Dr. Eric Miller

Department of Energy (DOE)
Office of Energy Efficiency and Renewable Energy (EERE)
Fuel Cells Technology Office (FTCO)

DOE and DoD Multi-topic Workshop
Advanced Materials Manufacturing (AMM) Session
Fort Worth, TX
October 9, 2014

Advanced Materials Manufacturing (AMM) Institute Stakeholders Workshop

WELCOME & THANK YOU!

from your friendly support staff: Eric Miller, David Forrest, Fred Crowson, Jessica Savell…

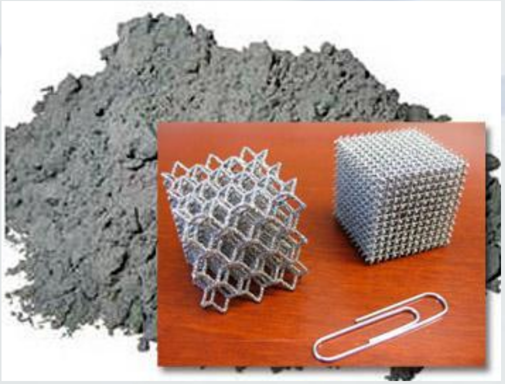
BRAINSTORMING RULES APPLY IN OUR EXPLORATIONS

(adding 'brutal honesty tempered by kindness and mutual respect')

Context: The First Manufacturing Innovation Institute
Additive Manufacturing/3D Printing – Youngstown OH

Prime Awardee: National Center for Defense Manufacturing and Machining

- Initial $30M federal investment matched by $40M industry, state/local
- Strong leveraging of equipment, existing resources
- Strong business development
- Tiered membership-based model, low cost to small business and nonprofits



- **Now at $50M federal, $60M co-invested**
- **OVER 100 Participating partners!**

Why America Makes?

America Makes
National Additive Manufacturing Innovation Institute

A Self Sustainable Institute Model

America Makes creates mechanisms for collaboration…

Cooperative Development of
- **Training**
- **Assessments**
- **Case Studies**

Pooling Resources / Pooling Risks

Cooperative Development of
- **Material Specs**
- **Process Specs**
- **Material Databases**
- **Design Rules**
- **Application Guides**

Solving Problems Collaboratively

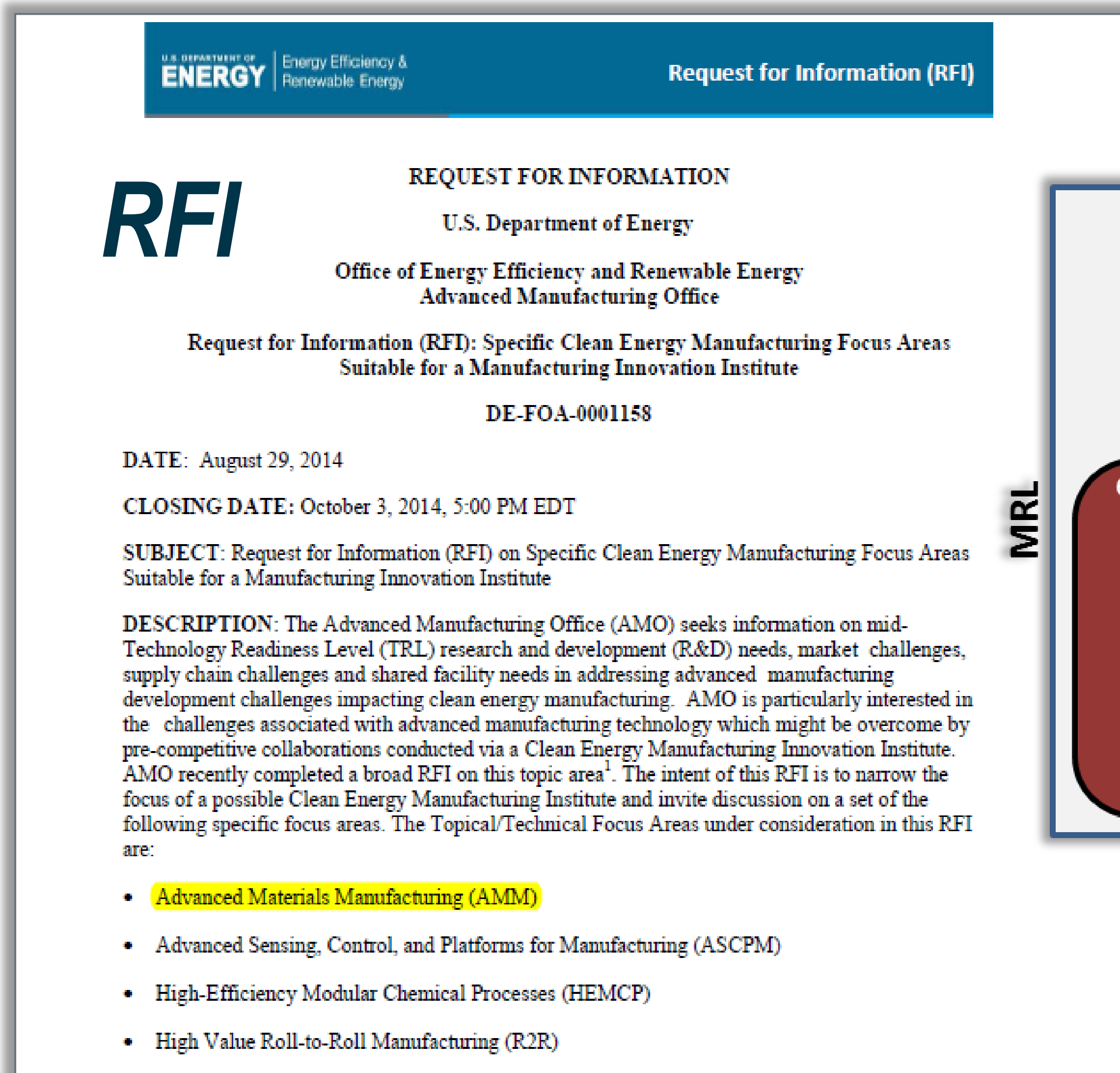
Work Shops, Working Groups, Projects

Public/Private Funded Projects
Crowd Funded Projects

Leveraging Community Knowledge

Knowledge Base, Online Collaboration Tools, Databases, Specifications, Application Guides, Curriculum

