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

FCTO Projects and the Materials Genome Initiative

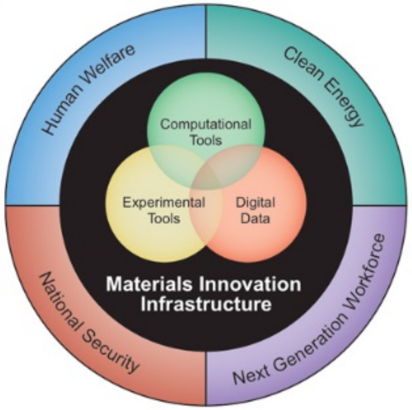
2 December 2014

Eric L. Miller, FCTO

with guest speakers from several exciting H_2 and fuel cells materials RD&D projects

Webinar Outline

- The Materials Genome Initiative (MGI)
- MGI for Clean Energy Applications and Industries
- MGI Methods and Tools Being Used in Current Hydrogen and Fuel Cell Technologies Research
  - *Catalyst materials for fuel cells and electrolyzers*
  - *Materials for solar water splitting technologies*
  - *Hydrogen handling materials*
  - *Hydrogen storage materials*



- Opportunities for Improved RD&D Coordination among Hydrogen and Fuel Cell Technologies with Other Clean Energy Technologies under an MGI Innovation Ecosystem

Materials Genome Initiative (MGI)

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http://www.whitehouse.gov/mgi

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Home • About the Materials Genome Initiative

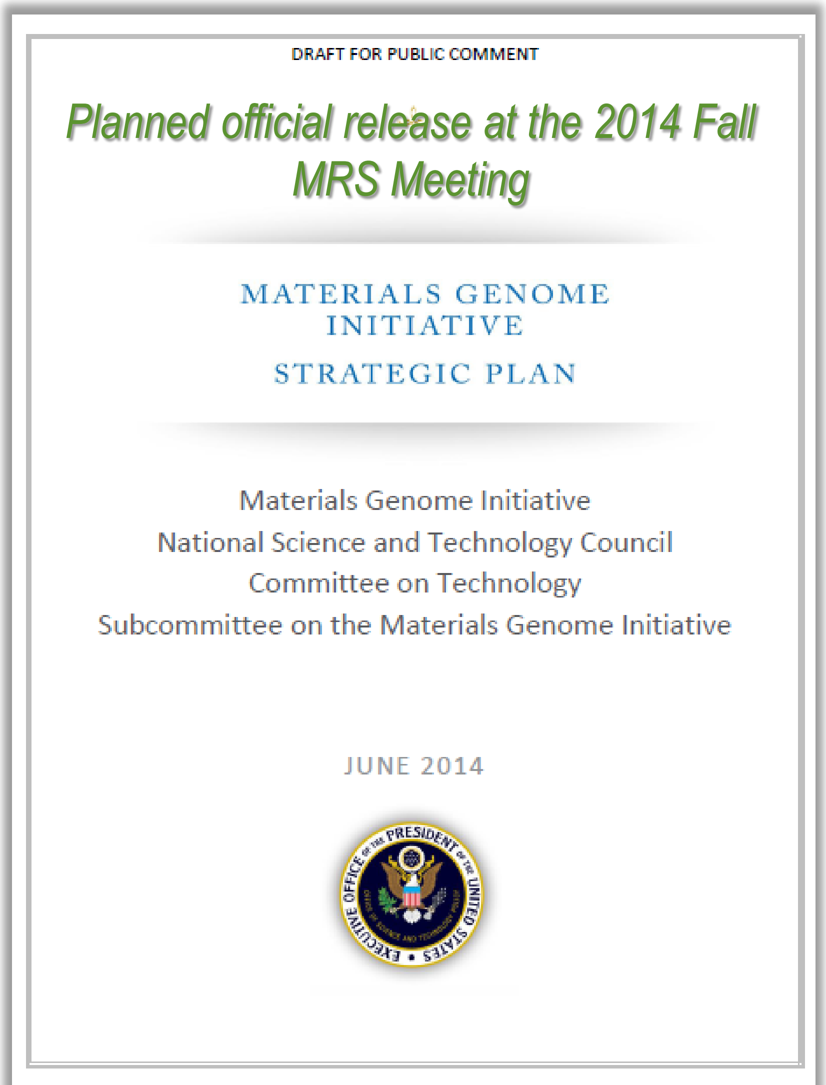
Materials Genome Initiative

About | Goals | Examples | News & Announcements | Federal Programs | External Stakeholder Activities | Contact Us

> "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

***Presidential Initiative* promoting materials innovations in the marketplace**

The MGI Mission


DRAFT FOR PUBLIC COMMENT

Planned official release at the 2014 Fall MRS Meeting

MATERIALS GENOME INITIATIVE

STRATEGIC PLAN

Materials Genome Initiative
National Science and Technology Council
Committee on Technology
Subcommittee on the Materials Genome Initiative

JUNE 2014

The MGI Vision:

"Advanced materials are essential to economic security and human well-being and have applications in multiple industries, including those aimed at addressing challenges in clean energy, national security, and human welfare. To meet these challenges, the Materials Genome Initiative will enable discovery, development, manufacturing, and deployment of advanced materials at least twice as fast as possible today, at a fraction of the cost."

Targeting a 2x acceleration of the materials-to-market process

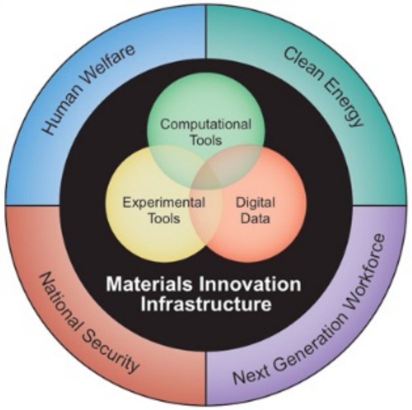
Four Key MGI Challenges*

(1) **Leading a culture shift in materials research** to encourage and facilitate an integrated team approach that links computation, data, and experiment and crosses boundaries from academia to industry;

(2) **Integrating experiment, computation, and theory** and equipping the materials community with the advanced tools and techniques to work across materials classes from research to industrial application;

(3) **Making digital data accessible** including combining data from experiment and computation into a searchable materials data infrastructure and encouraging researchers to make their data available to others;

(4) **Creating a world-class materials workforce** that is trained for careers in academia or industry, including high-tech manufacturing jobs.



