



Critical Materials Institute

AN ENERGY INNOVATION HUB

Creating Technological Options for Assuring Material Supply Chains

Rod Eggert, Deputy Director

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CYTEC
Delivering Technology Beyond Our Customers' Imagination™



Eck Industries, Inc.
Specialists in Premium Aluminum Castings



Molycorp



SIMBOL materials



United Technologies Research Center



BROWN



COLORADO SCHOOL OF MINES
EARTH • ENERGY • ENVIRONMENT

UCDAVIS
UNIVERSITY OF CALIFORNIA

FIPR
Florida Industrial and Phosphate Research Institute

IOWA STATE UNIVERSITY

PURDUE UNIVERSITY

RUTGERS
THE STATE UNIVERSITY
OF NEW JERSEY



THE Ames Laboratory
Creating Materials & Energy Solutions
U.S. DEPARTMENT OF ENERGY



Lawrence Livermore National Laboratory



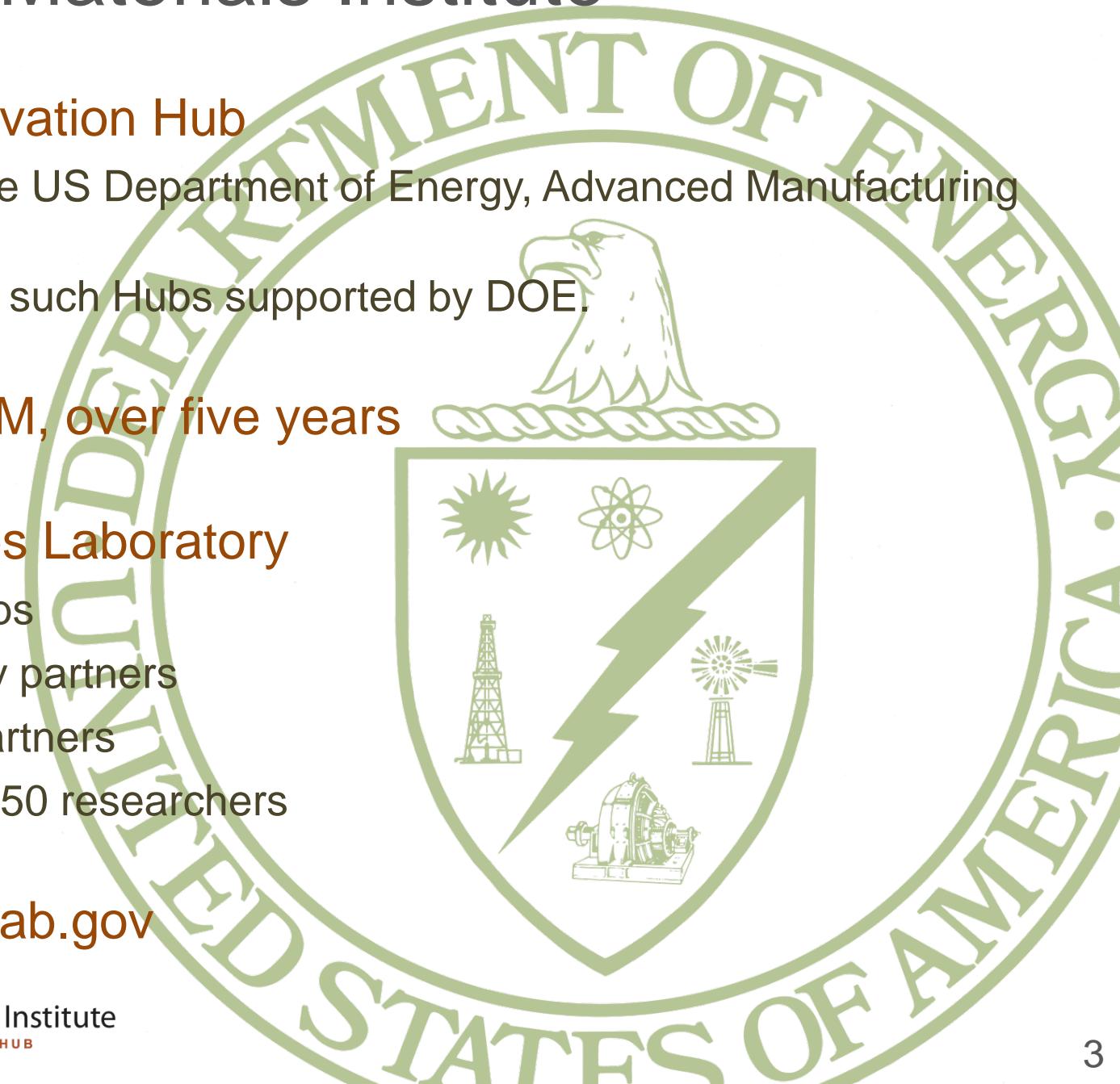
U.S. DEPARTMENT OF
ENERGY

Outline

- Overview
- Technical highlights
- Economic highlights
- Plans & final thoughts

The Critical Materials Institute

- An Energy Innovation Hub
 - Supported by the US Department of Energy, Advanced Manufacturing Office
 - One of only four such Hubs supported by DOE.
- Budget of \$120M, over five years
- Led by the Ames Laboratory
 - Four national labs
 - Seven university partners
 - Ten industrial partners
 - Approximately 350 researchers
- www.cmi.ameslab.gov



Mission

To assure supply chains
of materials critical to
clean energy technologies

- enabling innovation in U.S. manufacturing
- enhancing U.S. energy security

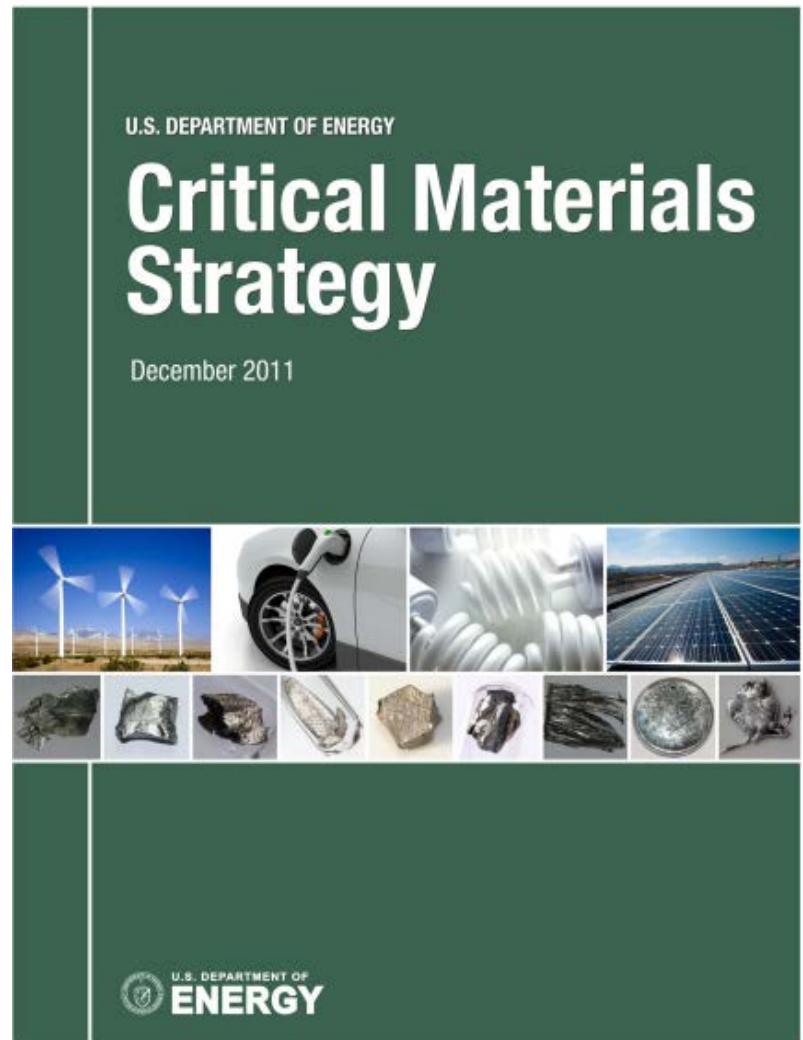




A three-pillared research strategy

Find ways to:

- diversify our sources
- provide alternatives to the existing materials
- make better use of the existing supplies through recycling and re-use



DOE

Industry Council
Iver Anderson (Ames)

Advisory Board
Gretchen Baier (Dow)

Operations

Cynthia Feller (Ames)

Finance

Carol Bergman (Ames)

Education & Outreach

Barry Martin (CSM)

Director

Alex King (Ames)

Deputy

Rod Eggert (CSM)

Commercialization

Deb Covey (Ames)

Technology Deployment

Iver Anderson (Ames)

Diversifying Supply

Bruce Moyer (ORNL), Lead
R. Scott Herbst (INL), Deputy

New Sources of Critical Materials

Transformational Processing

New Uses for Co-Products

Developing Substitutes

Tom Lograsso (Ames), Lead
Brian Sales (ORNL), Deputy

Strong Permanent Magnets with Reduced RE Content

Phosphors

Improving Reuse & Recycling

Eric Peterson (INL), Lead
Ed Jones (LLNL), Deputy

Source Preparation (Separation & Concentration)

Transformative Extraction & Materials Production

Crosscutting Research

Eric Schwengler (LLNL), Lead
Carol Handwerker (Purdue), Deputy

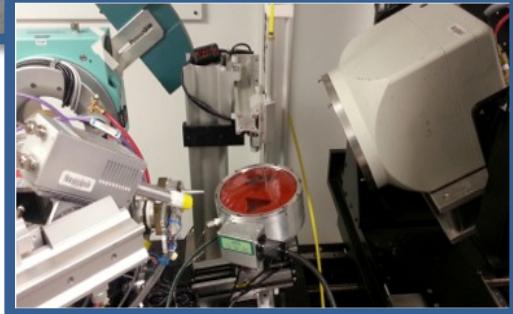
Enabling Science

Environmental Sustainability

Supply Chain & Economic Analysis

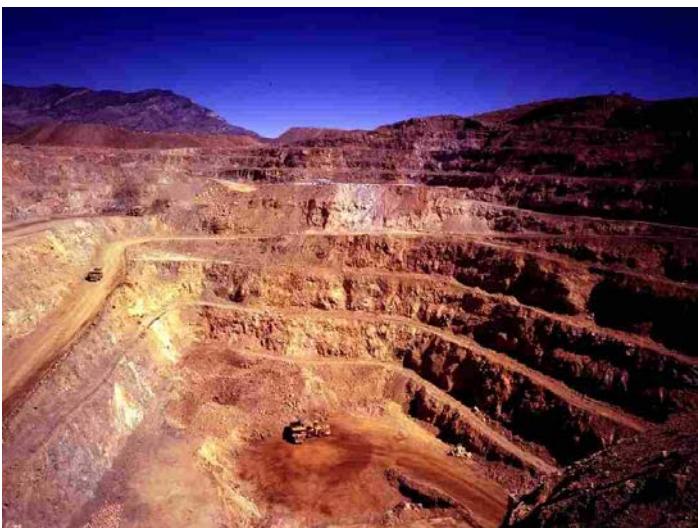
Salient facts

- Started operations on June 1, 2013
- 348 researchers & staff on payroll (80.9 FTEs)
- Several new facilities established
 - Improved criticality assessment capacity
 - Bulk combinatoric library production facility
 - Thin-film combinatoric library production facility
 - High-throughput analysis (with JCAP and JCESR)
 - Solvent exchange (SX) pilot scale test facility
 - Electrophoretic deposition capability
 - Filtration test facility
 - Toxicology test capability
 - Thermal analysis in high magnetic fields
 - Rapid magnetic property assessment
 - Rapid thermodynamic property assessment
 - Micro-x-ray fluorescence analysis capability
 - Adiabatic calorimeter.
 - Metal reduction capabilities
 - Robotic high-throughput catalyst development system
- Extensive industrial outreach
- 44 invention disclosures
- 13 patent applications

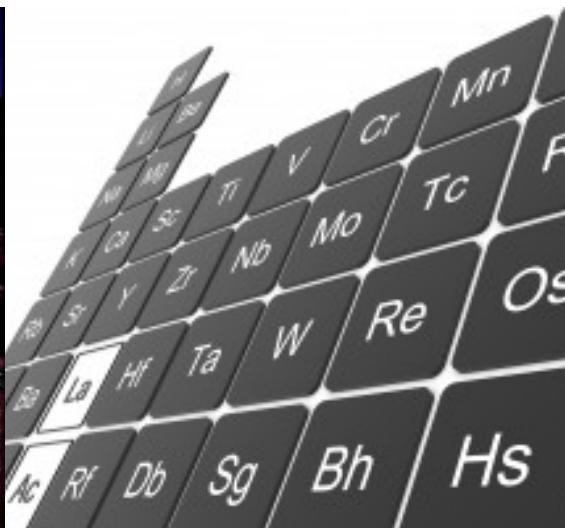


Five-Year Goals

Within its first five years, CMI will develop at least one technology, adopted by U.S. companies, in each of three areas:



Diversifying & expanding production



Developing substitutes



Reducing wastes



Invention Disclosures

1. Extraction of rare earth elements from phosphoric acid streams 
2. Recovery of neodymium from neodymium iron boride magnets
3. Membrane solvent extraction for rare earth separations  
4. Selective composite membranes for lithium extraction from geothermal brines
5. Methods of separating lithium-chloride from geothermal brine solutions
6. Extraction of rare earths from fly ash 
7. Recovery of Dy-enriched Fe alloy from magnet scrap alloy via selective separation of rare earth elements 
8. Aluminum nitride phosphors for fluorescent lighting 
9. Novel surface coatings to improve the functional properties of permanent magnets
10. Additive manufacturing of bonded permanent magnets using a novel polymer matrix

Invention Disclosures

11. Ceria-based catalyst for selective phenol hydrogenation under mild reaction conditions
12. Recycling and conversion of samarium cobalt magnet waste into useful magnet
13. Catalysts for styrene production
14. Task specific ionic liquids extractive metallurgy or rare earth minerals 
15. Separation of neodymium from praseodymium
16. High throughput cost effective rare earth magnets recycling system
17. Recycle of Fe Nd B Machine Swarf and Magnets 
18. Directly Printing Rare Earth Bonded Magnets
19. Procedure for Concentrating Rare-earth Elements in Neodymium Iron Boron-based Permanent Magnets for Efficient Recycling/Recovery
20. Enhancing Consumer Product Recycling via Rapid Fastener Eradication

