to different materials classes are needed

- Enable researchers at national labs, universities, and industry to have access to HTE facilities

- The HTE-MC would facilitate MGI-driven research while leveraging investment

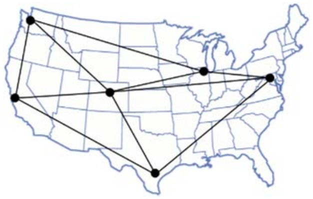
- Complement new science investments (EMN’s, NNMI, NSF)

The Collaborative Economy

airbnb HomeExchange.com FLIPKEY

UBER lyft TURO Getaround

KHAN ACADEMY simplilearn coursera



HTE-MC

How?

Collaboratory: a 1989 neologism (William A. Wulf, Computer Scientist at University of Virginia):

"...defined by...a 'center without walls,' in which the nation's researchers can perform their research without regard to physical location, interacting with colleagues, accessing instrumentation, sharing data and computational resources, …. accessing information in digital libraries."

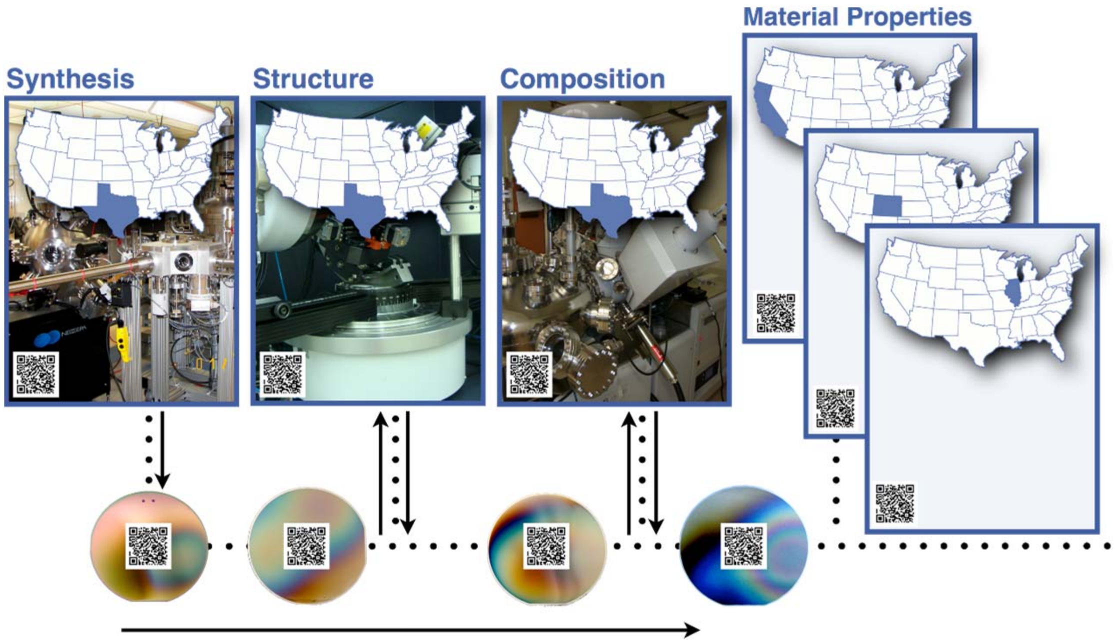
- The HTE-MC would consist of:
  - An integrated, delocalized network of HTE synthesis and characterization tools
  - A best-in-class materials data management platform

