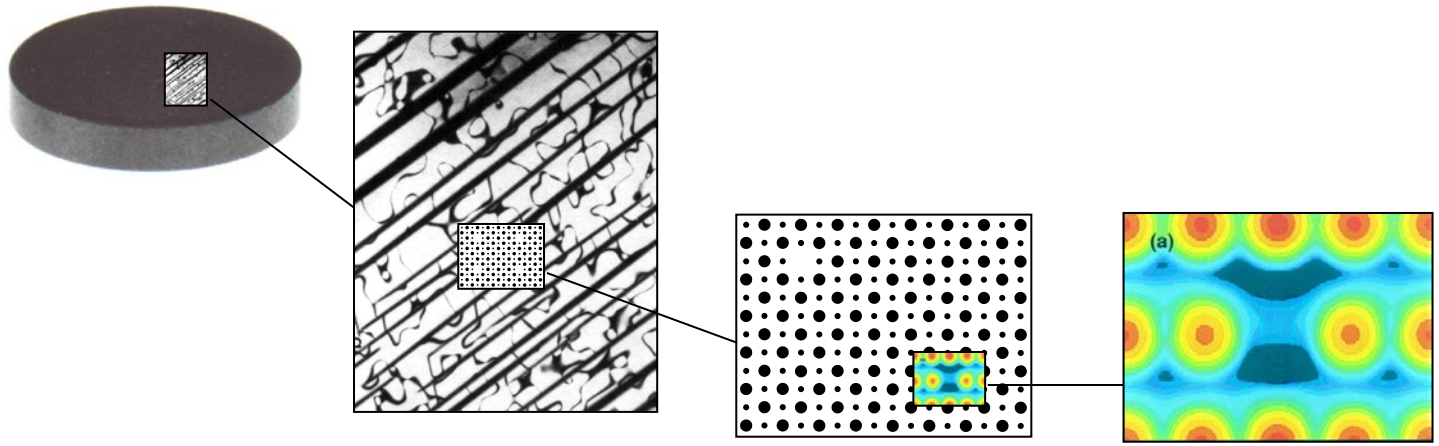
Towards an ab initio theory of temperature dependent and multi-scale phenomena in magnets



- **Complexity:** Applied magnetism – multiscale phenomena. Different physics at each inhomogeneous length scale
- Magnetic properties "feel" all length scales
- Combination of methods, linking length scales at finite temperatures
- **Goal:** New magnets by design

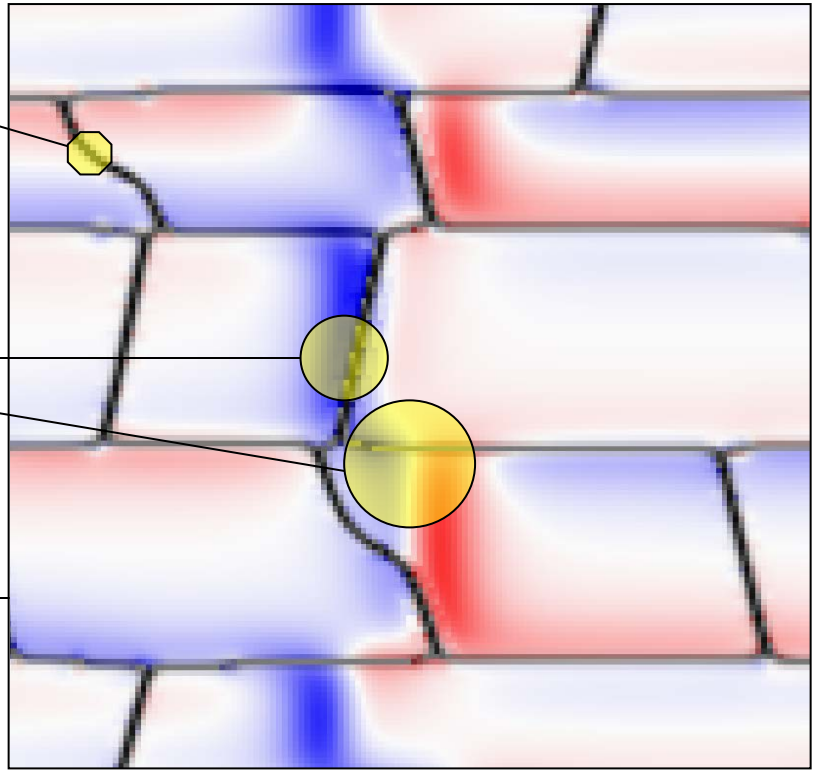
Theoretical multiscale modeling of magnets at finite temperatures

- **Ab initio calculations**
- Intrinsic and extrinsic properties of magnets

- **Atomistic models**
- Domain walls at defects

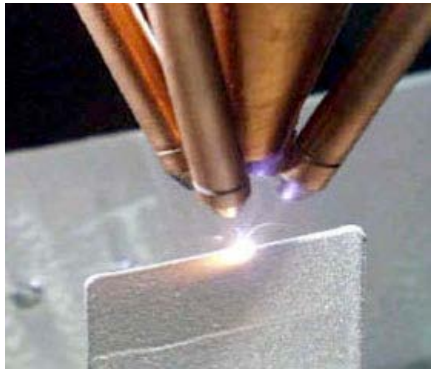
- **Micromagnetism**
- Domain structure
- Hysteretic properties