Invention Disclosures

- 
21. Automated Printed Circuit Board Disassembly by Rapid Heating 
 22. Electrochemistry Enabled Recovery of Value Metals from Electronics
 23. Synthesis of High Surface Area Mesoporous Ceria
 24. Self-Assembly of Low Surface Colloidal Nanoparticles into High Surface Area Networks
 25. Selective Chemical Separation of Rare-Earth Oxalates (CSEREOX)
 26. Carbothermic Preparation of SmCo_x ($x=5$ to 8.5) Permanent Magnets Directly from Sm_2O_3
 27. A One Step Process for the Removal of Nickel/Nickel Copper Surface Coating from the $\text{Nd}_2\text{Fe}_{14}\text{B}$ (neo) Permanent Magnets
 28. Engineering Caulobacter Surface Protein for Rare Earth Element Absorption
 29. Chemical Separation of Terbium Oxide (SEPTER) 
 30. Novel Methods towards Selective Surface Modification of $\text{Nd}_2\text{Fe}_{14}\text{B}$ Magnets to Achieve High Performance Permanent Magnets

Invention Disclosures

- 
31. Mesoporous Carbon and Methods of Use
 32. Castable High-Temperature Ce-Modified Al Alloys 
 33. High Command Fidelity Electromagnetically Driven Calorimeter (High-CoFi EleDriCal) 
 34. 3D Printable Liquid Crystalline Elastomers with Tunable Shape Memory Behaviors and Bio-derived Renditions
 35. The Separation of Ancylite by Way of Magnetic Separation and Froth Flotation 
 36. Recovering Rare Earth Metals using Bismuth Extractant 
 37. Structural Optimization of Complex Materials using High-throughput Hierarchical Decomposition Methods
 38. Novel 3D Printing Method to Fabricate Bonded Magnets of Complex Shape
 39. Rare Earth Free High Performance Doped Magnet
 40. Acid-free Dissolution and Separation of Rare-earth Metal

Invention Disclosures

41. Materials designed for Structural Direct Write Additive Manufacturing of Molten Metals
42. A Process for the Recovery of Mercury and Rare Earth Elements from Used Fluorescent Lamps
43. Multi-functional Liquid Crystalline Networks : 3D Printable liquid crystalline elastomers with tunable shape memory behavior and bio-derived renditions 
44. High performance magnets with abundant rare earth elements

Industrial Engagement Programs

• Team Members

- Participate in CMI research projects
- Share in the research costs
- Participate in the IP management plan

• Associates

- Sponsor research using CMI's assets
- May wholly own the resulting IP, subject to DOE rules & regulations

• Affiliates

- Participate in CMI meetings and information streams
- Pay an annual membership fee
- Get an “early look” at CMI intellectual property



CMI Affiliates



Education & Outreach

- Our education and outreach programs are focused on meeting the needs of the critical materials supply chain.
- *During the last year, we have*
 - Collected information from relevant industries to determine their HR needs.
 - Developed an inventory of college-level courses available for students working on critical materials.
 - Incorporated CMI research data in a chemical engineering design class at the University of Tennessee.
 - Convened a two-day research seminar for CMI graduate students and post-docs.
 - Delivered monthly webinars on topics related to CMI's objectives.
 - Inaugurated a critical materials exhibit in the Geology Museum of the Colorado School of Mines.

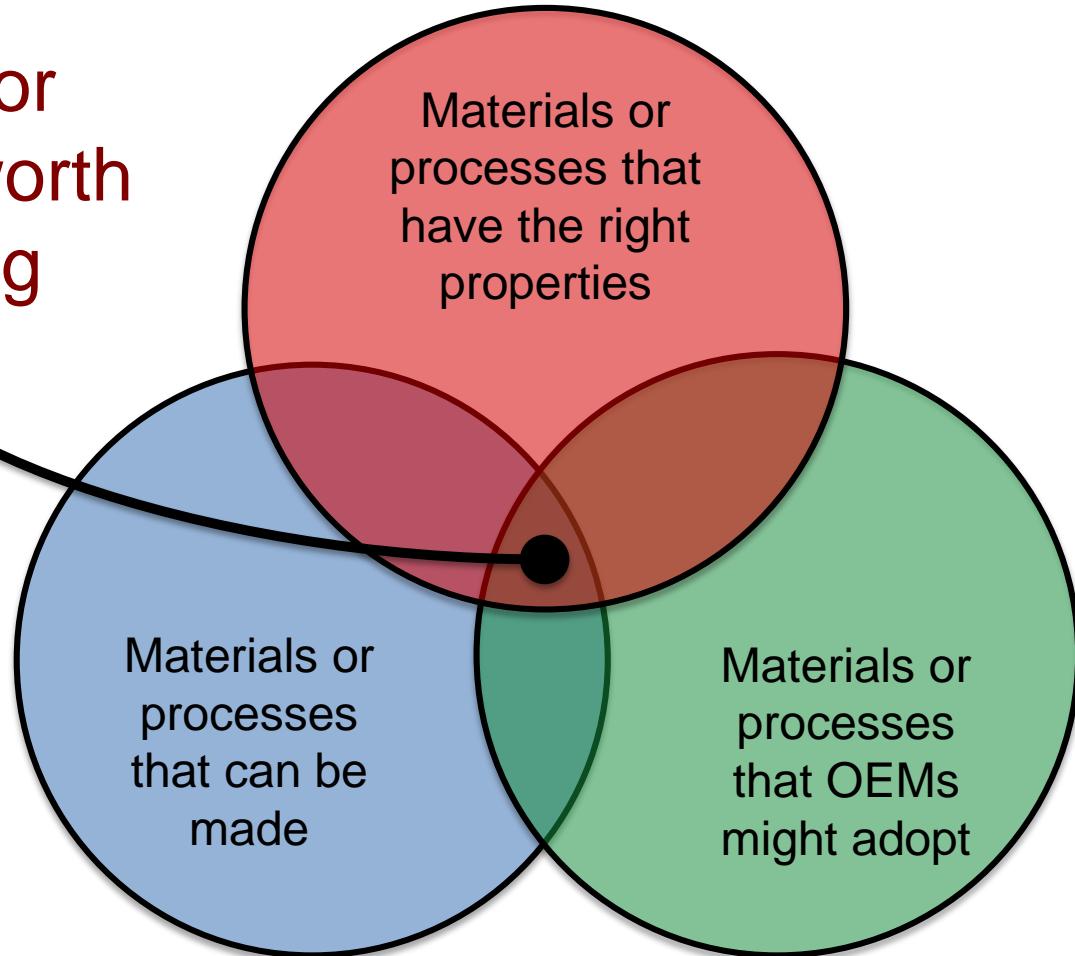


Outline

- Overview
- ***Technical highlights***
- Economic highlights
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The CMI technology development paradigm

Materials or
processes worth
developing



Technical Highlights from Year 3

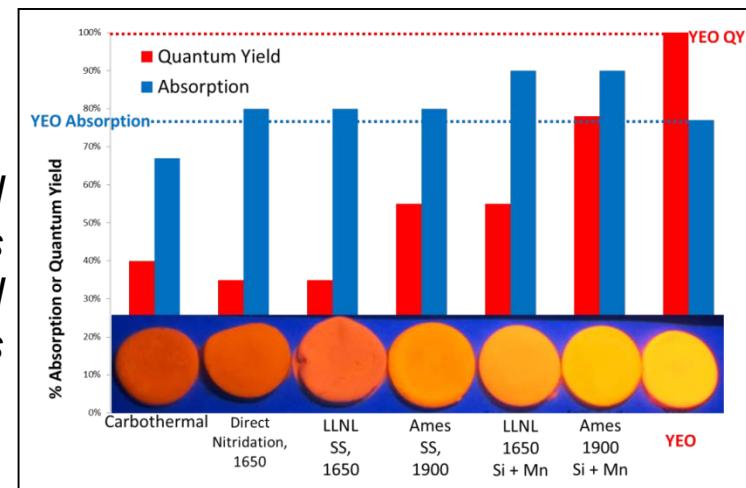
- CMI R&D moving rapidly toward commercialization.
- Key technical successes:



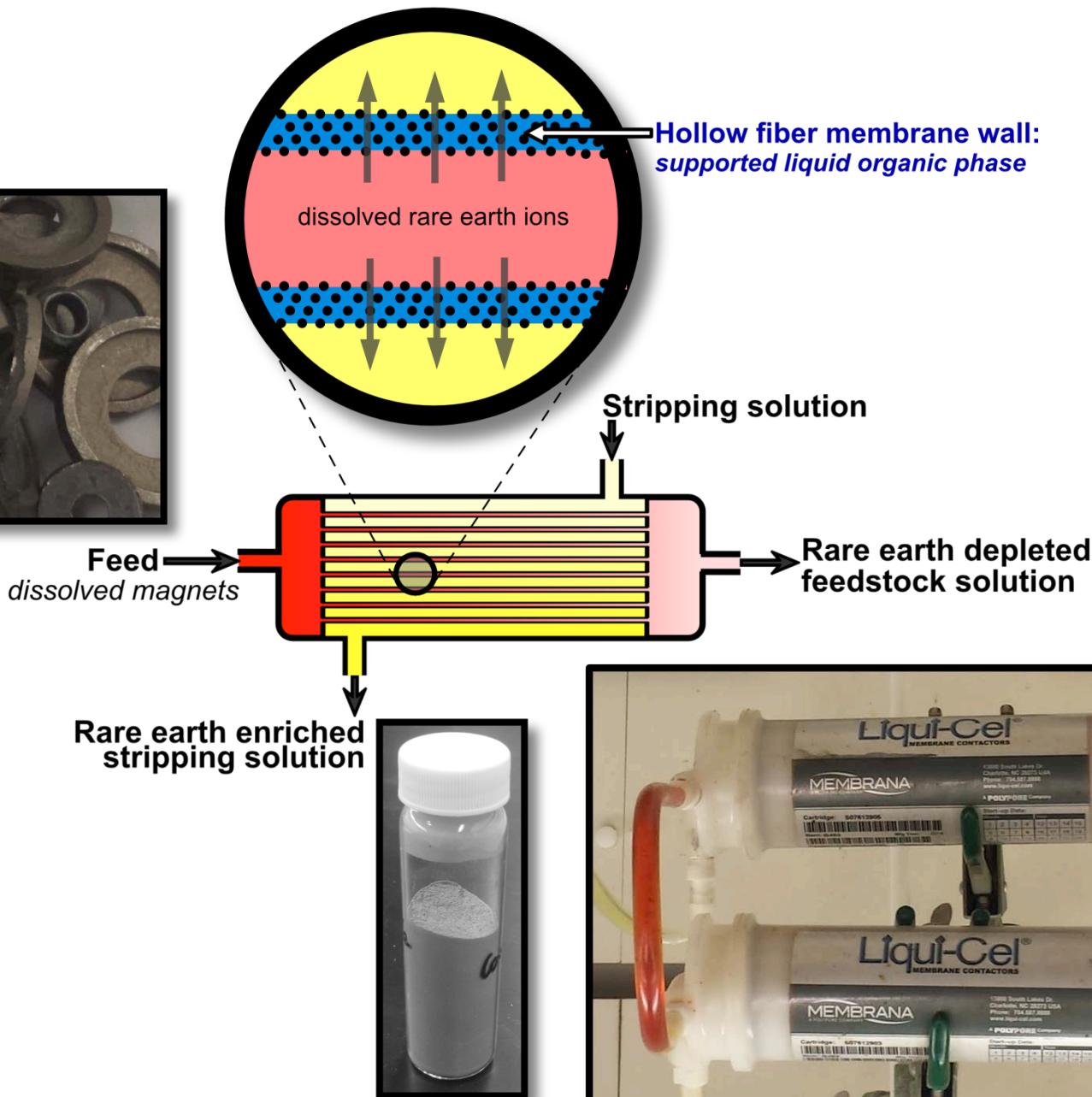
A membrane solvent extraction system for rare earth elements has been licensed to Momentum Technologies, LLC



A substitute for Eu-based red phosphor materials is approaching the required performance characteristics



A new Al-Ce-X alloy exhibits better performance than current casting alloys. It has been cast into a cylinder head for a commercial small gasoline engine and test-run in a generator set.



Development of New Casting Alloys

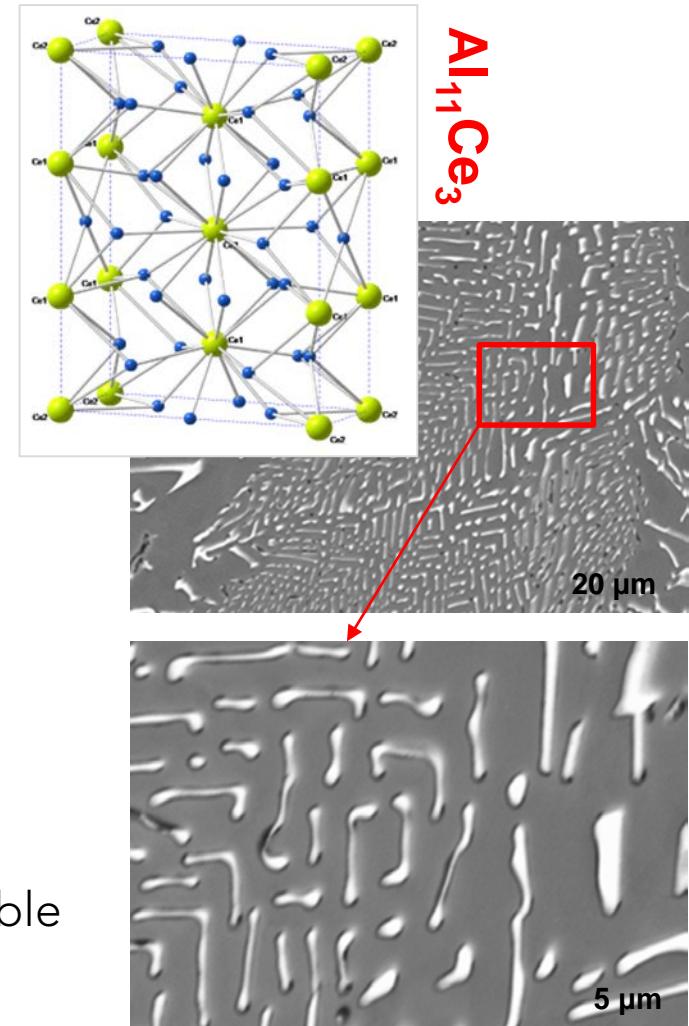
Project Background

Partnership Enabled Under CMI

- The Ames Laboratory
- Lawrence Livermore National Laboratory
- Eck Industries, Inc.
- Oak Ridge National Laboratory

Development of new ternary Al-Ce-X casting alloy for high temperature applications:

- As-cast mechanical properties – 30 ksi UTS
- Fine microstructure
- Reinforced with nanostructured intermetallic stable above 400°C