HTE-MC – *change states!!*

Materials Problems

Core Funding, Access Fees

Students



New Knowledge

Materials Solutions

AI-Ready Public Data

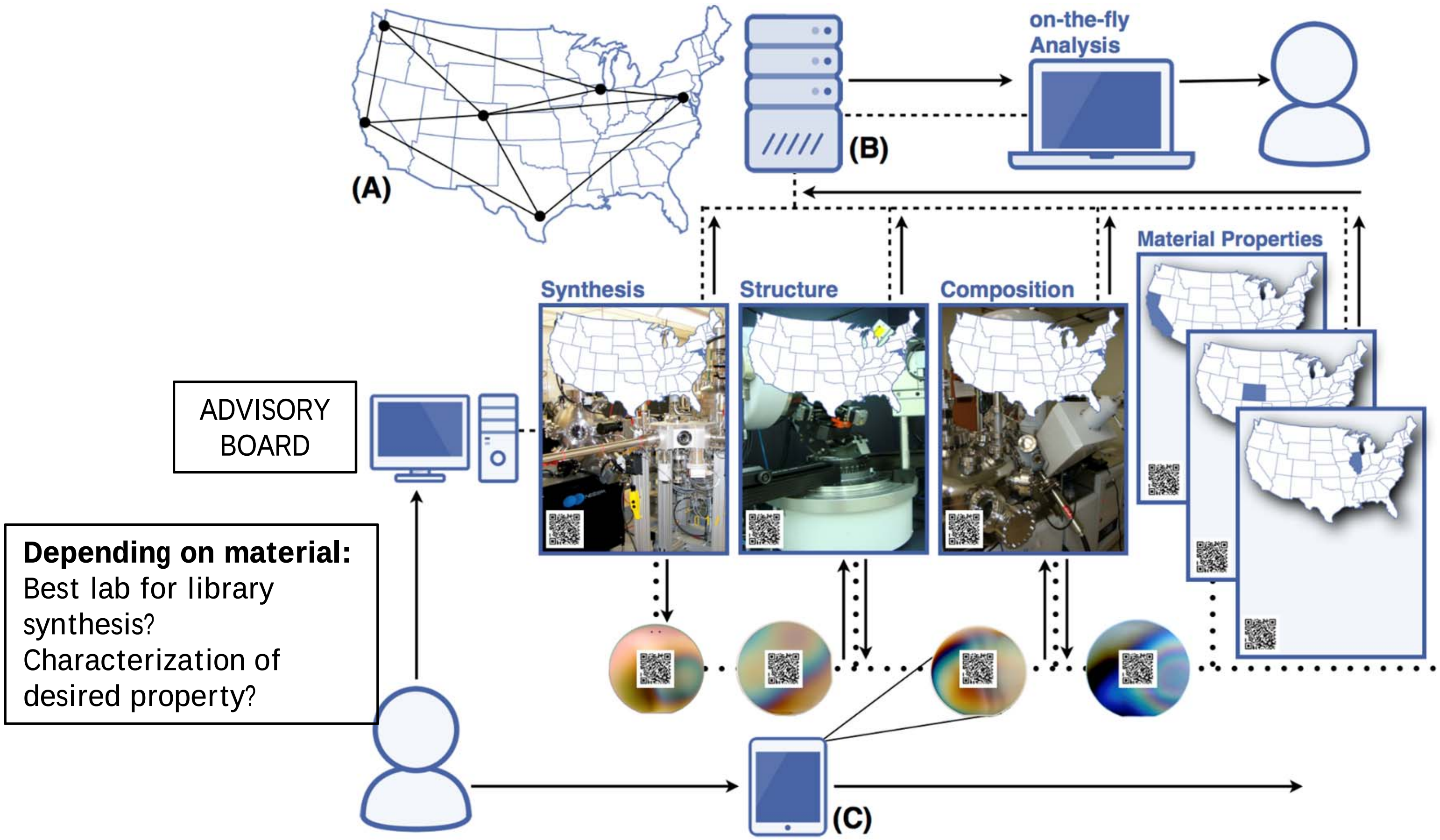
HTE Libraries

AI-Materials Infrastructure

New Mat. Commerce

Next Gen. Workforce

HTE - MC



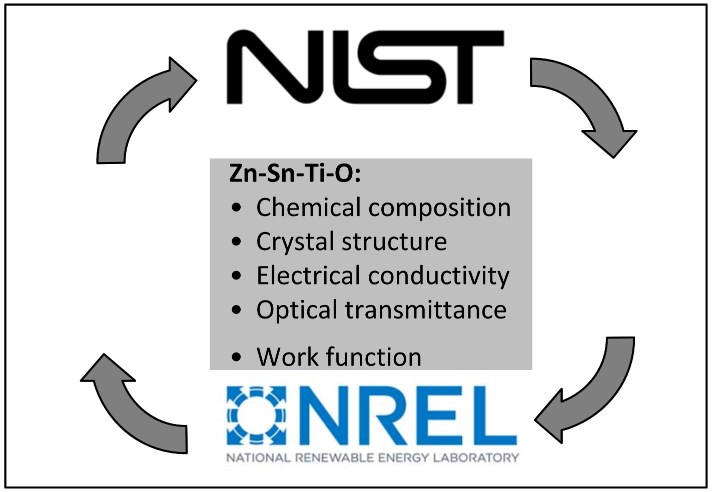
ADVISORY BOARD

Depending on material:
Best lab for library synthesis?
Characterization of desired property?