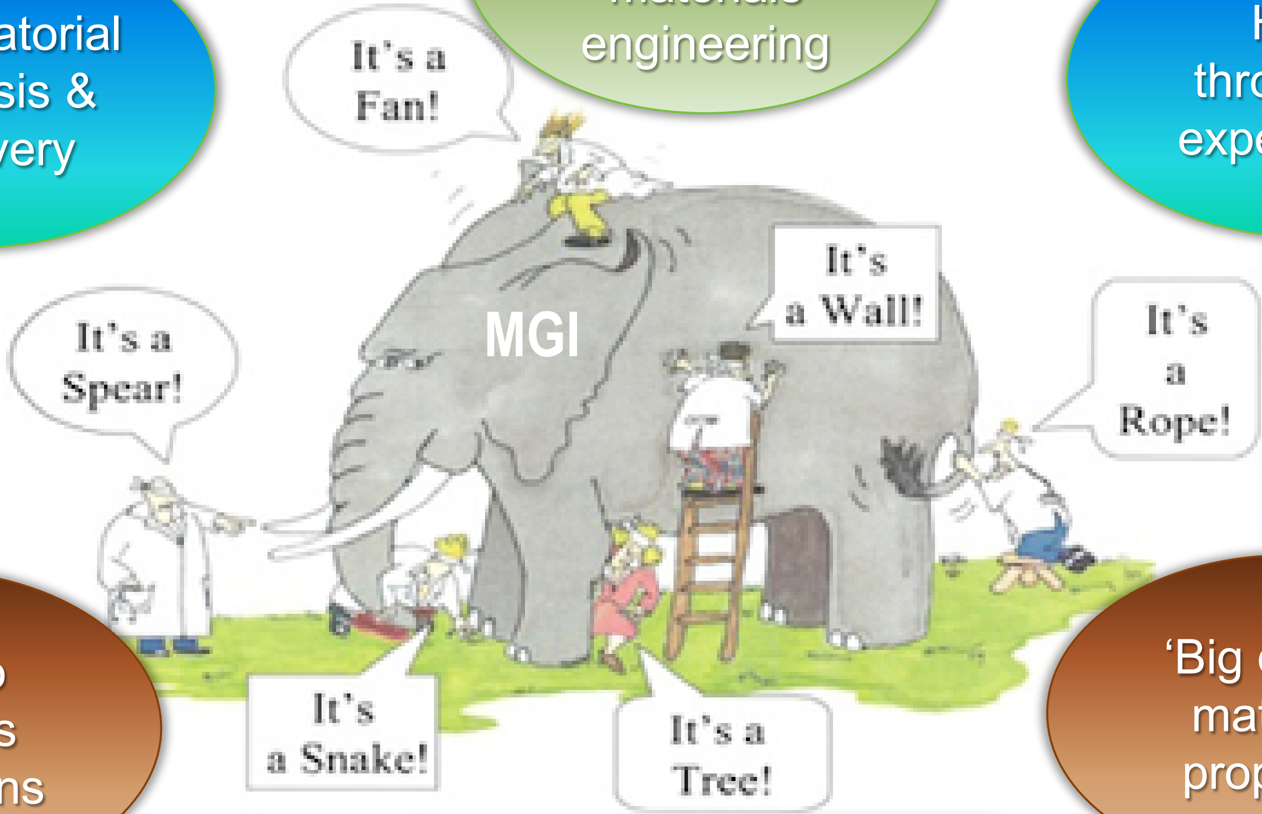
from the MGI Strategic plan

Different Perceptions of MGI

Combinatorial synthesis & discovery

Integrated computational materials engineering

High-throughput experiments



Ab-initio materials calculations

'Big data' of materials properties

MGI represents a multi-facetted "Innovation Ecosystem"

"Push" vs "Pull" in MGI Ecosystem

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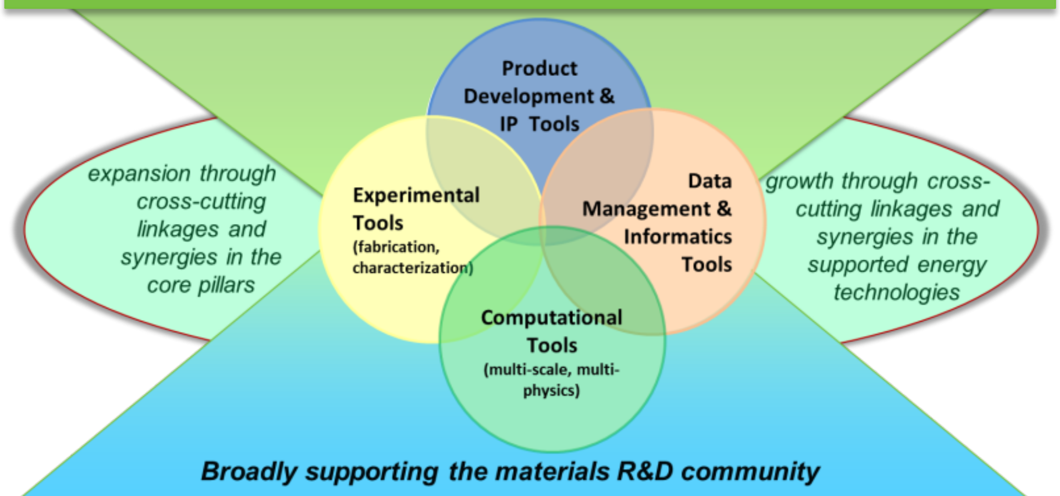
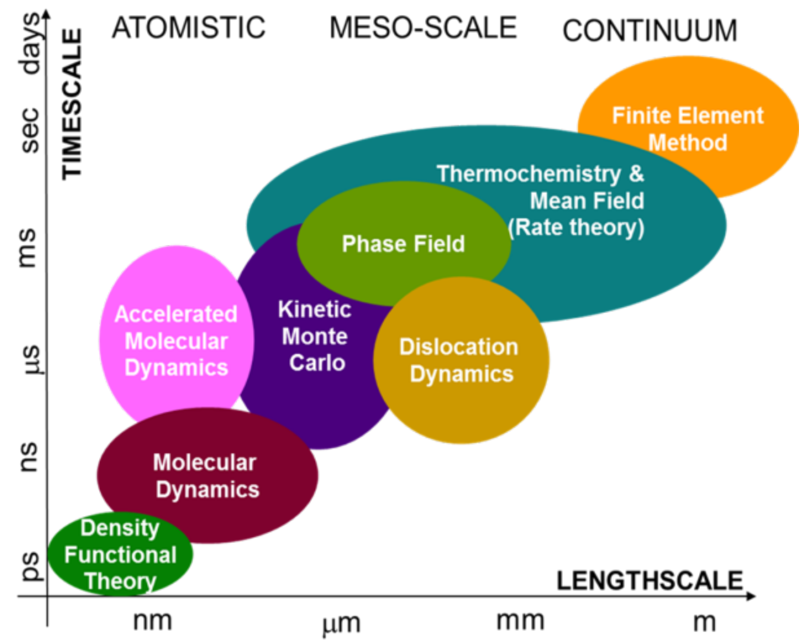
PRODUCTS by design, typically focuses on the 'high end' of the time and length scales in accelerated materials-to-market development