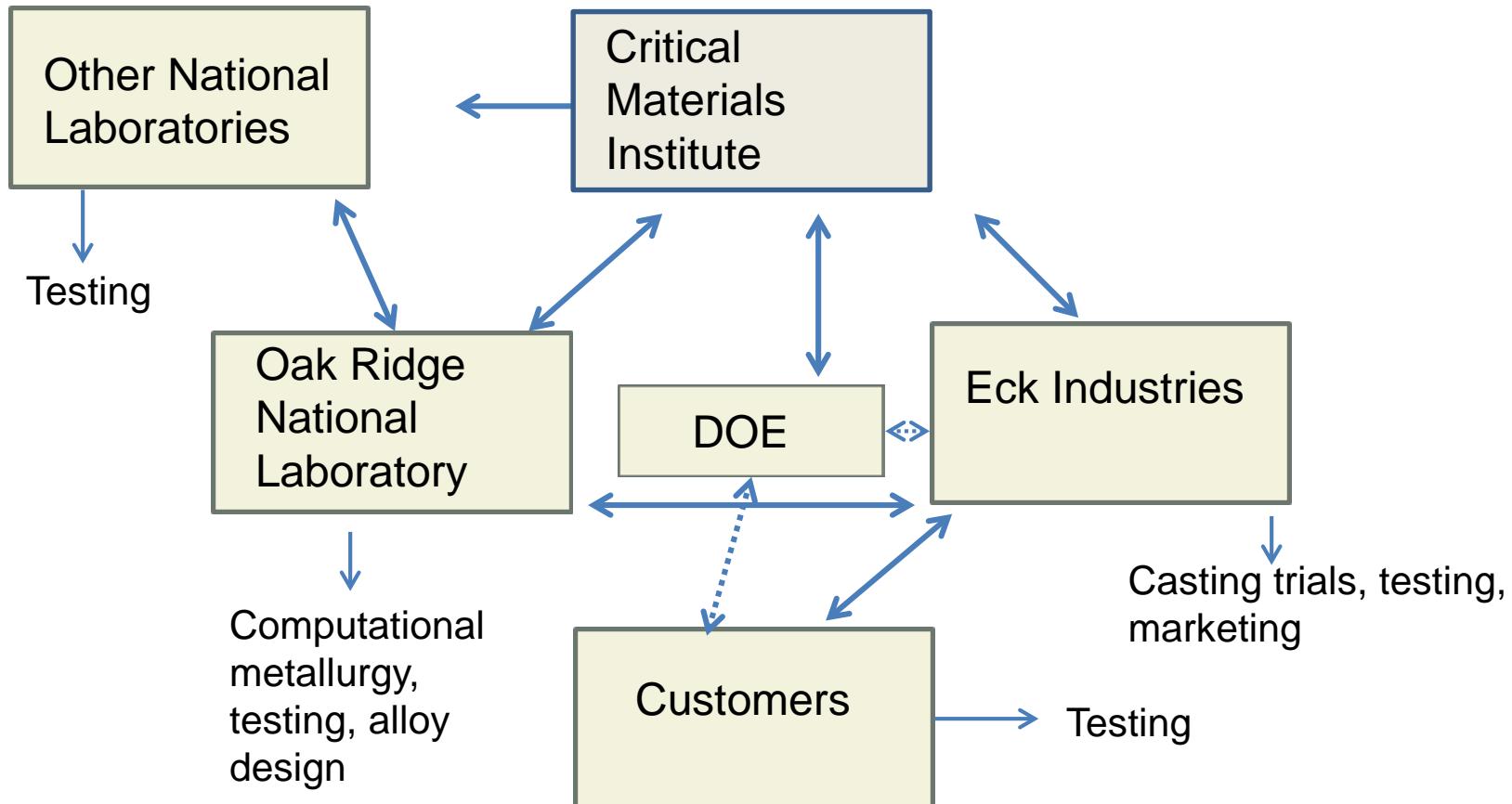


Strategy

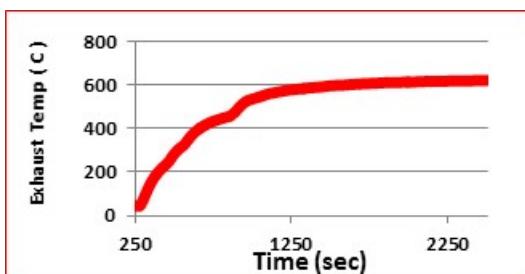
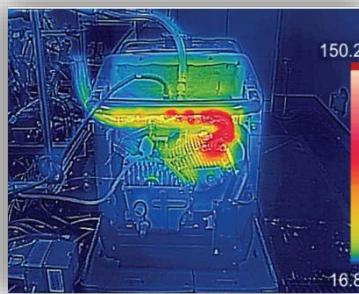
- Use abundant Ce in the form of Al-Ce alloys for high temperature applications
- Indirect stabilization of rare earth supplies
- Use computational metallurgy and applied R&D to rapidly commercialize improved higher temperature aluminum alloys
- High Ce levels in this alloy could use very large amounts of the element-4 billion pounds of aluminum are used in transportation annually



Partnership is the Key



Promising new cerium-aluminum alloy for high-temperature applications demonstrated in working engine



Top row: Mold and finished part, Above: Cylinder installed on engine with thermal imaging

Achievement:

A cylinder head made with the new alloy exhibited stable operation during full load testing on a commercial engine/genset at temperatures reaching 600°C.

Significance and Impact

The Al-Ce alloy offers high performance at lower costs and could boost America's rare earth mining industry by providing a high-volume automotive application for cerium, the most abundant rare earth element mined in excess. In turn, the economics of producing critical rare earths like neodymium for magnets improves.

Research Details

- Ternary Al-Ce-X alloy was selected for testing.
- Alloy was cast into 3D printed sand molds, then machined for engine use.
- The cast cylinder head was tested on a Honda 4-stroke engine/3 kW genset at temperatures reaching 600°C.

Computers Guide Development of Lanthanide Extractants

CMI publication on ligand design featured on journal cover

The image shows the journal cover of *Inorganic Chemistry*, Volume 55, Number 12, published on June 20, 2016. The cover features a computer monitor displaying a software interface for molecular design. On the left, labeled 'INPUT', is a chemical structure of a lanthanide complex with a central metal ion bonded to phosphine oxide ligands. A green arrow points from this input structure to a 'Link Database' section in the center, which contains a grid of various molecular linkages. Another green arrow points from the database to the 'OUTPUT' section on the right, where a tree-like network of generated chelate structures is shown, labeled with numbers 0001 through 0005. The title 'Computer-Created Chelates' is displayed above the monitor.

Achievement

A computer-aided molecular design approach has identified chelating agents to improve performance in liquid-liquid extractive separation of adjacent lanthanides from a collaboration between the Supramolecular Design Institute, Oak Ridge National Laboratory, Ames Laboratory, and Idaho National Laboratory.

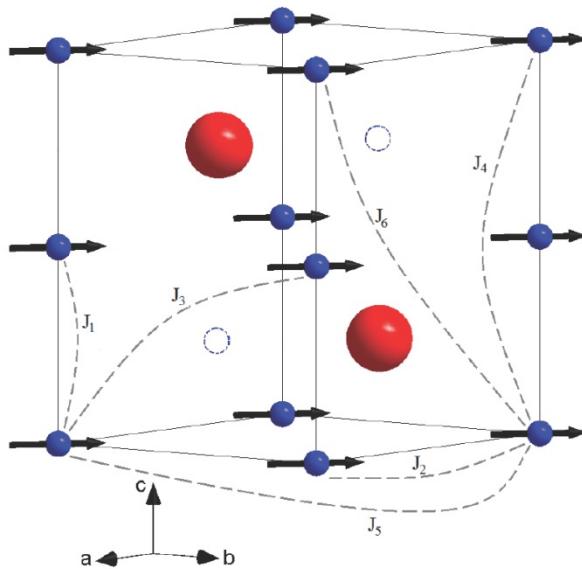
Publication featured on journal cover:

McCann, B. W.; De Silva, N.; Windus, T. L.; Gordon, M. S.; Moyer, B. A.; Bryantsev, V. S.; Hay, B. P. "Computer-Aided Molecular Design of Bis-phosphine Oxide Lanthanide Extractants" *Inorg. Chem.* **2016**, *in press* (DOI: 10.1021/acs.inorgchem.5b2995).