Global Identification and Tracking of Instruments, Samples, and Data

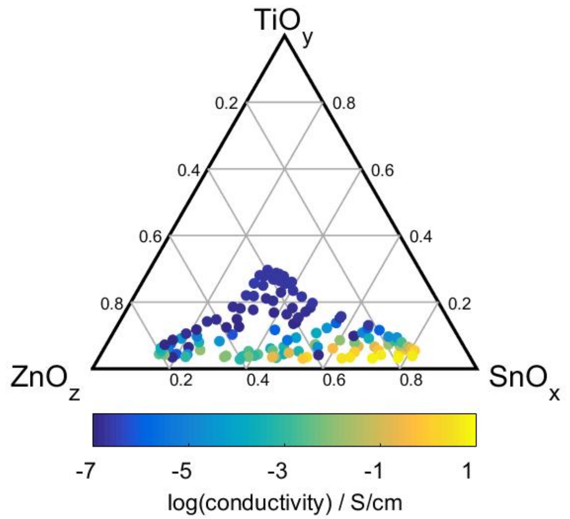
In Progress: HTEMC “Round Robin” Proof of Principle

Goal: test and improve the standards for exchange of data and sample among participant labs

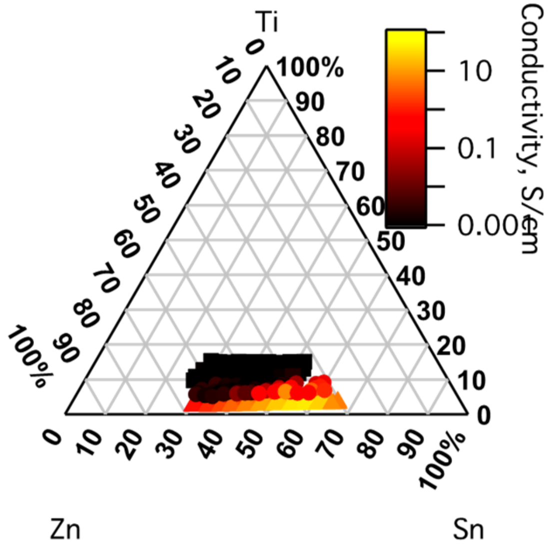


Zn-Sn-Ti-O:
- Chemical composition
- Crystal structure
- Electrical conductivity
- Optical transmittance
- Work function

NIST:



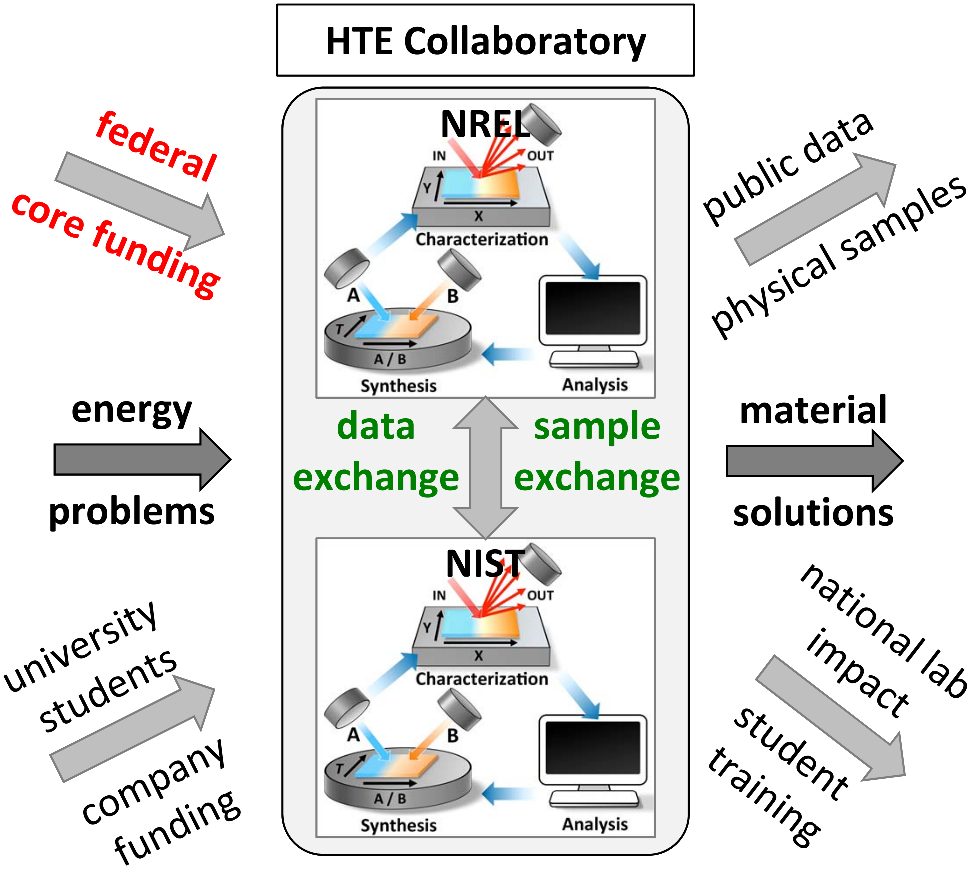
NREL:



Sample synthesis and measurements:

- *Synthesize*: Zn-Sn-Ti-O composition spread sample libraries using combinatorial PLD (@NIST) or sputtering (@NREL)
- *Measure*: Chemical composition, Crystal structure, Electrical conductivity, Optical transmittance, Work function
- *Exchange*: Sample libraries and associated data, repeat measurements