Why an Advanced Materials Manufacturing (AMM) Institute? *for Accelerating Clean Energy Technology Development*



U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Request for Information (RFI)

RFI

REQUEST FOR INFORMATION

U.S. Department of Energy

Office of Energy Efficiency and Renewable Energy
Advanced Manufacturing Office

Request for Information (RFI): Specific Clean Energy Manufacturing Focus Areas Suitable for a Manufacturing Innovation Institute

DE-FOA-0001158

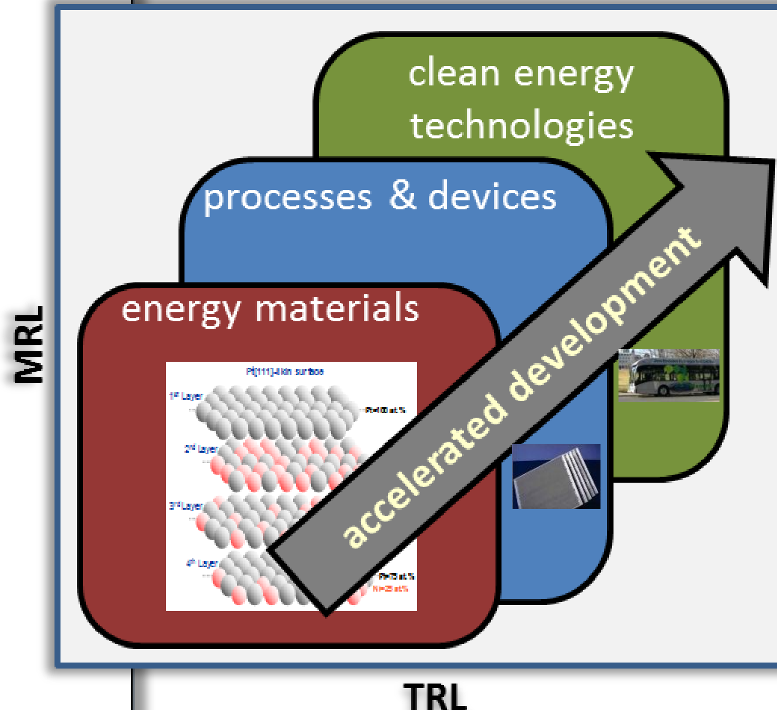
DATE: August 29, 2014

CLOSING DATE: October 3, 2014, 5:00 PM EDT

SUBJECT: Request for Information (RFI) on Specific Clean Energy Manufacturing Focus Areas Suitable for a Manufacturing Innovation Institute

DESCRIPTION: The Advanced Manufacturing Office (AMO) seeks information on mid-Technology Readiness Level (TRL) research and development (R&D) needs, market challenges, supply chain challenges and shared facility needs in addressing advanced manufacturing development challenges impacting clean energy manufacturing. AMO is particularly interested in the challenges associated with advanced manufacturing technology which might be overcome by pre-competitive collaborations conducted via a Clean Energy Manufacturing Innovation Institute. AMO recently completed a broad RFI on this topic area[1]. The intent of this RFI is to narrow the focus of a possible Clean Energy Manufacturing Institute and invite discussion on a set of the following specific focus areas. The Topical/Technical Focus Areas under consideration in this RFI are:

- Advanced Materials Manufacturing (AMM)
- Advanced Sensing, Control, and Platforms for Manufacturing (ASCPM)
- High-Efficiency Modular Chemical Processes (HEMCP)
- High Value Roll-to-Roll Manufacturing (R2R)



Addresses both technology- and manufacture- readiness to move materials to market in clean energy applications

SPOILER ALERT! *USE YOUR YELLOW CARD TO RESPOND*

Q5: Does an AMM Central-Institute and/or Distributed Consortium Make Sense, and if so, What Does it Look Like?

Include, for example:

- **Your name(s), affiliation and expected AMM role***
- **Model for *CORE CAPABILITIES* and leveraged partnerships (with initial government investment)**
- **Benefits to clean energy technologies, *US MANUFACTURING* (*and Mankind*)**
- **Orchestration of *INDUSTRY PULL* with *SCIENTIFIC PUSH* in new RD&D paradigm**
- **Benefits in leveraging *SYNERGIES* among computation, experiments and informatics**
- **Advantages in exploiting *COMMONALITIES* among different materials classes**
- ***METRICS* to gauge success in accelerated development time, *COST SAVINGS*, etc.**
- **Emphasis on *COMMUNITY BUILDING* (instead of empire building)**
- **Emphasis on key role of *HUMAN EXPERTISE* in tandem with *TECHNOLOGY RESOURCES***
- **Long-term *SUSTAINABILITY* of institute/consortium**

****Roles Including: Clean Energy Technology Developers/ Integrators/ Users/ Companies; Materials Tool Developers / Integrators/ Users/ Companies; and Others….***

Other Cards for Today's Festivities:

PINK: Your "Dance Card"

Keeping track of colleagues you'd like to network with during our 'working lunch' (and possibly beyond!)

BLUE : General Answer-Board Cards

Archiving your thoughtful responses to our session's four focus questions

(Feel free to use 'regular' pen; Please write legibly)

DOE's Clean Energy Materials R&D Challenges:
Spanning Numerous Materials Classes

Can an AMM Approach Integrating MGI* Toolsets and Expertise Facilitate Acceleration of Clean Energy Product Development?

Structural Materials

lightweight alloys & composites
cars, buses, wind turbines, fuel tanks...

advanced optical absorbers
PV, solar fuels, solar purifiers..

Optical Materials

efficient solid-state converters
thermoelectrics, LED lighting…

high temp materials
CSP, combustion, geothermal...

advanced membranes
batteries, fuel cells, purifiers...

WBG semiconductors
power electronics, grid integration..

electrode materials
batteries, fuel cells, electrolyzers…

energy storage materials
thermal, thermochemical...

Thermal Materials

non precious catalysts
fuel cells, electrolyzers, reformers...