End-Use-Specific Industry Pull in a Techno-Economic Framework

leveraging cross-cutting synergies to accelerate materials qualification



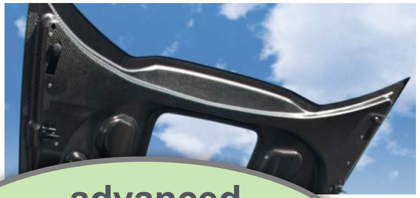


Scientific PUSH of MGI's computation, experimental & data tools

Multi-physics/multi-scale scientific methodologies continue to expand, including much-needed bridges between the scales

More industry "pull" needed in this big materials-to-market challenge

Clean Energy Materials Challenges



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

alternative fuels
advanced combustion, bio/synthetic fuels…

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

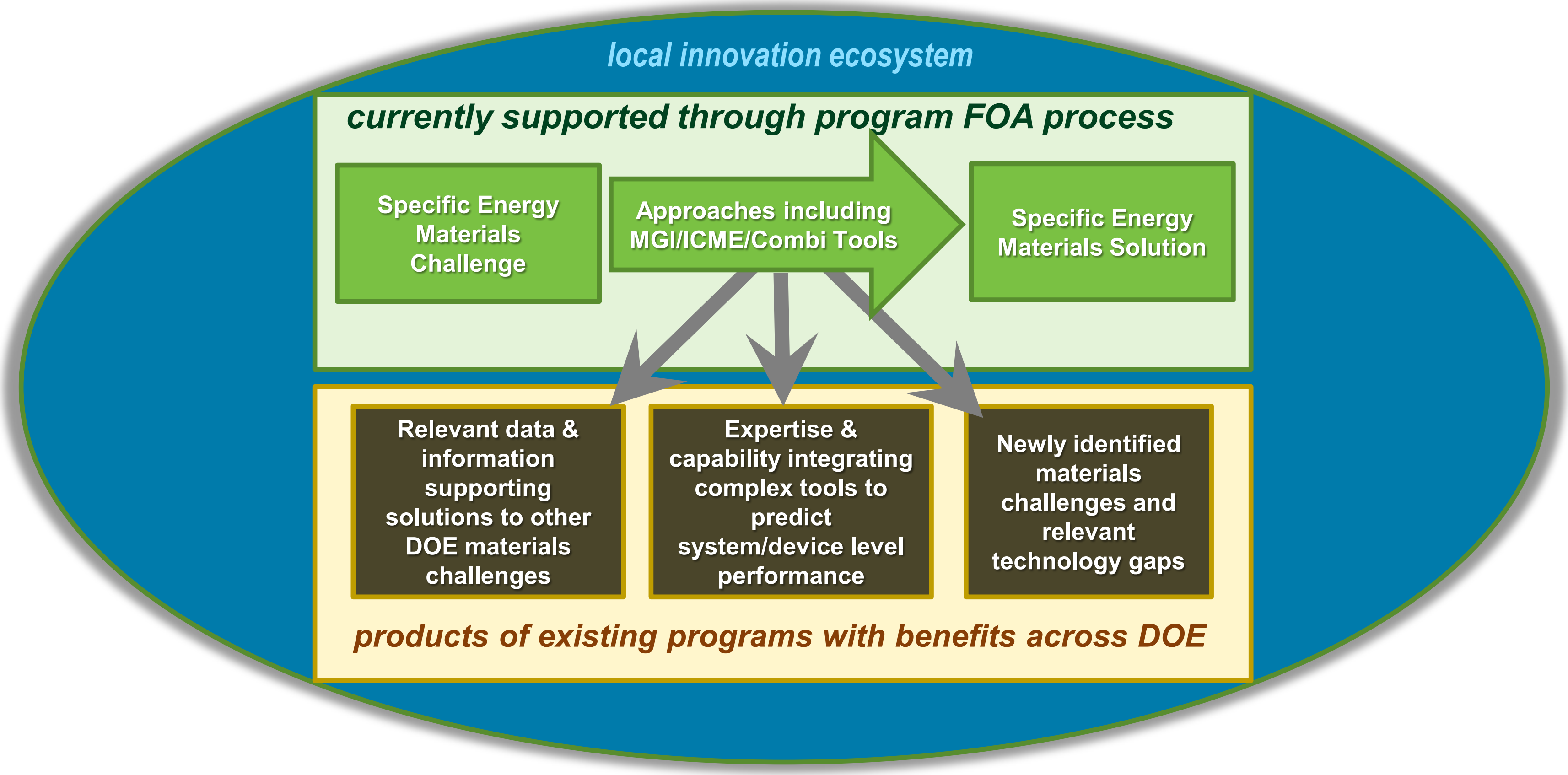
Electronic Materials

Chemical Materials

Numerous materials classes are vital to “Clean Energy Technologies”

Coordinated MGI RD&D at DOE Offers:

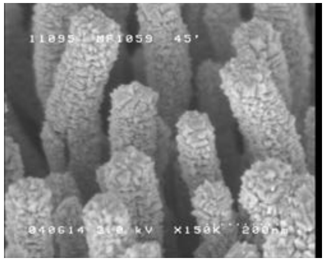
- Computational/Experimental/Big Data Synergies
- Cross-Cutting Technology Impact
- Significant Cost Savings in Shared Resources

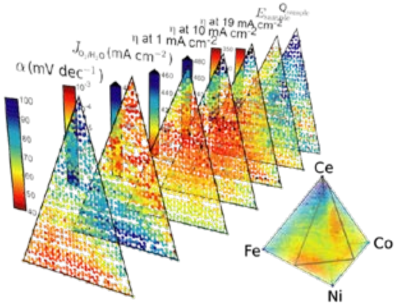


… better leveraging of DOE's current materials development work

Early MGI Adoption in H_2 & Fuel Cells

Showcase of Projects in Fuel Cell and Hydrogen Production, Delivery & Storage





- **Advanced Cathode Catalysts for PEM Fuel Cells**
  PI: M. K. Debe (3M Co., retired); Dalhousie U.,ANL,JPL
- **High-Throughput Synthesis & Testing of non-PGM PEMFC cathode catalysts and PGM cathodes**
  PI: Debbie Myers (ANL), ORNL, and LANL
- **JCAP High Throughput Experimentation**
  PI: J.M. Gregoire, Caltech; J. Jin, J.B. Neaton and K.A. Persson, LBNL
- **New Metal Oxides for Efficient Hydrogen Production via Solar Water Splitting**
  PI: Y. Yan, The University of Toledo
- **Surface Validation: III-V Materials for Photoelectrolysis**
  PI: T. Deutsch (NREL), C. Heske (UNLV), T. Ogitsu (LLNL)
- **High Efficiency Solar Thermochemical Reactor for Hydrogen Production**
  PI: A.H. McDaniel (SNL), ASU, Bucknell, DLR, CSM, Northwestern, & Stanford
- **Materials for Solar Thermochemical Water Splitting**
  PI: C. Musgrave, A. Weimer, C. L. Muhich, K. Weston, Brian Ehrhart (CU Boulder)
- **Hydrogen Compatible Materials**
  PI: B. Somerday (SNL), C. San Marchi (SNL), I2CNER (U. Illinois, Kyushu U.)
- **Innovative Development, Selection & Testing to Reduce Cost & Weight of Materials for BOP Components**
  PI: Jonathan Zimmerman and SNL, Carpenter Technology Corporation
- **Improving the Kinetics & Thermodynamics of $Mg(BH_4)_2$ for H_2 Storage**
  PI: Brandon Wood (LLNL), with SNL &University of Michigan