HTE Materials Collaboratory



HTE Collaboratory

federal core funding

energy problems

university students

company funding

public data

physical samples

material solutions

national lab impact

student training

data exchange

sample exchange

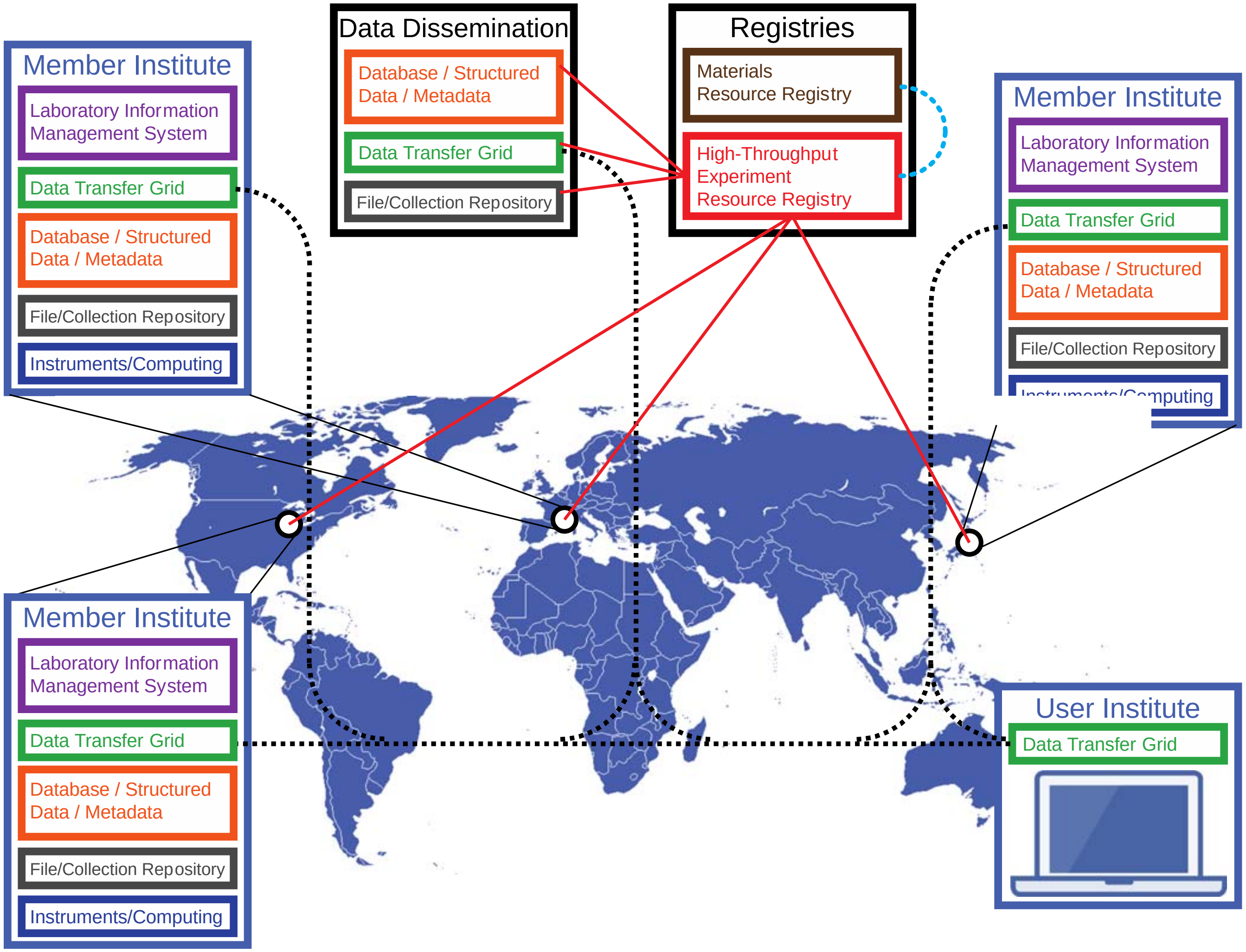
Problems:

- HTE equipment is very expensive and requires dedicated personnel to operate and maintain
- The materials synthesis routes and characterization techniques are diverse enough that no single institution can have all the necessary equipment

Solution:

- “Library” samples can be synthesized and characterized at geographically distributed locations
- Collaboratory will operate on demand from customers (Start-ups, academia, government agencies) with support from core federal funding (*like synchrotrons*)

High-Throughput Experimental Materials Collaboratory (HTEMC)