Electronic Materials

alternative fuels
advanced combustion, bio/synthetic fuels…

Chemical Materials

****Materials Genome Initiative***

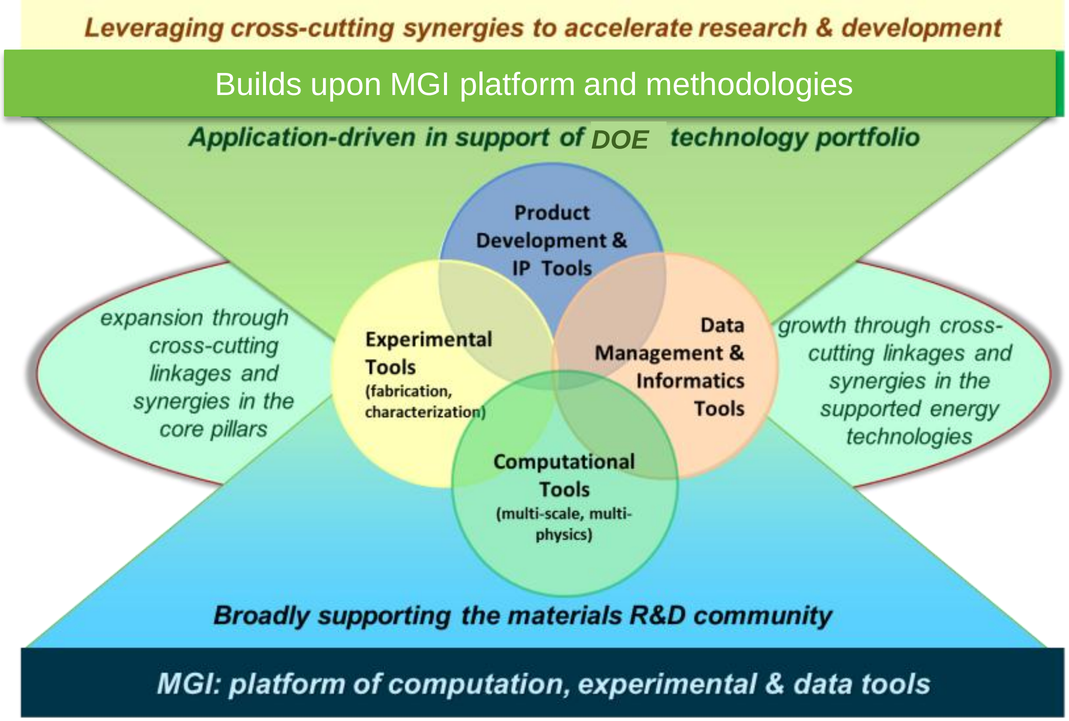
AMM is a Pillar in the DOE Clean Energy Manufacturing Initiative: *Independent of the "Institute/Consortium" Implementation*

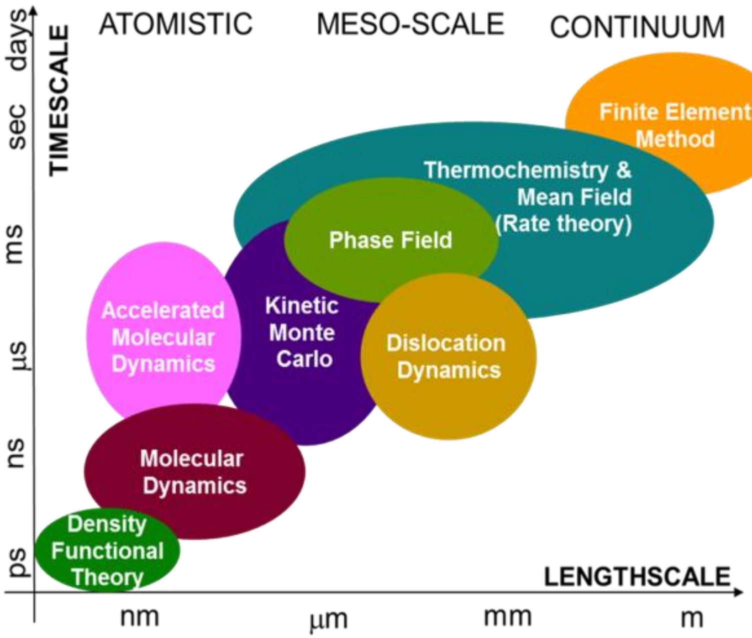
- **Serves as a strategic resource in DOE's broader *Materials Genome Initiative for Clean Energy***
- **Fosters public/private partnerships that:**
  – Identify and develop advanced materials and processes for clean energy product development
  – Provide common resources for high throughput computational , experimental and 'big data' activities emphasizing applied, energy materials challenges
  – Provide accessible and standardized archives of materials models and complementary experimental/computational materials data
  – Provide an accessible brain trust of professionals highly skilled in computational materials techniques, such as *Integrated Computational Materials Engineering*
  – Provide access to expert scientists and engineers able to leverage high throughput experimental methods for solving industry-relevant materials problems
  – Provide access to expertise in clean-energy-application materials classes

Materials Genome Initiative for Clean Energy: *Foundation for a Potential AMM Institute/Consortium*

Expands on the *Materials Genome Initiative (MGI)* approach, combining multi-scale, multi-physics computational methods with high-throughput synthesis and characterization for intelligent, focused development of improved *MATERIALS, PROCESSES & PRODUCTS* for clean energy technologies

Accelerates materials to market through a focus on process and end-use manufacturing





Materials, devices and PRODUCTS by design integrating and expanding the best experimental and computational tools