MGI methods already support the DOE Fuel Cell Technologies Office mission

Template for Showcased Project Summaries

Technical Objective and Relevance to Fuel Cell Technologies Office Goals

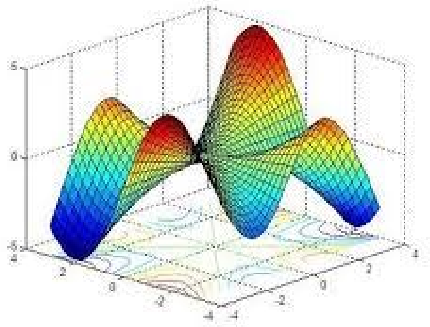
- …..
- …..

(include specific challenges being addressed in functional materials/interfaces)

Project Technical Approach & Example Results

- …..
- …..

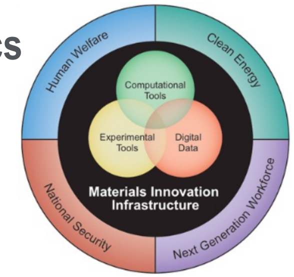
(include specific successes and limiting factors encountered in the approach to date)



MGI Elements Incorporated: theory, computational, experimental, informatics -including high-throughput & combinatorial techniques

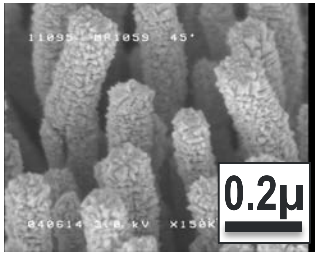
- …..
- …..

(include successes, challenges and recommended improvements)



Technical Objective and Relevance to FCTO Goals

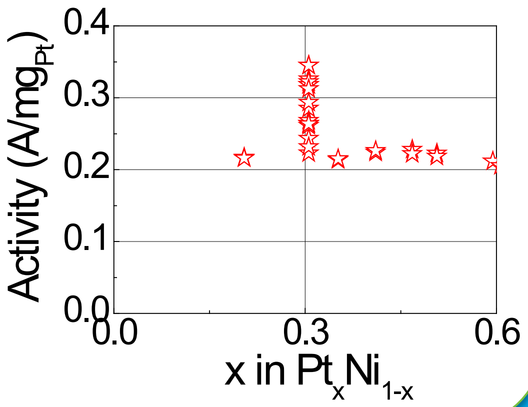
- Development of high activity, durable, and lower cost ORR cathode electrocatalysts amenable to high volume manufacturing.
- Durability, cost are key factors for PEMFC commercialization.



3M NSTF

Project Technical Approach & Example Results

- Using combinatorial catalyst fabrication (PVD) and high-throughput screening, rapidly evaluate wide ranges of catalyst fabrication variables to determine property trends and identify improved ORR catalysts.
- *Example: Unexpected activity spike at $Pt_{30}Ni_{70}$.*



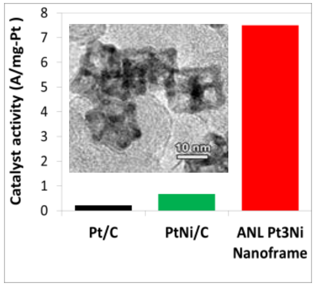
MGI Elements Incorporated

Experimental, Informatics (including high-throughput & combinatorial)

- PVD combinatorial catalyst fabrication is relatively straightforward.
- Primary challenge has been development of high-throughput characterization methods which accurately predict performance in end-use.

High-Throughput Synthesis & Testing of non-PGM PEMFC Cathode Catalysts and PGM Cathodes *PI: D. Myers (ANL), ORNL, and LANL*

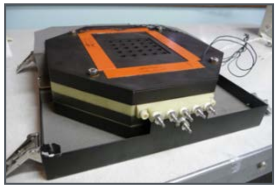
Technical Objective and Relevance to FCTO Goals



- Translate the activity benefits of advanced Pt-based PEMFC cathode electrocatalysts into the maximum increase in fuel cell performance, which will decrease PEMFC cost while increasing efficiency and durability
- Accelerate the development of high activity and stable non-PGM cathode catalysts for PEMFCs, eliminating the need for Pt and greatly reducing PEMFC system cost

Project Technical Approach & Example Results

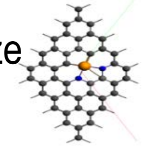
Twenty-five electrode fuel cell test fixture for combinatorial testing of fuel cell cathode performance

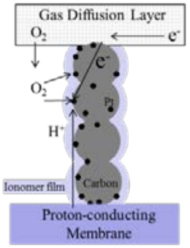


- Develop and utilize methods for rapid throughput fabrication, *ex situ* structural and property characterization, and combinatorial testing of cathode catalyst layers
- Develop and utilize equipment and methods for the high-throughput synthesis and oxygen reduction reaction (ORR) activity testing of non-PGM catalysts

MGI Elements Incorporated:

- Density functional theory (DFT) screening of the interaction of active site structures with reactants/products
- High-throughput fabrication and combinatorial testing of cathode catalyst layers to maximize reactant (O_2 and H^+) transport to catalyst sites
- High-throughput synthesis and activity/durability screening of non-PGM electrocatalysts

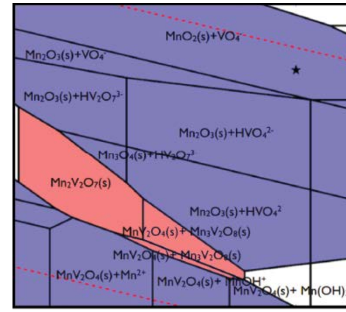


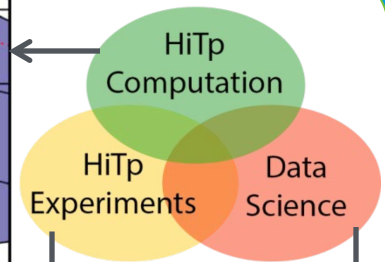


PI: J.M. Gregoire, Caltech; J. Jin, J.B. Neaton and K.A. Persson, LBNL

Technical Objective and Relevance to FCTO Goals

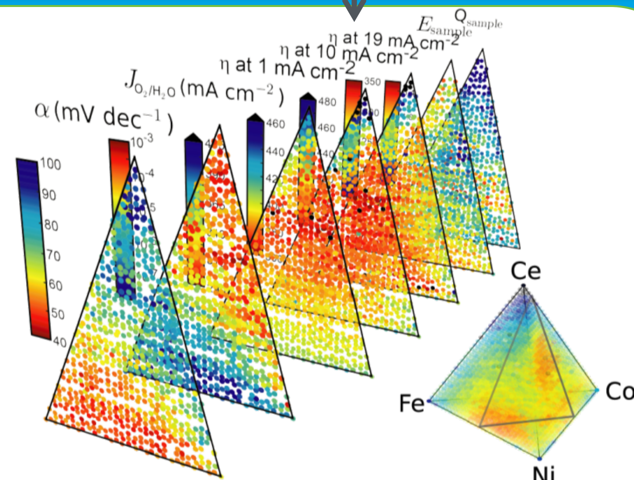
- Discover electrocatalysts, light absorbers and interfaces to advance solar fuels technology
- Identify non-precious functional materials. The electrochemical conditions are relevant to fuel cells.