Data Dissemination

Database / Structured Data / Metadata

Data Transfer Grid

File/Collection Repository

Registries

Materials Resource Registry

High-Throughput Experiment Resource Registry

Member Institute

Laboratory Information Management System

Data Transfer Grid

Database / Structured Data / Metadata

File/Collection Repository

Instruments/Computing

Member Institute

Laboratory Information Management System

Data Transfer Grid

Database / Structured Data / Metadata

File/Collection Repository

Instruments/Computing

Member Institute

Laboratory Information Management System

Data Transfer Grid

Database / Structured Data / Metadata

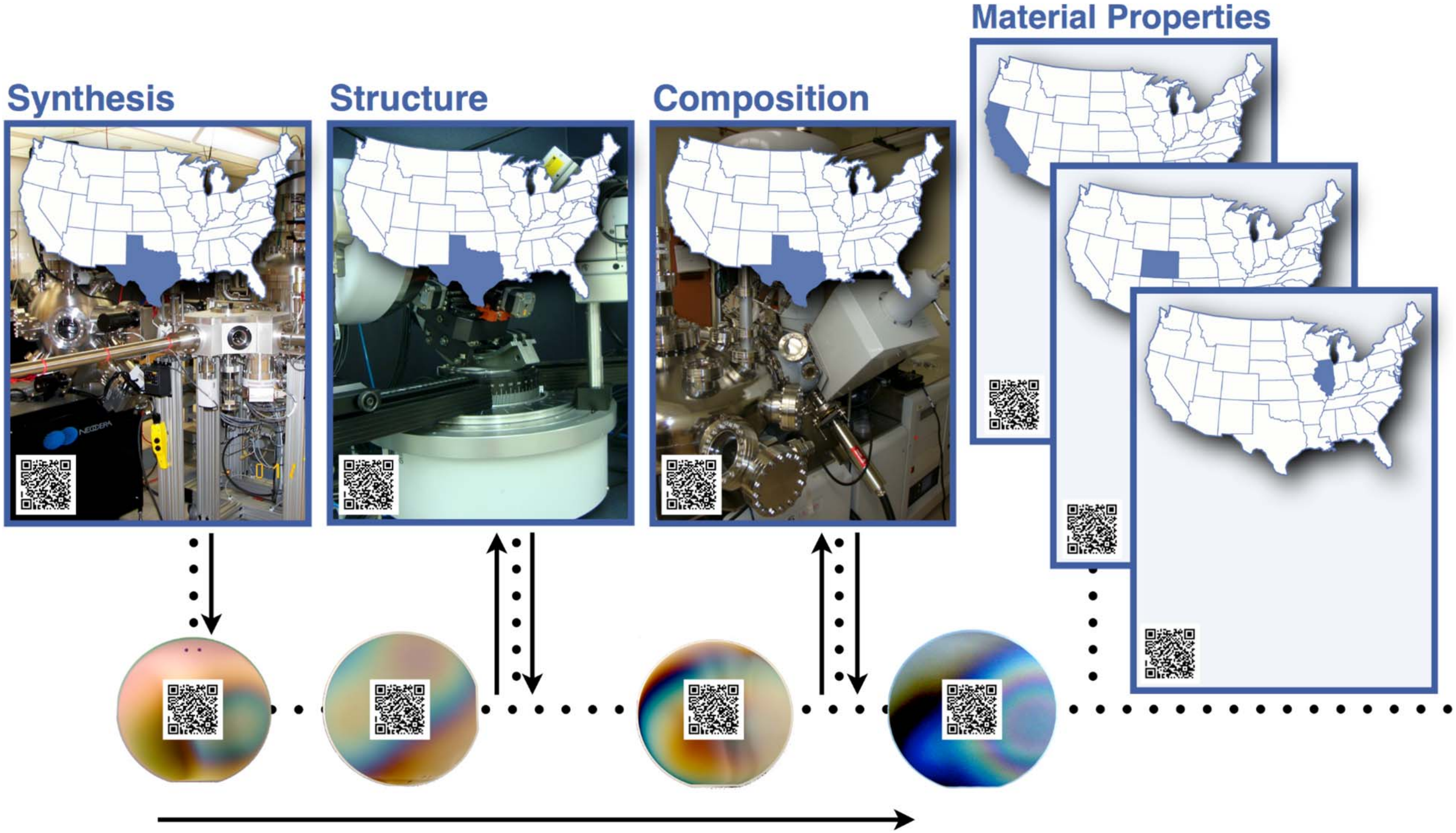
File/Collection Repository

Instruments/Computing

User Institute

Data Transfer Grid

HTE Registry: Tracking of Digital and Physical Artifacts



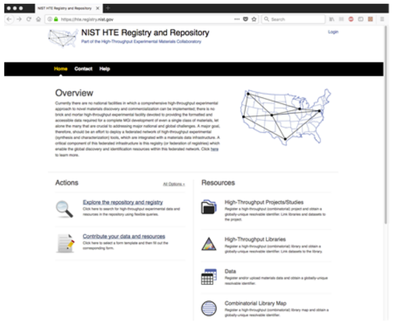