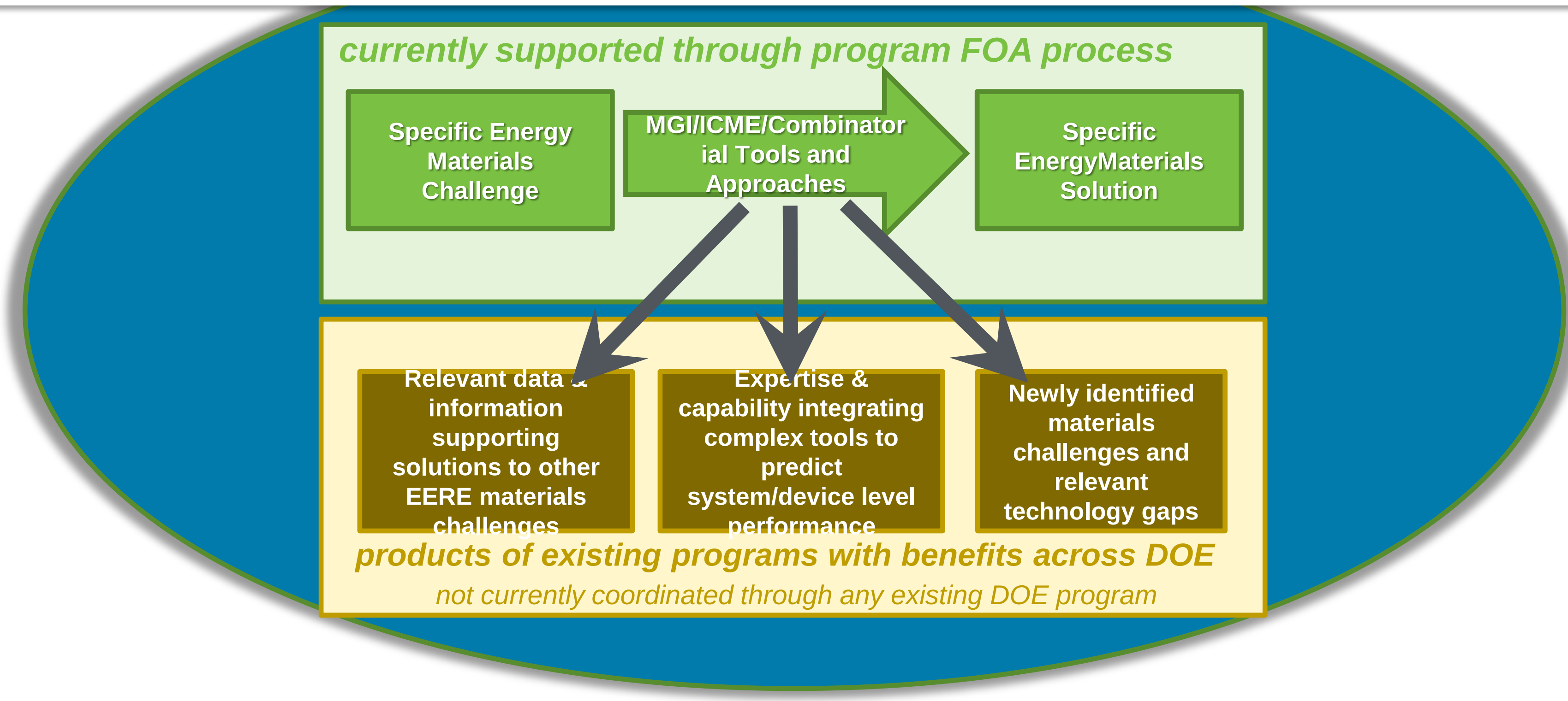
Utilizes multi-physics/multi-scale methodologies and models relevant to accelerated materials-to-market development

Why an AMM Institute/Consortium Could Make Sense..

- **Bridges *INDUSTRY PULL* with the *SCIENTIFIC PUSH***
  - **OSTP has embraced this as a vital and under-represented component of MGI.**
- ***Builds and maintains foundational resources and expertise***
  - **Individual companies/universities have developed their own data, tools, models, and expertise—but these resources fall into disuse without ongoing support and development. It is difficult for most institutions to support permanent in-house staff with the highly specialized skills, laboratory instruments, and computational power needed.**
- ***Serves as a resource where manufacturers can focus on advancing their own applications and businesses***
  - **There's insufficient payoff for most individual companies to make the investments necessary for advancing the Materials Genome infrastructure. AMM-CEMGI would focus on shared resources and take a custodial role of customized experimental and computational tools, models, and hard-won data.**

An AMM Institute/Consortium Approach Offers…

a better way to do what we are already doing in the materials development space



- **Computational/Experimental/Big Data Synergies:** The AMM consortium's combination of computational and experimental methods is ideally suited for accelerated materials discovery and development.
- **Cross-Cutting Technology Impact:** Applying AEMGI techniques in solving specific clean energy materials challenges produces large volumes of "remnant" data and information which could prove extremely valuable to solving materials challenges in other energy technology development efforts.
- **Significant Cost Savings in Shared Resources:** The cost of AMM resources needed to cover the broad spectrum of materials R&D critical to DOE and EERE would be prohibitive if built-up separately.

Doing it the "Right" Way, with Clearly Defined:

Mission Priorities

- **Emphasizing clean-energy benefits**, including identification of key technologies in the DOE's clean energy portfolio that could be advanced through the AMM material-to-market paradigm, and how application of AMM to cross-cutting technology thrusts with common materials R&D needs could broadly accelerate progress across the DOE Offices.
- **Formulating a high-impact strategy**, determining the most productive balance of application-specific materials design and broadly enabling material discovery, and emphasizing the benefit of different integrated computational/experimental/synthesis approaches towards addressing clean energy technology needs.
- **Targeting early stage success,** identifying the technology thrusts offering the 'lowest hanging fruit' (i.e. highest potential for early product-to-market successes) that should be targeted for initial implementation of the AMM R&D approach.

Operational Parameters

- **Delineating the core capabilities** in computation & modeling, experimental synthesis & characterization, data management & informatics, and product development & intellectual property management that would best define the scope and boundaries of an effective AEMGI consortium.
- **Identifying an optimal consortium/partnership model** for the AMM public/private partnership, including specification of constructs for managing resources and funding activities involving the core capabilities, and clear definition of DOE's role in consortium support.
- **Determining a critical mass for early deployment** in the core capabilities needed to start up the AMM Institute/Consortium (including resources, facilities, expertise, staffing, etc.); and identifying mechanisms needed to ensure growth and sustainability.