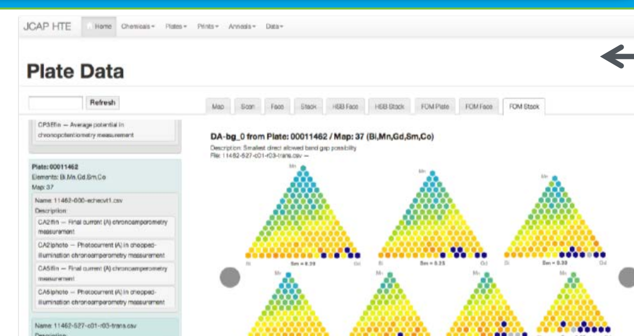
Project Technical Approach & Example Results

- Theory-guided HiTp evaluation of material libraries synthesized using scalable manufacturing techniques
- High throughput experiments with requisite data quality to enable robust data informatics
- Recent discoveries include new classes of electrocatalysts and illuminating data relationships



MGI Elements Incorporated

- Advancement of high throughput experimental and computational methods, and their mutual integration
- Data analytics and access via custom user interface
- Development of composition-property informatics



Technical Objective and Relevance to FCTO Goals

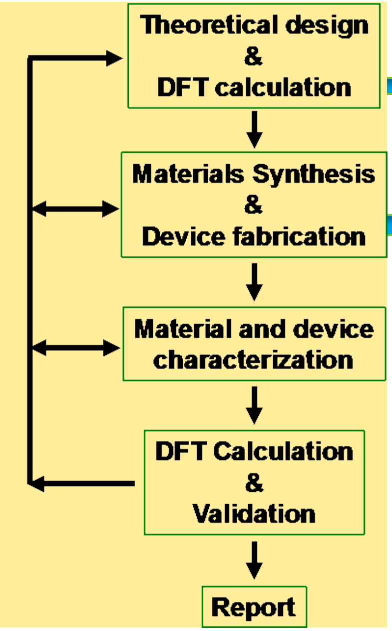
- Fundamental principles will be developed and validated for designing novel multi-component metal oxides with physical, optical, chemical, and electronic properties optimized for PEC hydrogen production.
- Novel bulk and thin-film methods will be developed for synthesizing the targeted metal oxides to enable validation of the technologies in functioning PEC water splitting devices.
- The fundamental properties of the new oxides, junctions, interfaces, and devices and the stability of the new oxides will be characterized and understood to provide critical feedback to further validate the design criteria.
- Postdocs, graduate students, and undergraduate students will be trained to provide young scientists for future renewable energy research. K-12 outreach and industry communication will be carried out to promote public awareness and to make a broader impact.

Results not Available yet (initial project stage)

MGI Elements Incorporated:

theory, computational, experimental, informatics

- Fundamental design principles and density-functional theory calculation.
- Targeted synthesis and experimental characterization and validation
- Iterative feedback loop: Theory design ➔ Synthesis ➔ Characterization ➔ Understanding ➔Theory re-design •••••

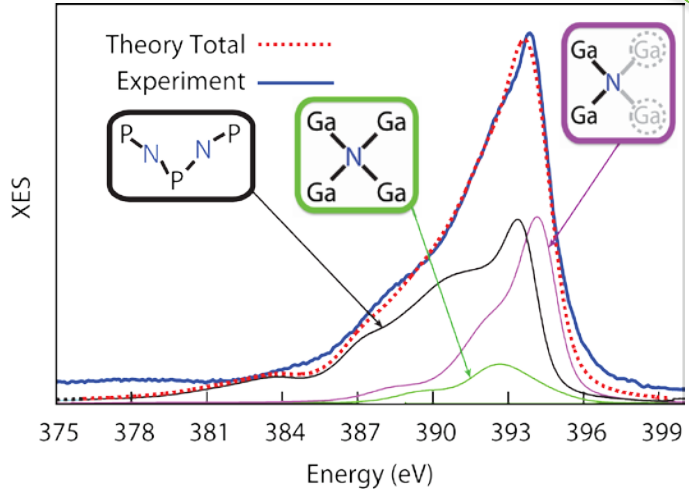


Understanding Semiconductor Photocorrosion for Economical Solar H_2

- Achieving renewable hydrogen economically produced by photoelectrolysis requires stabilizing semiconductor/electrolyte interface for long durations under harsh conditions
- Use advanced *spectroscopy* and *theory* to identify corrosion initiation mechanism and design processes to modify the surface in order to mitigate it

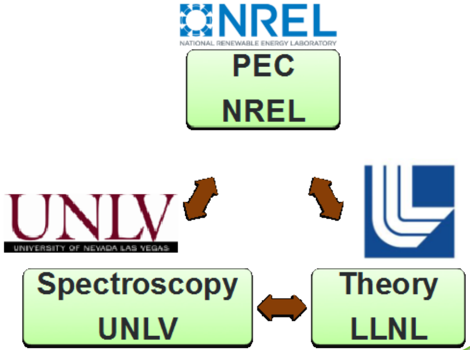
Correlate Spectroscopy with Theory on Nitrided p-$GaInP_2$ System: Establish Base for Predictive Capabilities

- Based on observation that nitridation led to stabilized $GaInP_2$ surface: Model the *local* nitrogen environment to understand measured spectra
- Theoretical N_2^+ implanted $GaInP_2$ nitrogen K-edge XES spectrum by LLNL constructed from various types of nitrogen impurity states as well as the experimental XES measured by UNLV group at LBNL synchrotron



MGI Elements Incorporated: theory, modeling, experimental

- ✓ Encourage and enable integrated R&D
- ✓ Enable creation of accurate, reliable simulations
- ✓ Support creation of accessible materials data repository (sharepoint)
- ✓ Provide opportunities for integrated research experiences



Solar Thermochemical Reactor for Efficient H_2 Production

PI: A.H. McDaniel (SNL), ASU, Bucknell, DLR, CSM, Stanford and Northwestern

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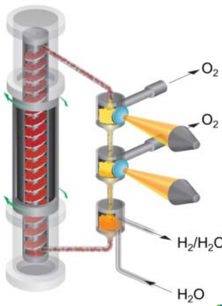
Technical Objective and Relevance to FCTO Goals