Infrastructure Model: Dissemination

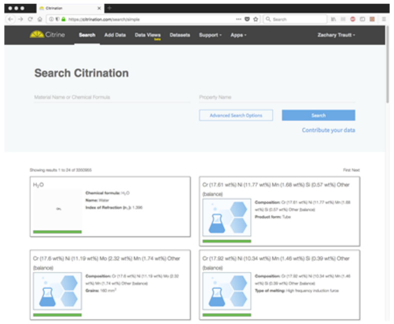
Data Dissemination

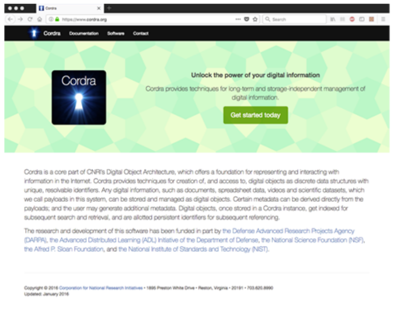
Database / Structured Data / Metadata

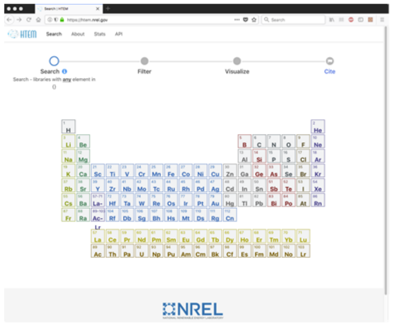
Data Transfer Grid

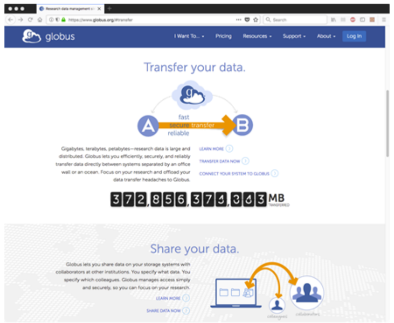
File/Collection Repository

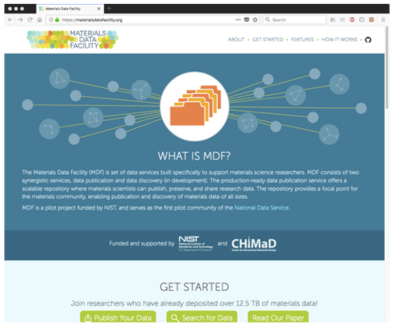


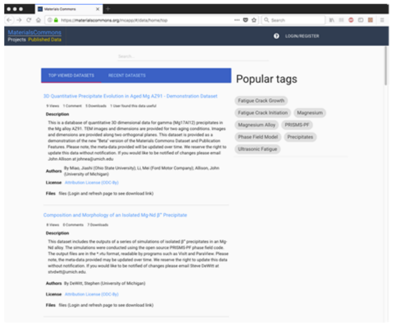


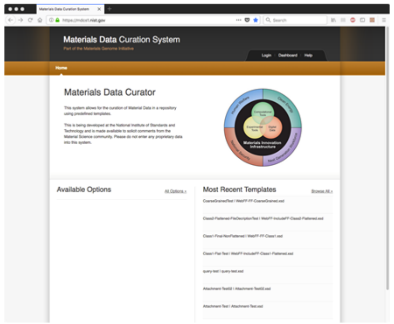


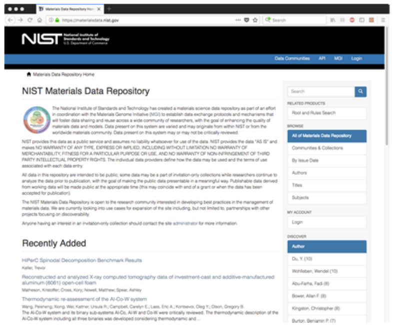








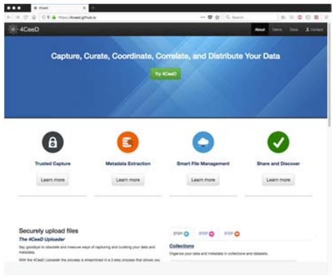




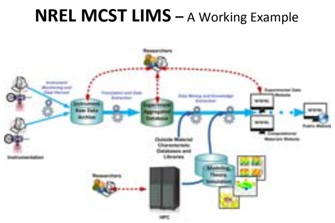
Infrastructure Model: Members

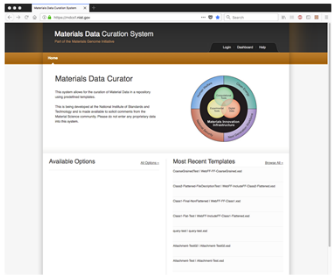
Member Institute

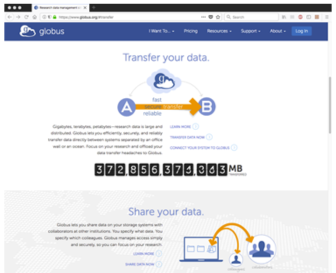
- Laboratory Information Management System
- Exchange & Integration
- Database / Structured Data / Metadata
- File Management
- Instruments/Computing