What an AMM Institute/Consortium Might Look Like

structural lightweight materials thrust

extreme environment materials thrust

functional materials interfaces thrust

leveraging unique capabilities for fast-tracking materials to market, while expanding and enhancing the tools & methods in the core

AMM CORE INSTITUTE/CONSORTIUM

unique set of in-house capabilities in accelerated energy-materials development

Advanced Modeling, Computing, and Simulation Capabilities

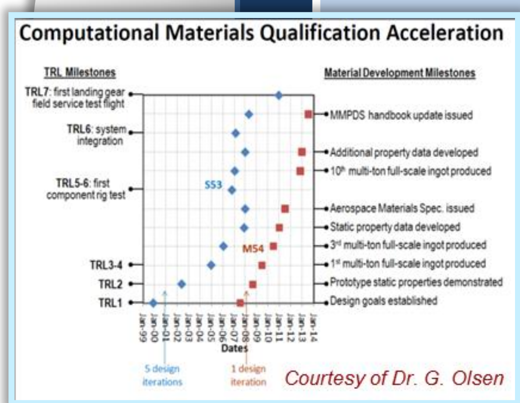
leveraging and expanding on the current MGI multi-physics, multi-scale computational base

feedback pathways

High Throughput Synthesis, Characterization & Analysis Capabilities

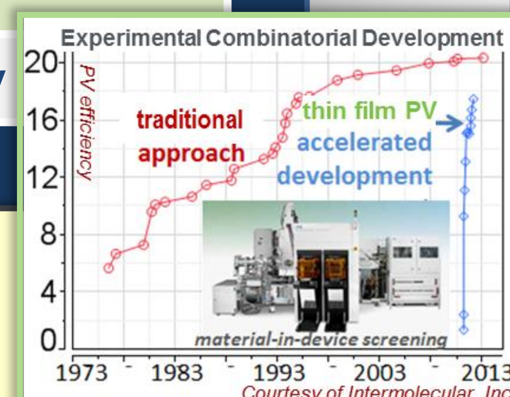
high productivity combinatorial discovery & development tailored to specific energy end uses

linkages in methods / data / intellectual property



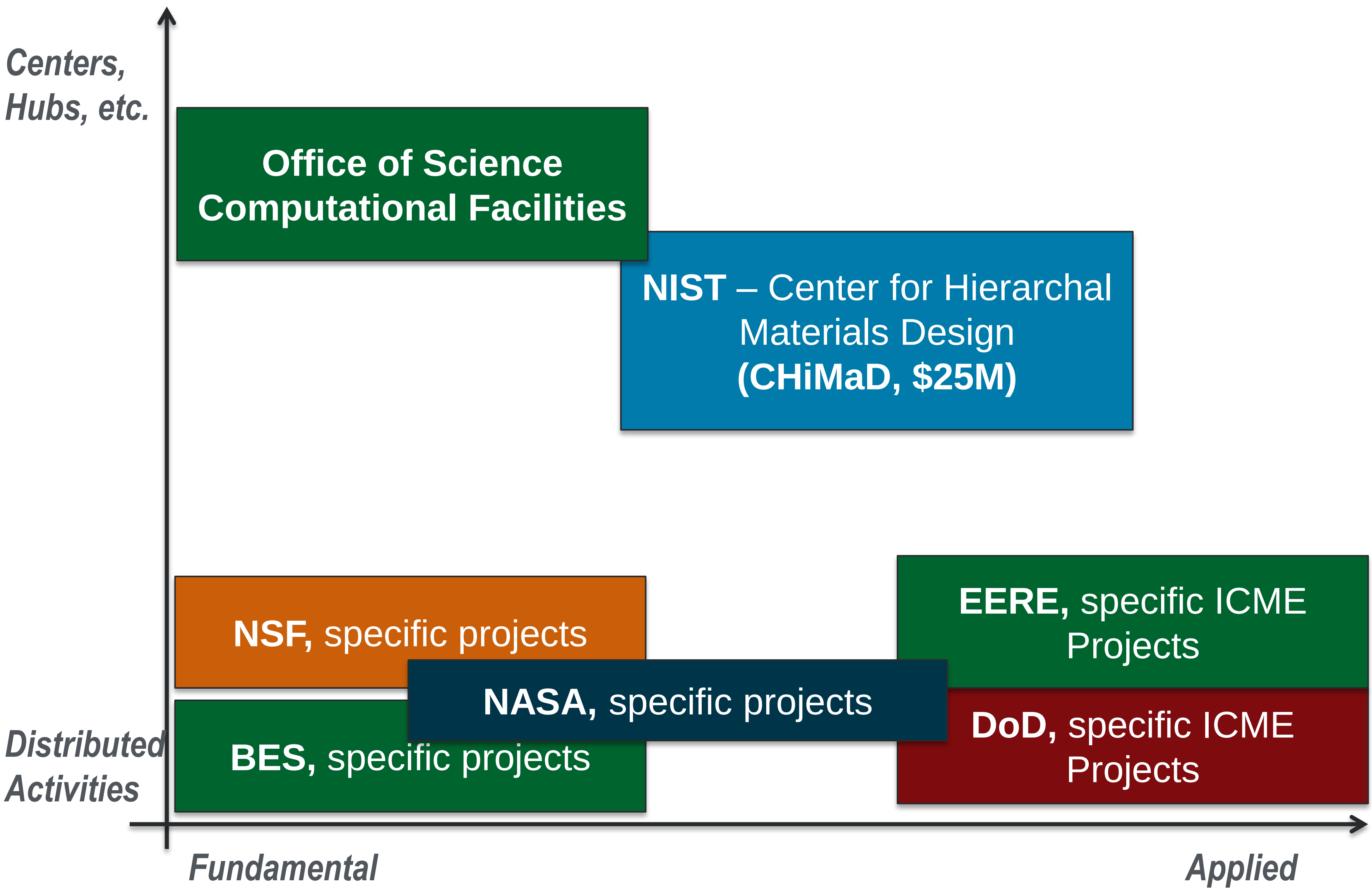
Courtesy of Dr. G. Olsen

Combines multi-physics, multi-scale computation with high-throughput synthesis and characterization for intelligent, focused materials RD&D in different clean energy technology thrusts