- Demonstrate that solar-driven thermochemical water-splitting can meet FCTO targets for H_2 production cost (\$2/gge) and process efficiency (26%).
- Design redox materials/chemistries with tailored thermodynamic properties.
  - $325<\Delta H^o(\delta)< 425$ kJ/mol O, $150<\Delta S^o(\delta)< 300$ kJ/mol O $MO_x \rightarrow MO_{x-\delta} + \delta/2\ O_2$

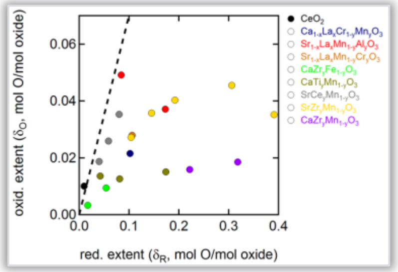


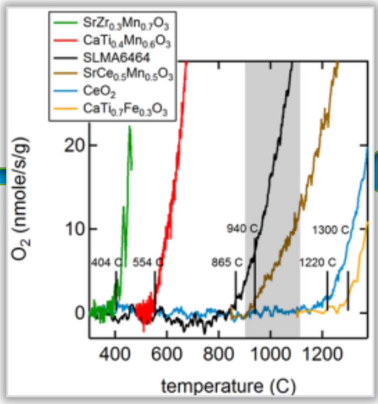
Project Technical Approach (*past practice*)

- Low-throughput synthesis and screening guided by chemical intuition.
  - Search focused on known or suspected fast O-ion conductors
  - Introduced (Sr, Mn) doped $LaAlO_3$ perovskite **to solar fuels community**

A.H. McDaniel et al., *Energy Environ. Sci.*, 2013, **6**, 2424–2428

- Great breadth of possible perovskite formulations limit the approach.
- Search for stoichiometric redox chemistries even more challenging.





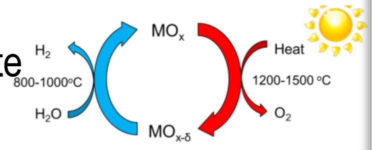
MGI Elements Incorporated (*future practice*)

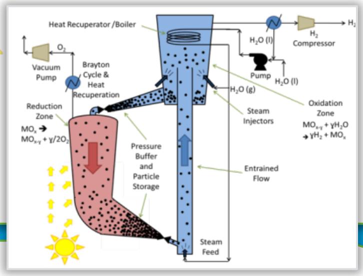
- HT DFT (Prof. Chris Wolverton @ Northwestern University, http://oqmd.org).
- Understand how simple substitutions effect thermochemistry.
  - Sr(Ce, Zr)MnO_3 radically changes redox behavior
- Is DFT+U valid for the complex oxides of interest, and can we formulate design rules?

PI: C. Musgrave (CU Boulder), A. Weimer, C. Muhich, K. Weston, B. Ehrhart

Technical Objective and Relevance to FCTO Goals

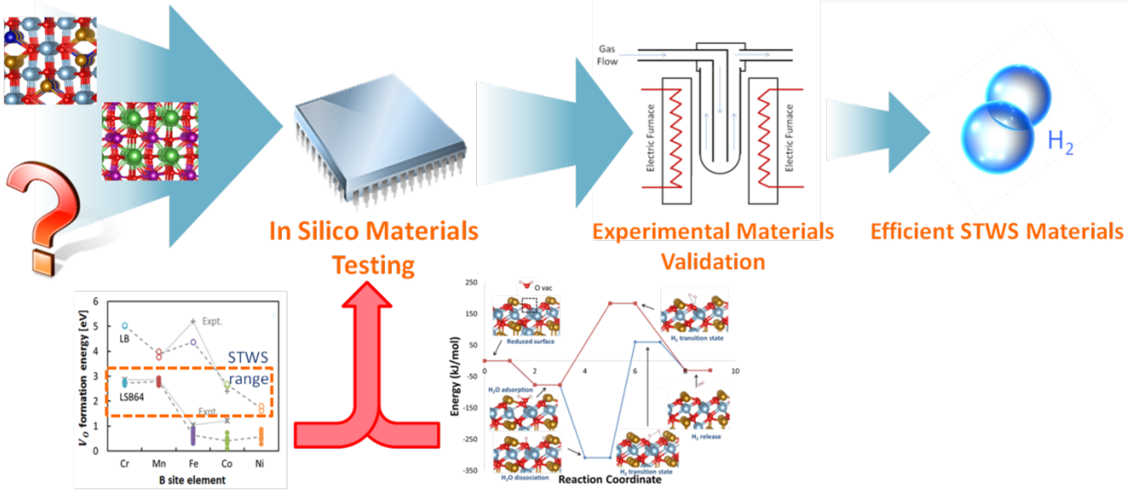
- Solar thermochemical particle flow reactors using novel hercynite materials that produce more H_2 over a wider temperature range & at lower temperature than conventional ferrite cycles





Project Technical Approach

- Computational prototyping of hercynite & related materials integrating theory and experimentation
- Using both thermodynamic and kinetic filters in optimization of materials for quasi-isothermal solar water splitting



Thermodynamic Filters

Kinetic Filters

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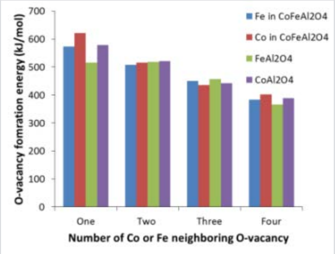
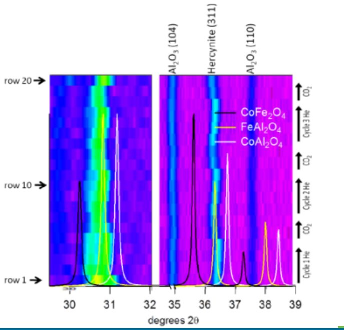
- Density functional theory and experimental:
  $FeAl_2O_4 \geq Co_{0.5}Fe_{0.5}Al_2O_4 > CoAl_2O_4$
- General thermodynamics predict O-vacancy mechanism
- HTXRD and EDS analysis experimentally corroborate O-vacancy mechanism

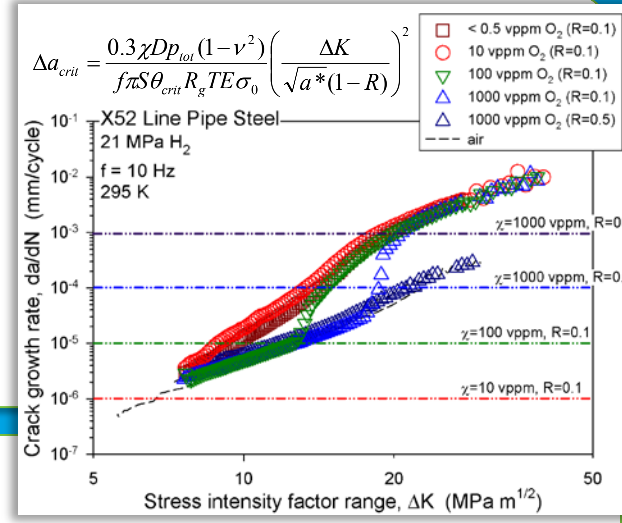




PI: B. Somerday (SNL), C. San Marchi (SNL), I2CNER (U. Illinois, Kyushu U.)