HostDesigner, Version 3.0 - General purpose molecular design software available at no cost from <http://sourceforge.net/projects/hostdesigner-v3-0/>

ParFit, Version 1.0 - Software to automate parameterization of force field models required to evaluate and rank candidates is available at no cost from <https://github.com/fzahari/ParFit>

Spin Waves in the Itinerant Ferromagnet MnBi



Above: Crystal Structure of MnBi. Dashed lines indicate magnetic coupling paths between Mn atoms.

Below: Inelastic neutron scattering data along different directions. The black line is the theoretical fit.

Achievement:

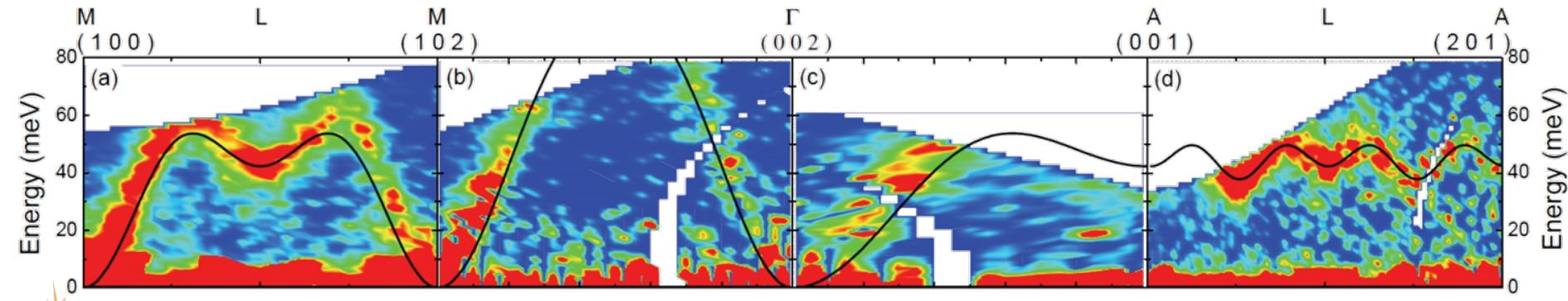
First experimental measurement of spin waves in MnBi, a candidate material for non-rare earth permanent magnets.

Impact:

The interactions between nearest neighbor Mn atoms are strongly antiferromagnetic, a result corroborated by DFT. The spin waves and the ferromagnetic ground state are only explained if several (up to 6th) next-nearest neighbor interactions are included. This surprising result will impact our understanding of other potential ferromagnets.

Details:

- First crystals of MnBi ever grown large enough to perform neutron diffraction.
- Experiments performed at the ORNL Spallation Neutron Source.



Outline

- Overview
- Technical highlights
- ***Economic highlights***
- Plans & final thoughts

Perspective: strategic to operational

- Criticality assessment and underlying economics
- Life cycle assessment
- System dynamics
- Technological roadmapping

Strategic

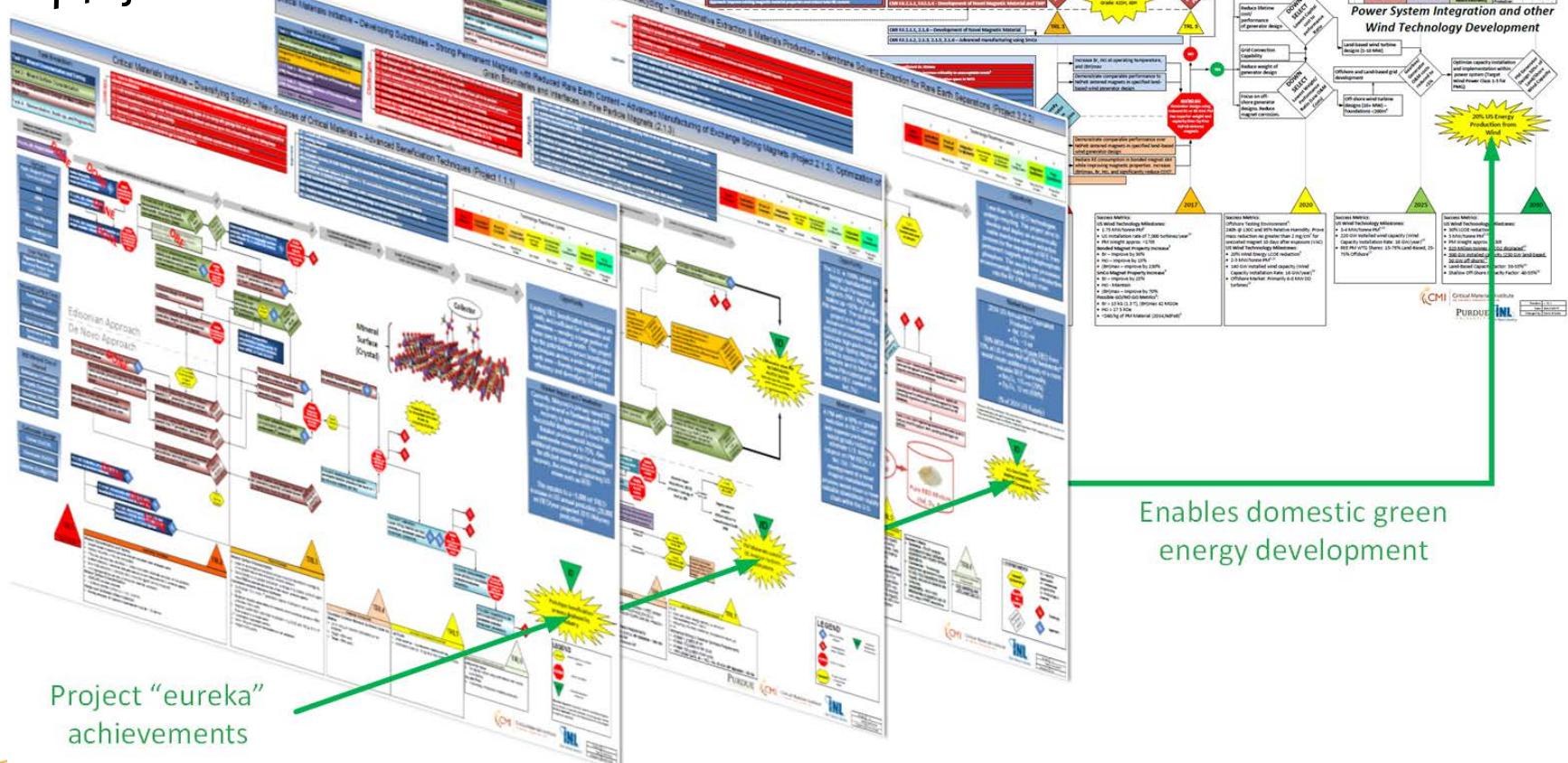


Operational

Roadmap Integration

Green Energy Technology Roadmap

Project Roadmaps



What is ‘critical’ for carbon abatement?