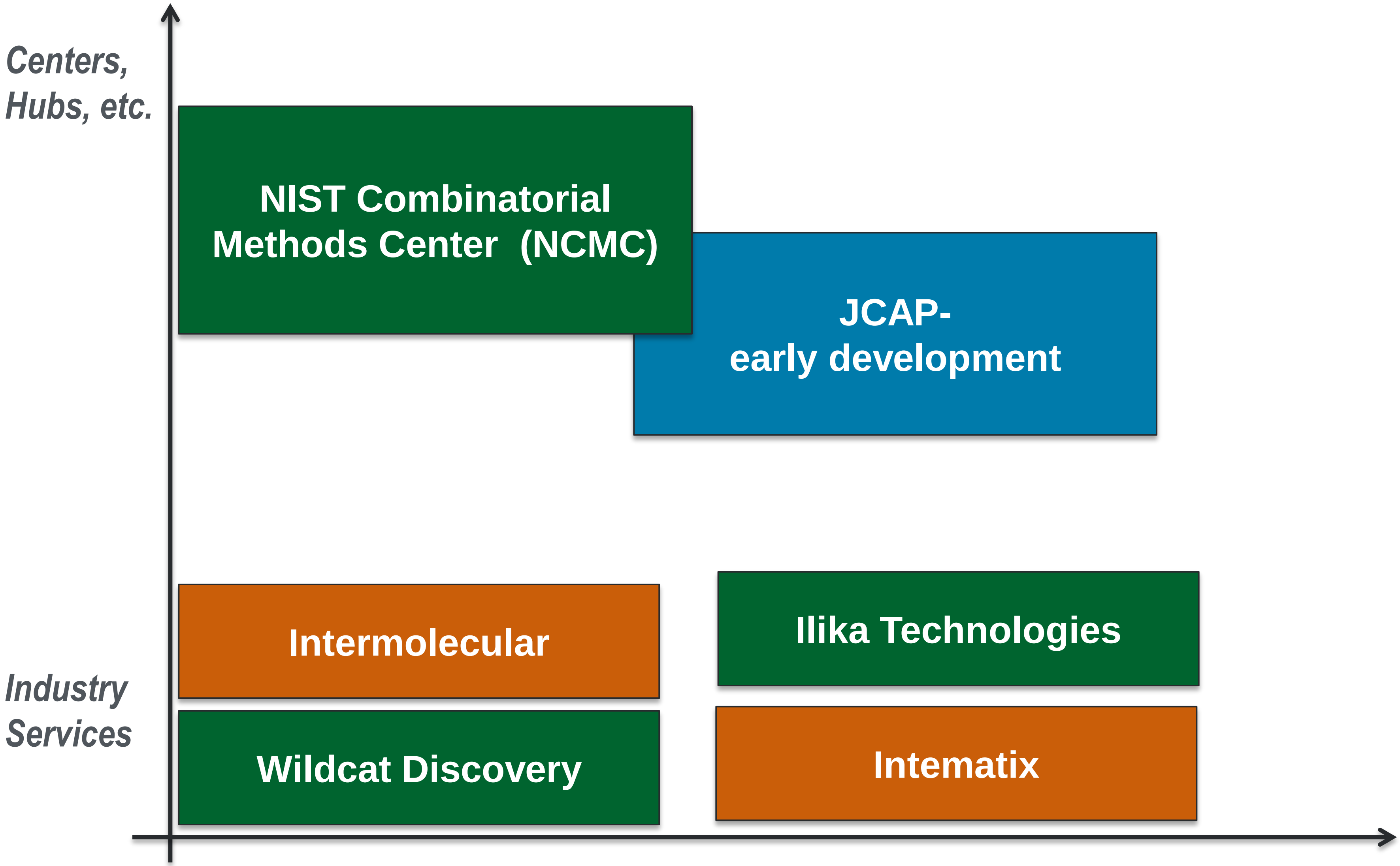


Courtesy of Intermolecular, Inc.

Leveraging Existing MGI-related Activities (to be updated): *Building Appropriate Bridges*



Leveraging Existing Combinatorial Resources (to be updated): *Building Appropriate Bridges*



Roadmap for Today's AMM Workshop Session

Vigorous Discussions: Industry-Pull and Scientific-Push Stakeholders

- ***What EXPERIENCES (good and bad) have you had with materials development for clean energy (or other) applications and products?***
- ***What GAPS in resources (equipment and expertise) and resource accessibility have inhibited your efforts at materials development for specific end-uses?***
- ***What EXISTING RESOURCES in computation, experimentation, and 'big data' (including MGI and other) can be leveraged by AMM for accelerating the materials-to-market process?***
- ***What AMM INSTITUTE/CONSORTIUM FRAMEWORK could serve to build and maintain foundational resources and expertise while best leveraging synergistic existing resources for accelerating materials-to-market in clean energy applications; and where would you fit into such a framework?***

Today's Objective: Constructing a model AMM Framework with Core Capabilites and Leveraged Partnerships

PARTNERS: Toolset Developers and Integrators

4A

CORE: Management Tools & Expertise (including scientific, manufacturing, intellectual property, etc.)

4B

PARTNERS: Clean Energy Application Developers and Manufacturers

4C

CORE: Computational and Modeling Tools & Expertise (including high-throughput)

4D

CORE: Experimental Tools & Expertise (including combinatorial and high-throughput methods)

4E

CORE: Materials Expertise in Clean Energy Materials Classes

4F

CORE: Data and Informatics Tools & Expertise

4G

Bridges to External Resources: Broader MGI and Other Materials R&D Efforts

4H

Breakout Session 4b: Experiences/Lessons-Learned in Applied Materials Development

QUESTION 1:

The application-driven approach aims to accelerate the material design/advanced materials manufacturing process. What are your experiences, good and bad, using computational/experimental tools (including 'high-throughput' methods) in application-specific materials development efforts?

Please provide quantitative metrics for success in terms of performance and development time, when appropriate.

Question 1: Experiences in Applied Materials Development (50 min)

Include on card: relevant sector ***1A, 1B, etc.***

Application/Material(s);
Toolset(s) and Expertise Employed ;
Resource Requirements;
Metrics on Performance/Development Time

(include name, affiliation, & AMM role, along with any elaborating details on back of card)

	Structural / Environmental Materials		Other	Functional Materials/ Interfaces	
	computational	*experimental*		*computational*	*experimental*
positive	1A	1B	1C	1D	1E
mixed	1F	1G	1H	1I	1J
less positive	1K	1L	1M	1N	1O

Breakout Session 4c: Gaps and Access Limitations in Current Tool Sets and Expert Resources

QUESTION 2:

What are the gaps and access-limited challenges in the advanced experimental tools (e.g. synthesis and characterization tools) or computational/ modeling tools (including high-throughput methods) that are available for solving application-specific materials development problems, and what additional development work, validation work, or integration/interoperability work, if any, would be most beneficial to accelerating the development process?

Question 2:
Gaps in Tools and Available Resources (50 min)

Include on card: relevant sector
2A, 2B, etc.