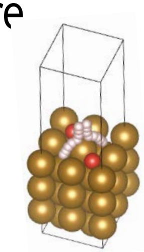
Technical Objectives and Relevance to FCTO Goals

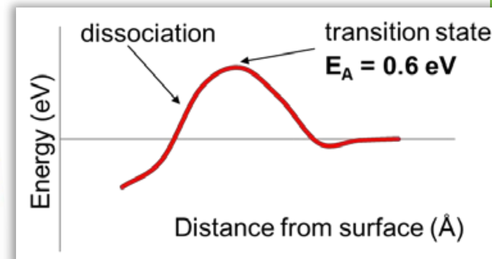
- Objectives: enhance materials testing efficiency, establish interactive materials database, enable materials selection, develop predictive models of H_2-assisted crack growth
- Support FCTO goals to facilitate deployment of safe and cost-effective components for H_2 delivery and storage



Project Technical Approach & Example Results

- Approach: perform specialized materials testing in high-pressure H_2, apply results in concert with modeling to interpret mechanisms and governing variables
- Example: coupled experiments and modeling revealed mechanism for trace O_2 inhibition of H_2-accelerated cracking





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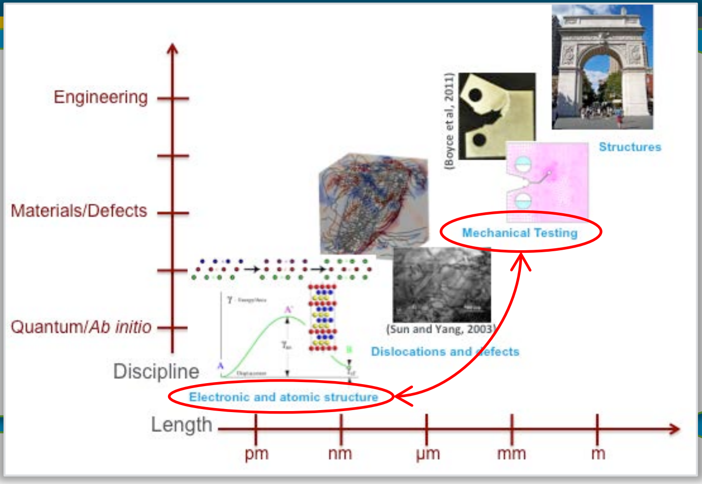
- Successes: integrated experiments and modeling, evolving database for mechanical properties of materials in H_2 gas
- Challenges: applying advanced tools to identify basic H_2-induced damage mechanisms

Innovative development, selection & testing to reduce cost & weight of materials for BOP components

J. Zimmerman (SNL) and Carpenter Technology Corporation



Technical Objective and Relevance to FCTO Goals

- Develop computational approaches to identify or develop low cost (i.e. low nickel), high performance (i.e. hydrogen embrittlement [HE] resistant) austenitic stainless steels used in BOP components.
- Accelerate materials discovery & development through an atomic-scale understanding of physical properties and their correlation with, and connection to macroscopic mechanical performance.

Project Technical Approach

- Use density functional theory (DFT) to provide reliable estimates of stacking fault energy (SFE) and other atomic-level properties for austenitic stainless steels.
- Evaluate the correlation between SFE and metrics of hydrogen embrittlement (*e.g*. ductility, fatigue life).
- If correlation is verified, use optimization approaches to efficiently explore alloy composition space to identify low nickel content, high SFE materials.
- If correlation is not verified, identify alternative atomic-scale properties that can be tied to macroscopic performance.

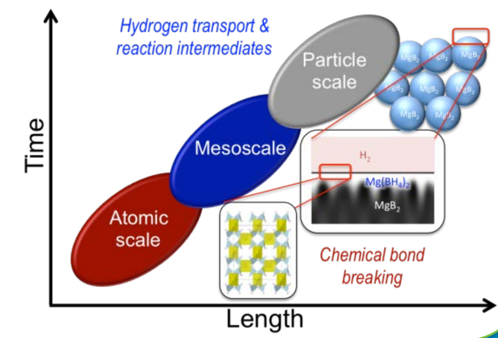
MGI Elements Incorporated

- Materials discovery through 'first principles' calculations (*guided* high-throughput computing)
- Integration of Experiment, Computation and Theory through…
    - Correlation between calculated atomic properties and experimentally quantified performance metrics
    - Quantification of property and performance variations between commercial alloys and "model" materials
    - Use of both sophisticated algorithms and experimental findings to define compositional space being explored
- Development of data analytics to enhance the value of computational data

Improving the Kinetics & Thermodynamics of $Mg(BH_4)_2$ for H_2 Storage *PI: B. Wood (LLNL), SNL &University of Michigan*

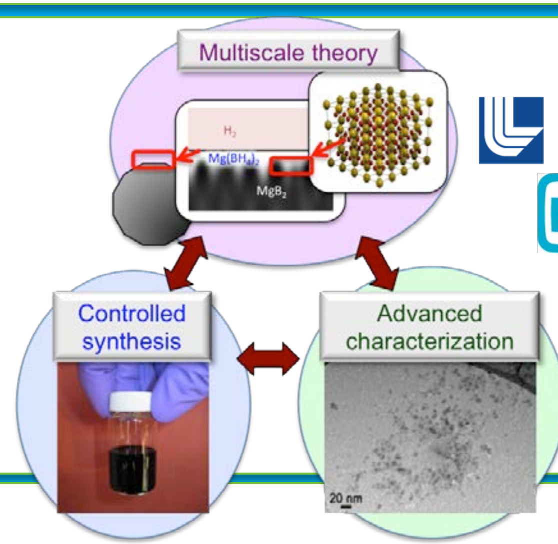
Technical Objective and Relevance to FCTO Goals

- Chemical hydrides such as $Mg(BH_4)_2$ are attractive candidates for compact, lightweight, and safe hydrogen storage tanks for fuel cell vehicles, but they absorb and release hydrogen **too slowly**
- To understand these limitations and develop a practical material that meets DOE targets, we use a combined **theory/synthesis/characterization** approach that integrates **multiple length/time scales**