Scope

- World
- 2016-2030
- 9 Technologies, 27 Elements

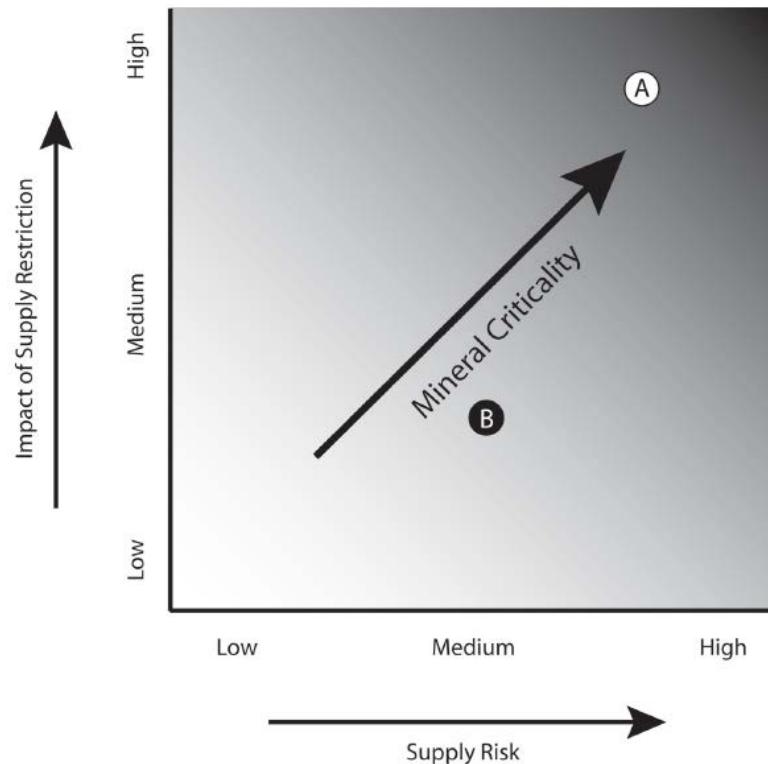
9 technologies*

- Photovoltaics
- Wind
- Advanced vehicles, including fuel cell
- Lighting
- Catalytic converters
- Nuclear power
- Gas turbines
- Batteries for electricity storage
- Vehicle lightweighting

*From DOE *Quadrennial Technology Review 2015*. Did not evaluate hydrogen electrolysis or thermoelectrics.

Method

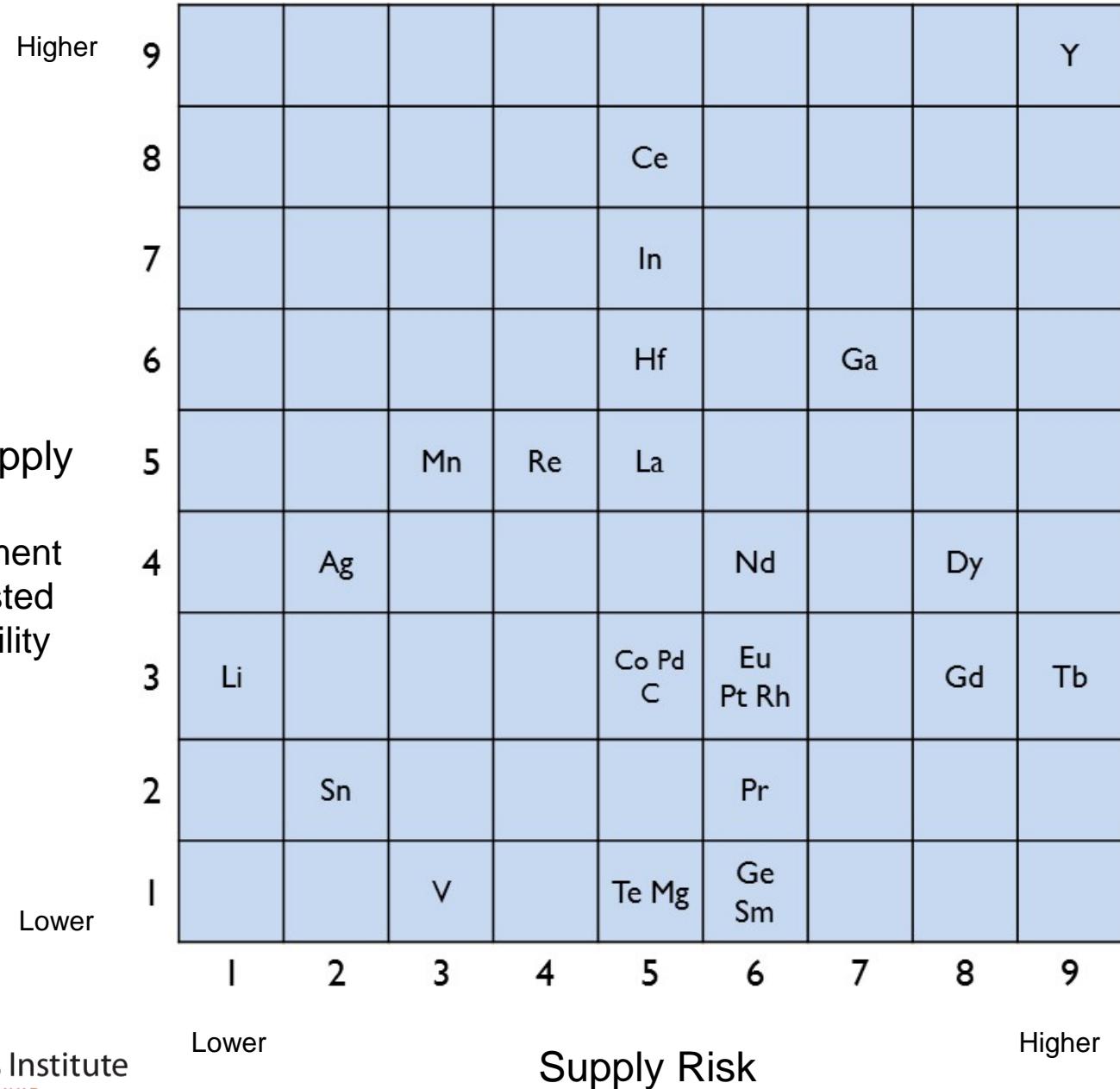
- Supply risk
 - Adjusted producer diversity
 - Risk of demand shock
 - Co-production risk
- Impact of a supply disruption
 - Carbon abatement
 - Substitutability



Source of figure: National Research Council (2008)

World 2016-2030

Preliminary
Impact of Supply
Disruption –
carbon abatement
potential adjusted
for substitutability



World 2016-2030

Rare Earths

Impact of Supply Disruption – carbon abatement potential adjusted for substitutability