Application/Material(s);
Gaps in Toolset(s) and Expertise;
Resource Needs and Limitations;
Expected Improvements in Results;

(include name, affiliation, & AMM role, along with any elaborating details on back of card)

	Structural / Environmental Materials	Other	Functional Materials/ Interfaces
Computational tools and expertise: multi-scale, ICME, etc.	*2A*	*2B*	*2C*
Information and data (deficits & surplus): informatics tools and expertise	*2D*	*2E*	*2F*
Experimental tools and expertise: synthesis, characterization (including high-throughput, combinatorial, etc.)	*2G*	*2H*	*2I*

Breakout Session 4d: Existing Resources and Leveraging Opportunities

QUESTION 3:

What are the pros and cons of existing efforts at multiple U.S. institutions developing fundamental material data, property data, advanced materials computational tools, high throughput characterization methods, and deep knowledge about the relationships between composition, processing, structure, and properties and where are there gaps that may be addressed with the proposed DOE approach?

Question 3:
Existing Resources & Leveraging Opportunities (50 min)

Include on card: relevant sector ***3A, 3B, etc.***

Existing Resource Type/Scope/Sponsor
Toolset(s) and Expertise;
Accessibility & Bridging Opportunities

(include name, affiliation, & AMM role, along with any elaborating details on back of card)

	Structural / Environmental Materials	Other	Functional Materials/ Interfaces
Application-driven manufactured materials	*3A*	*3B*	*3C*
Cross-cutting; multi-scale, multi-physics	*3D*	*3E*	*3F*
Fundamental; atomic to molecular scale	*3G*	*3H*	*3I*

Breakout Session 4e: AMM Core Infrastructure and Leveraged Partnerships

QUESTION 4:

What core infrastructure components and specific relevant capabilities/tools would be required for a central facility or institute to support an AMM-based approach to various materials challenges versus distributed model leveraging or expanding on existing capabilities; and what is the availability and ease of access of advanced computing/experimental tools from specific institutions relevant to application-driven problem? What AMM framework (potentially including central core capabilities and expertise, leveraged partner resources, and coordinated linkages with MGI and other materials R&D efforts) would be best suited to build a versatile and expandable R&D community in accelerated materials development for clean energy applications, uniting, curating, and coordinating resources in a way that preserves intellectual property and maximizes the benefits for U.S. industrial competitiveness?

Question 4:
Core Infrastructure and Leveraged Partnerships (60 min)

Include on card: relevant sector
4A, 4B, etc.

Capability Type with Toolset(s) and Expertise;
Proposed Entity with Resource Requirements;
Expected Inputs-to and Outputs-from AMM;
Accessibility & Bridging Opportunities

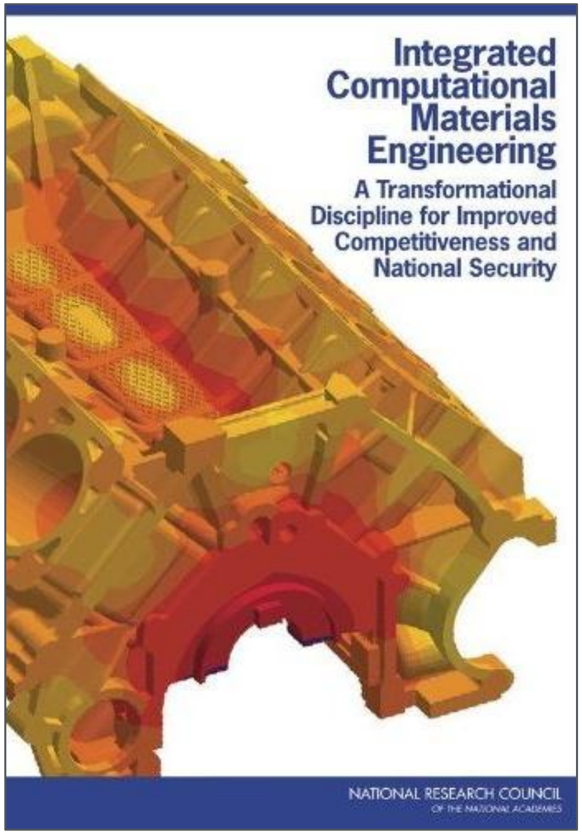
(include name, affiliation, & AMM role, along with any elaborating details on back of card)

PARTNERS: Toolset Developers and Integrators ***4A***	**CORE:** Management Tools & Expertise (including scientific, manufacturing, intellectual property, etc.) ***4B***		**PARTNERS: Clean Energy Application Developers and Manufacturers** ***4C***
	CORE: Computational and Modeling Tools & Expertise (including high-throughput) ***4D***	**CORE:** Experimental Tools & Expertise (including combinatorial and high-throughput methods) ***4E***	
	CORE: Materials Expertise in Clean Energy Materials Classes ***4F***		
	CORE: Data and Informatics Tools & Expertise ***4G***		

Bridges to External Resources: Broader MGI and Other Materials R&D Efforts
4H

BACKUP

Integrated Computational Materials Engineering (ICME) Materials Genome Initiative (MGI)



ICME: A growing discipline in materials science and engineering

Replace and/or augment conventional experimental techniques with computational and high throughput techniques to generate material properties used for engineering analysis

MGI: A White House Office of Science and Technology Policy (OSTP) Initiative

Advance and integrate experimental tools, computational tools, and data to reduce the time from discovery to deployment for new materials

The Materials Genome Initiative (MGI)

Integrating experimentation, modeling, and theory

- Developing new models
- Implementing models to develop new tools
- Integrating tools to develop new frameworks

Building the foundation for a materials data infrastructure

- Developing best practices and standards for materials data
- Enabling and supporting data infrastructure

Driving a fundamental shift in materials research culture

- Emphasizing cross-discipline, cross-agency, and industry-academic research
- Promoting data sharing, distribution, and citation

Equipping the next-generation materials workforce

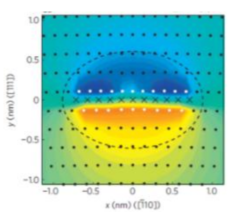
- Connecting early-career researchers with industry
- Developing curricular and training programs
- Establishing co-op/intern/detail opportunities

Integrated Computational Materials Engineering (ICME)