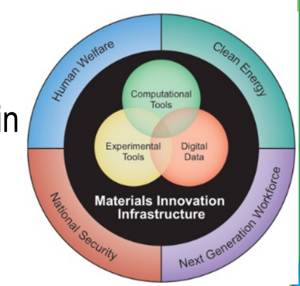
Project Technical Approach

- Focus on scalable, cost-effective optimization by reducing particle size or using metal additives, guided by close feedback between theory and experiment teams
- Multiscale modeling of diverse chemical processes during hydrogen uptake and release in $Mg(BH_4)_2$ nanoparticles using state-of-the-art supercomputing facilities at LLNL
- Novel synthesis & characterization approach for direct vallidation and verification of predictions using advanced experimental capabilities at Sandia



MGI Elements Incorporated

- Tightly integrated **theory-synthesis-characterization** effort is intended to **accelerate the feedback and development** cycle
- **Multiscale framework** integrates all relevant chemical and physical processes to mimic **actual operation** in a tank, and can be easily applied to any chemical hydride using calculated and/or measured parameters from a **materials database**
- Addresses challenges of **"real" materials** beyond ideal theoretical descriptions to evaluate suitability for **industrial** use



Industry Successes with MGI

- High-throughput research has produced several revolutionary technologies and will play an important role in the MGI, ***connecting theoretical predictions to materials synthesis.***

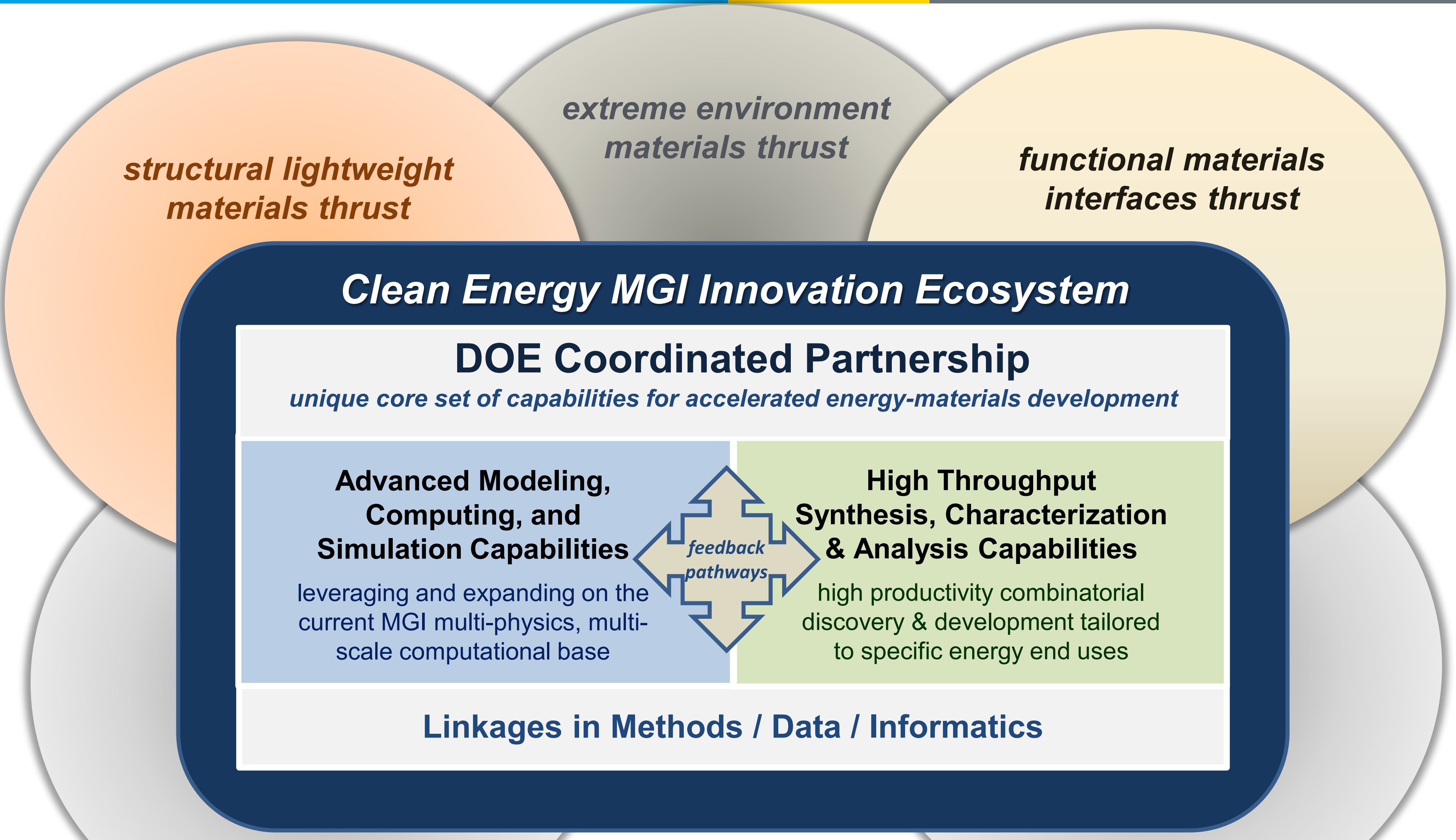
- There are several examples of High-throughput work producing radically new materials, one is in the development of olefin block copolymers by the *Dow Chemical Company.* This well described work* produced materials predicted by theory, optimized production and led to the rapid commercialization of a class of ***new polymers that are now made at commercial scales.***

Hustad, Phillip D., Roger L. Kuhlman, Daniel J. Arriola, Edmund M. Carnahan, and Timothy T. Wenzel. "Continuous production of ethylene-based diblock copolymers using coordinative chain transfer polymerization." Macromolecules **40, no. 20 (2007): 7061-7064.*

Large companies have the resources to establish MGI-based innovation ecosystems in their RD&D- A government-supported collaborative approach including shared resources could broaden access

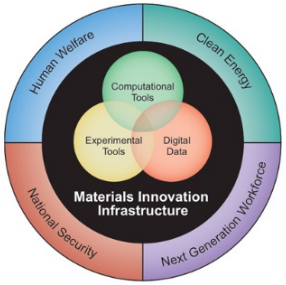
DOE Coordination Opportunity

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



Intelligent, focused materials RD&D in different clean energy technology thrusts, leveraging unique capabilities for fast-tracking materials to market, while expanding the tools & methods in the core

Coordinated MGI Activities Can…



- **Bridge *<u>INDUSTRY PULL</u>* with the *<u>SCIENTIFIC PUSH</u>***
  - **OSTP has embraced this as a vital component of MGI.**
- ***Build and maintain 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 required specialized skills, laboratory instruments, and computational power.**
- ***Develop 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. A coordinated MGI approach in clean energy would build and maintain shared resources, including customized experimental and computational tools, models, and hard-won data.**

Mahalo Nui Loa!

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http://energy.gov/eere/transportation/hydrogen-and-fuel-cells

Panel Discussion

- What are the main opportunities and challenges you see in broader adoption of MGI principles in the commercial development of your technologies?