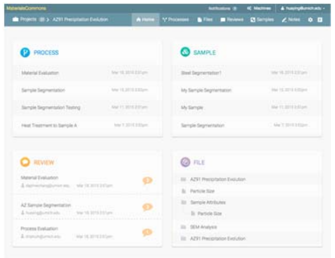


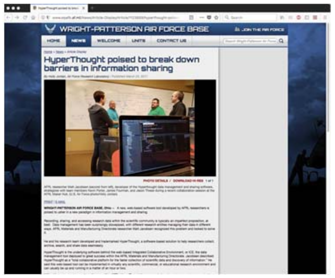
NREL MCST LIMS – A Working Example

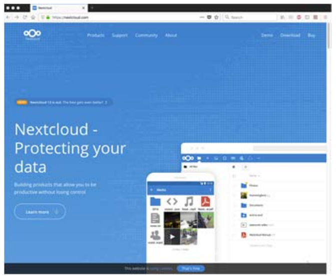


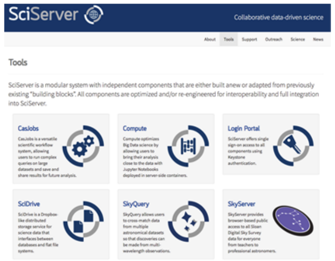


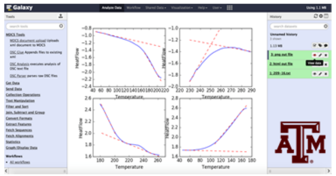




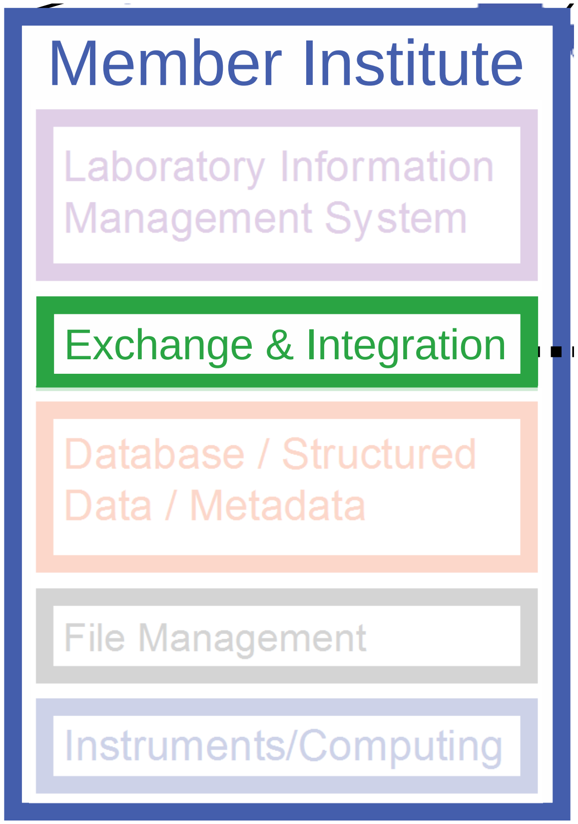








Infrastructure Model: Members



Member Institute

Laboratory Information Management System

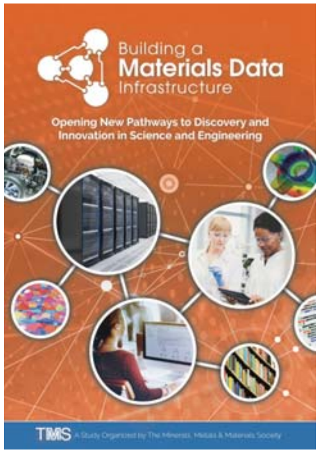
Exchange & Integration

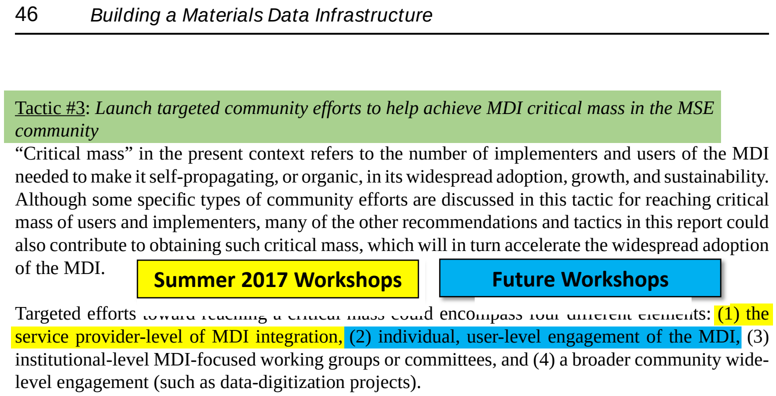
Database / Structured Data / Metadata

File Management

Instruments/Computing

Motivation





46 *Building a Materials Data Infrastructure*

Tactic #3: *Launch targeted community efforts to help achieve MDI critical mass in the MSE community*

"Critical mass" in the present context refers to the number of implementers and users of the MDI needed to make it self-propagating, or organic, in its widespread adoption, growth, and sustainability. Although some specific types of community efforts are discussed in this tactic for reaching critical mass of users and implementers, many of the other recommendations and tactics in this report could also contribute to obtaining such critical mass, which will in turn accelerate the widespread adoption of the MDI.