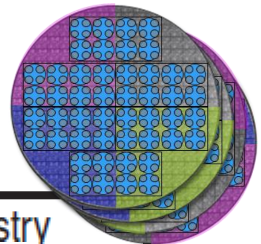
Start

"We want to reduce weight of a shock tower by 15% using Mg alloys while costing no more than $18.50 to produce and integrate into the vehicle"

Atomic Scale Models

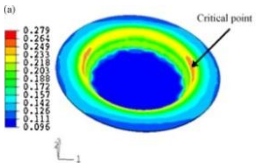


Material Property Measurements



Bulk Measurement

Macro-scale Models

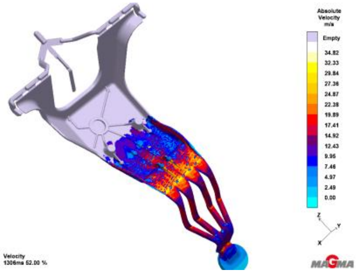


J. Allison, *JOM*, ***63***, *15-18, 2011.*

Chemistry
Thermodynamics
Diffusion

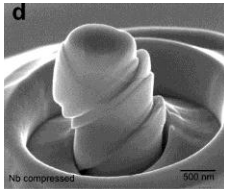
Manufacturing Process Simulation — Quantitative Processing-Structure Relationships — Quantitative Structure-Property Relationships — Constitutive Models — Engineering Product Performance Analysis

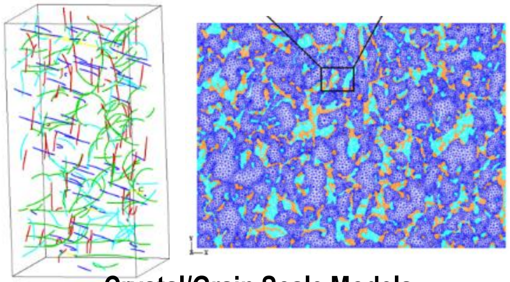
- Process & product optimization
- Innovation



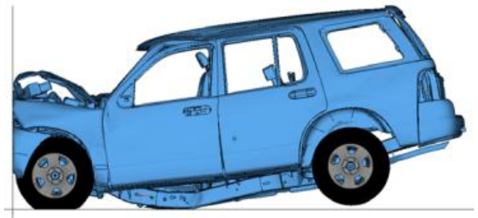
Manufacturing Process Models

Fine-scale Measurement



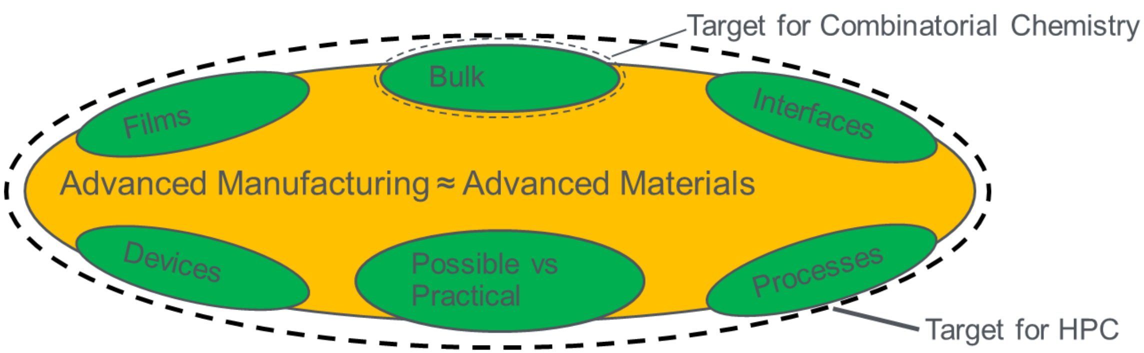


Crystal/Grain Scale Models

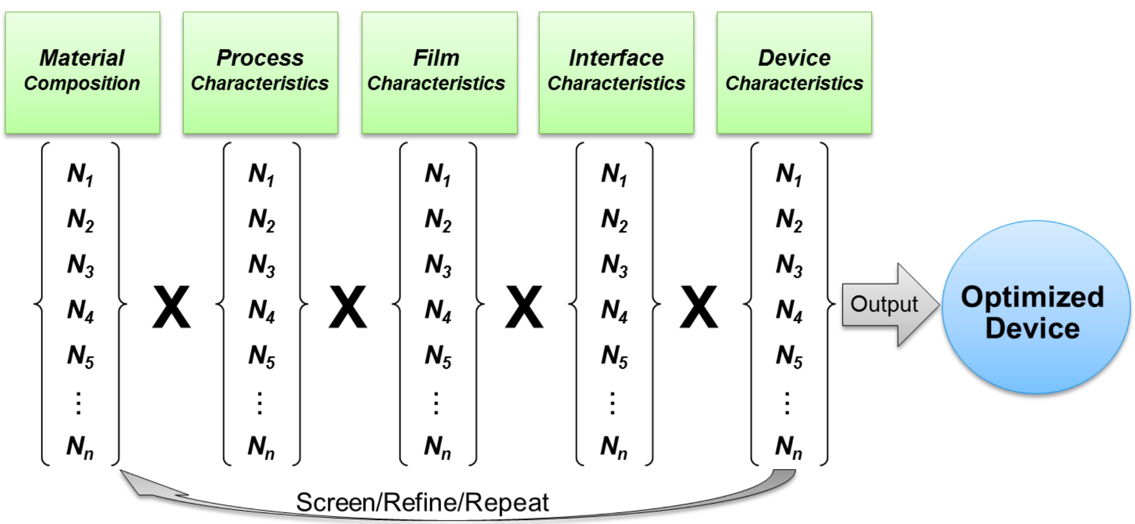


System Level Model

Combinatorial Chemistry with High-Throughput Screening



- Advanced manufacturing and materials are a <u>very complex</u> phase space
- Combinatorial chemistry revolutionized industries with complex materials challenges (e.g. drug discovery and catalysts)
- Extensions of the approach could do the same for advanced manufacturing



- Combinatorial strategies can be applied to <u>multi-dimensional</u> systems
- Appropriate for the complexity of advanced materials/device/ manufacturing
- Can impact and accelerate multiple advanced materials programs

INTERMOLECULAR
FAST FORWARD THINKING