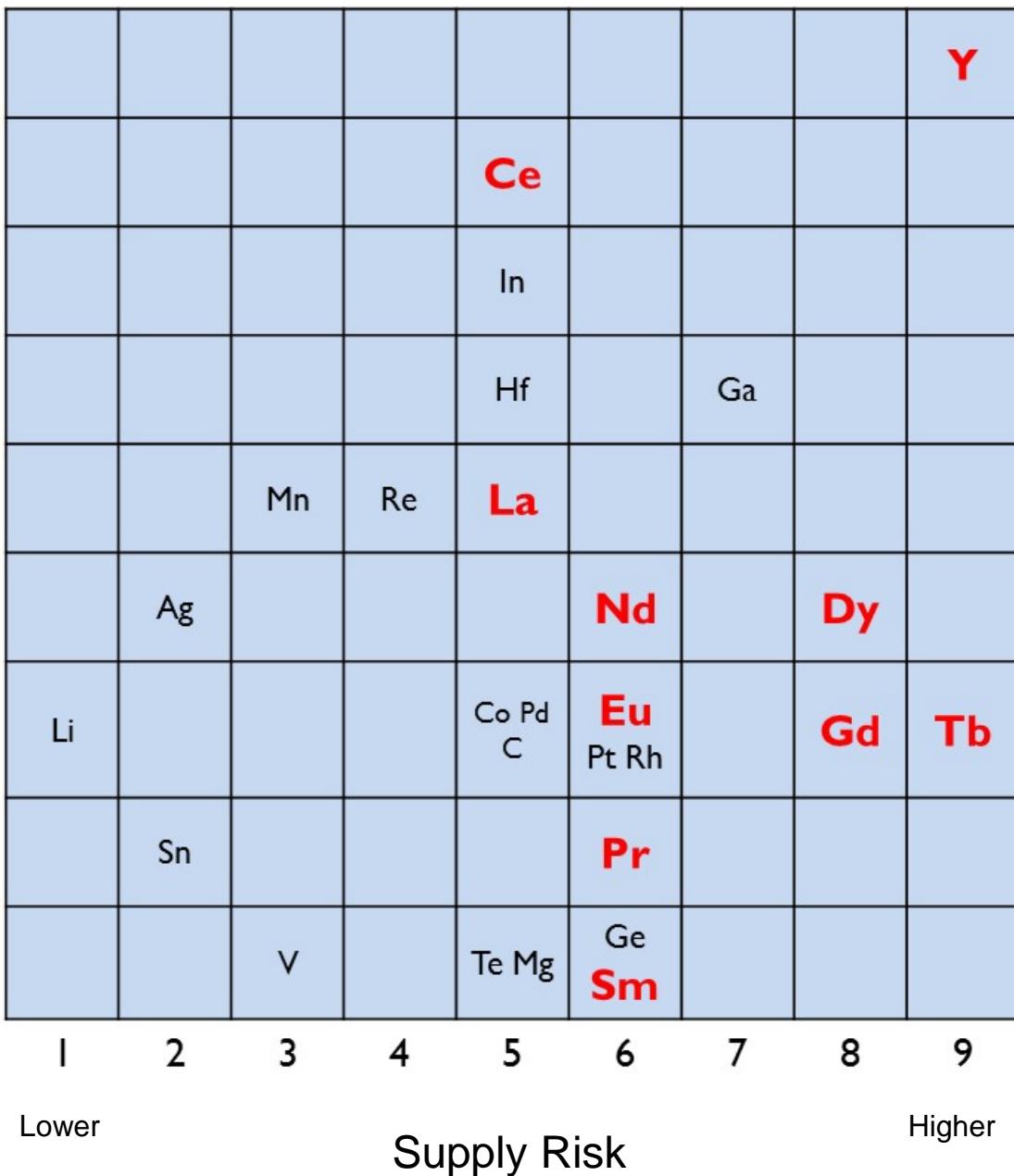
Preliminary

Higher

Lower



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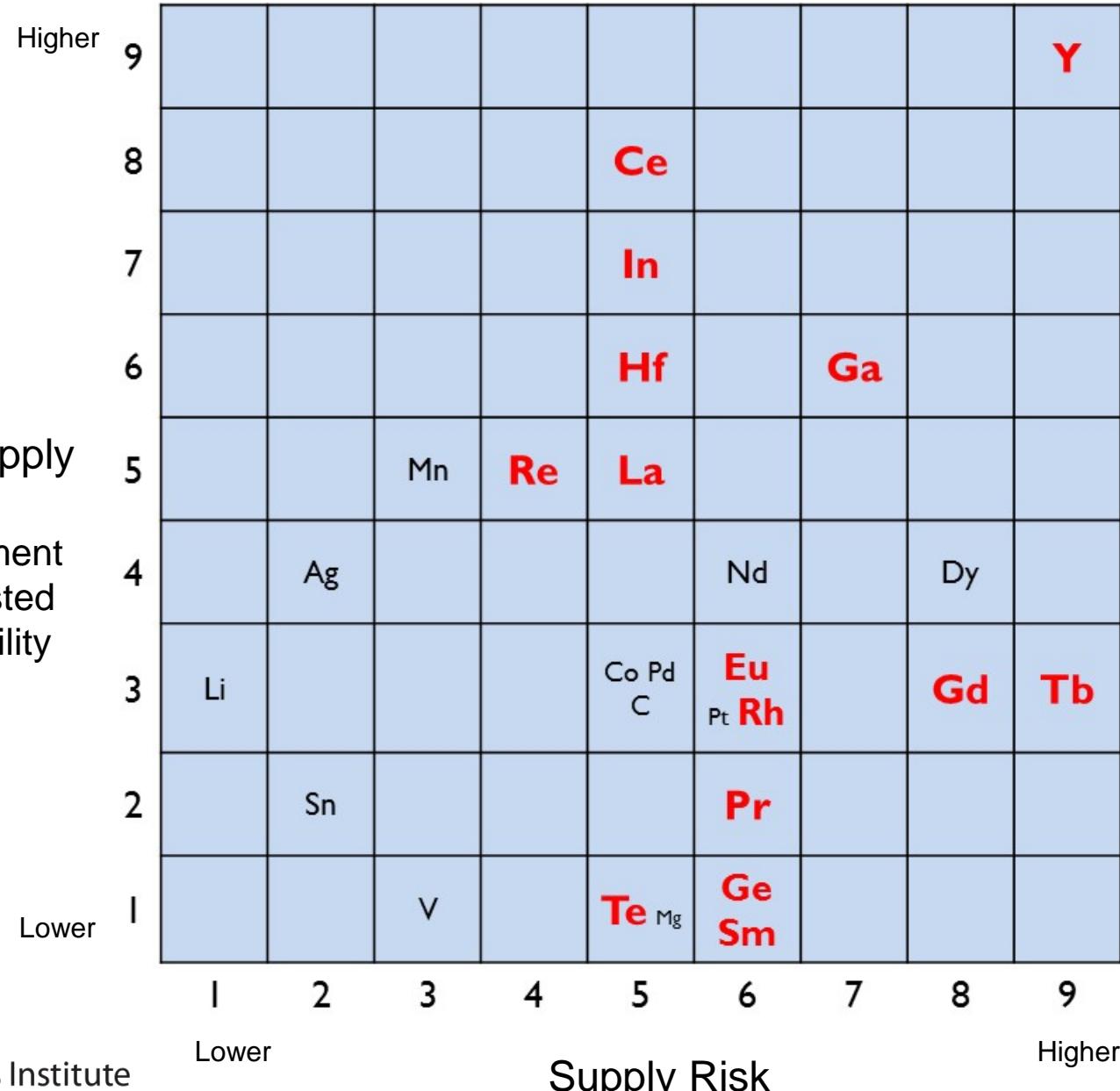


World 2016-2030

Byproducts

Impact of Supply Disruption – carbon abatement potential adjusted for substitutability

Preliminary



Outline

- Overview
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- ***Plans & final thoughts***

Plans for Years 4-5

July 1, 2016 - June 30, 2018

- Continued focus on commercialization
- Metrics aligned with AMO standards for NNMI facilities
- Four strategic themes
 - Develop advanced manufacturing technology that is adopted for clean energy manufacturing
 - Train an advanced manufacturing workforce
 - Enrich the innovation ecosystem
 - Be substantially self-sustaining after 5 (more) years