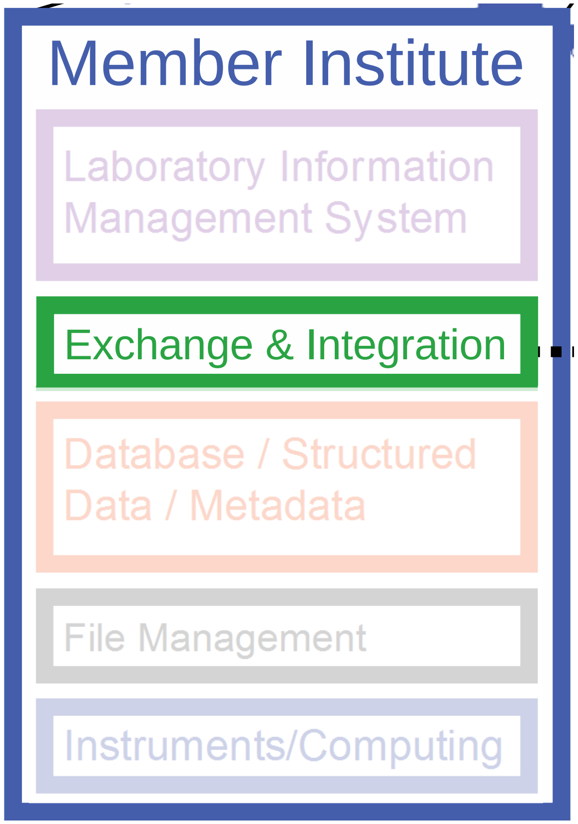
Summer 2017 Workshops

Future Workshops

Targeted efforts toward reaching a critical mass could encompass four different elements: (1) the service provider-level of MDI integration, (2) individual, user-level engagement of the MDI, (3) institutional-level MDI-focused working groups or committees, and (4) a broader community wide-level engagement (such as data-digitization projects).

Report available for free download at www.tms.org/MDIstudy

Infrastructure Model: Members



Member Institute

Laboratory Information Management System

Exchange & Integration

Database / Structured Data / Metadata

File Management

Instruments/Computing

2017 Platform Integration Hack-a-Thon

Part 1, Week of July 17, Dayton OH

Announced as:

*LIMS-to-LIMS integration

Attendees from:

AFRL, UIUC, Granta, NanoHUB, GaTech, MarkLogic

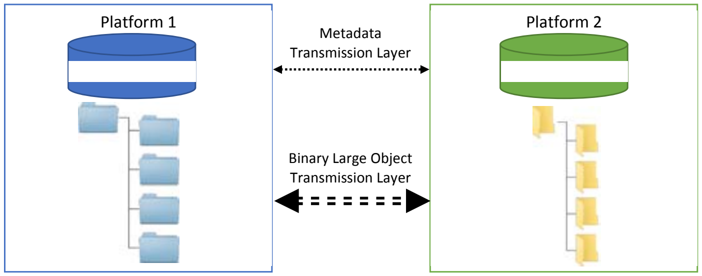
Part 2, Week of Sept. 11, Dayton OH

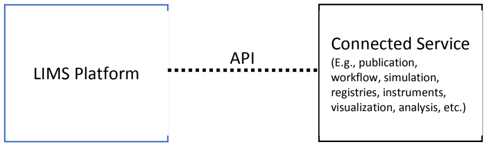
Announced as:

LIMS-to-other service integration

Attendees From:

AFRL, NIST, Citrine, Granta, LLNL, LBL, MDF, NanoHUB, BlueQuartz, SciServer, Materials Commons





*Laboratory Information Management System