- **Statistical averaging**



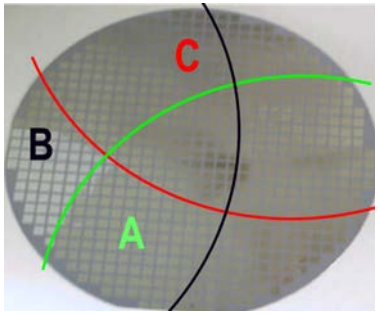
Rapid Assessment Methods

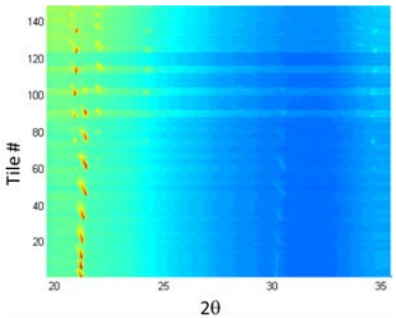
- Rapid Synthesis
- Mico-to-bulk

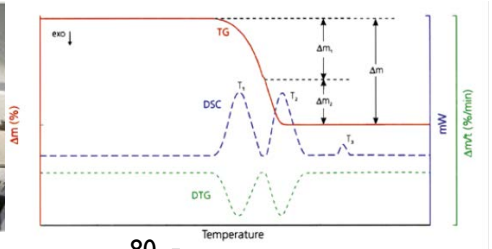


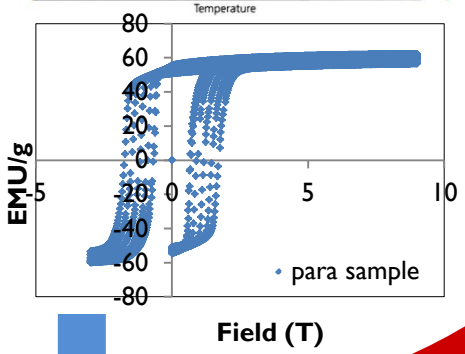
Rapid Characterization

Parallel analysis of structure and properties









Focus Area 2

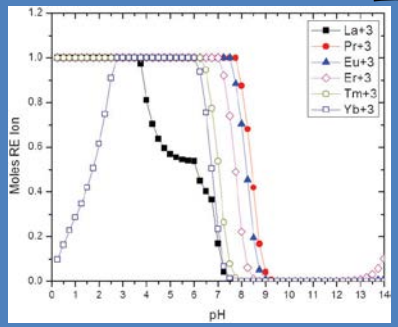
Develop permanent magnets with decreased rare earth content

Techniques:

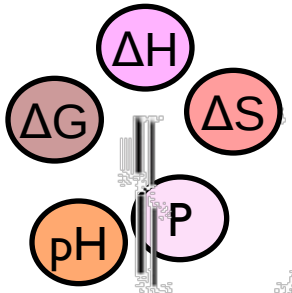
- ab initio
- Thermodynamic modeling
- Materials informatics

FA 4 Crosscut Team-Thermodynamics

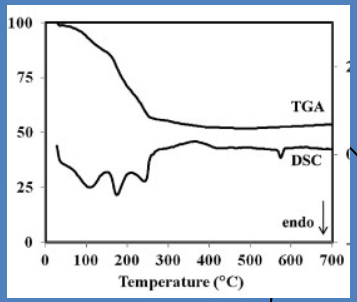
Solubility

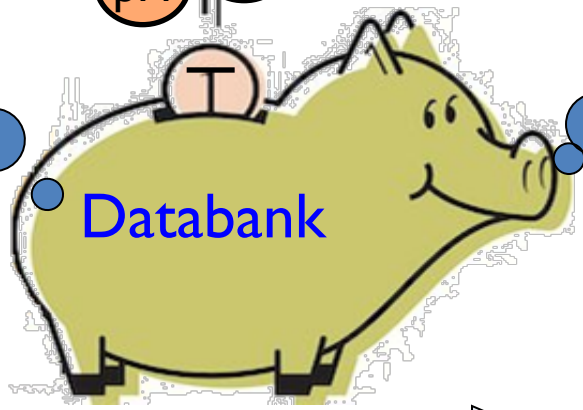


Data Deposit



Calorimetry





Input

- Precursors, target products
- Reaction condition (T, P, pH)

OLI Simulation Engine

Output

- Phase equilibria
- Optimum process

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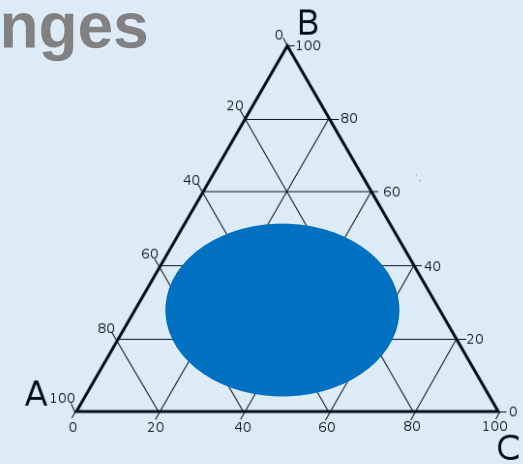
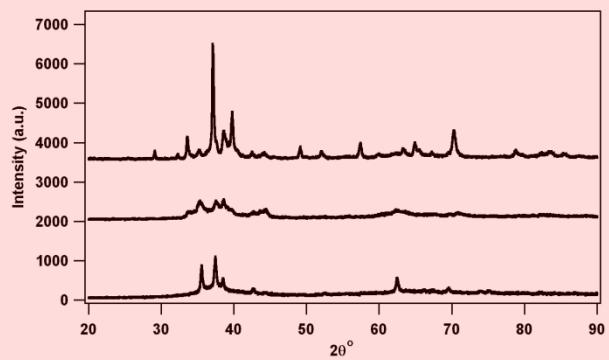
Combinatorial Materials Science

Synthesize libraries over composition ranges



- Characterize:
  Structural, Magnetic, Mechanical, etc.



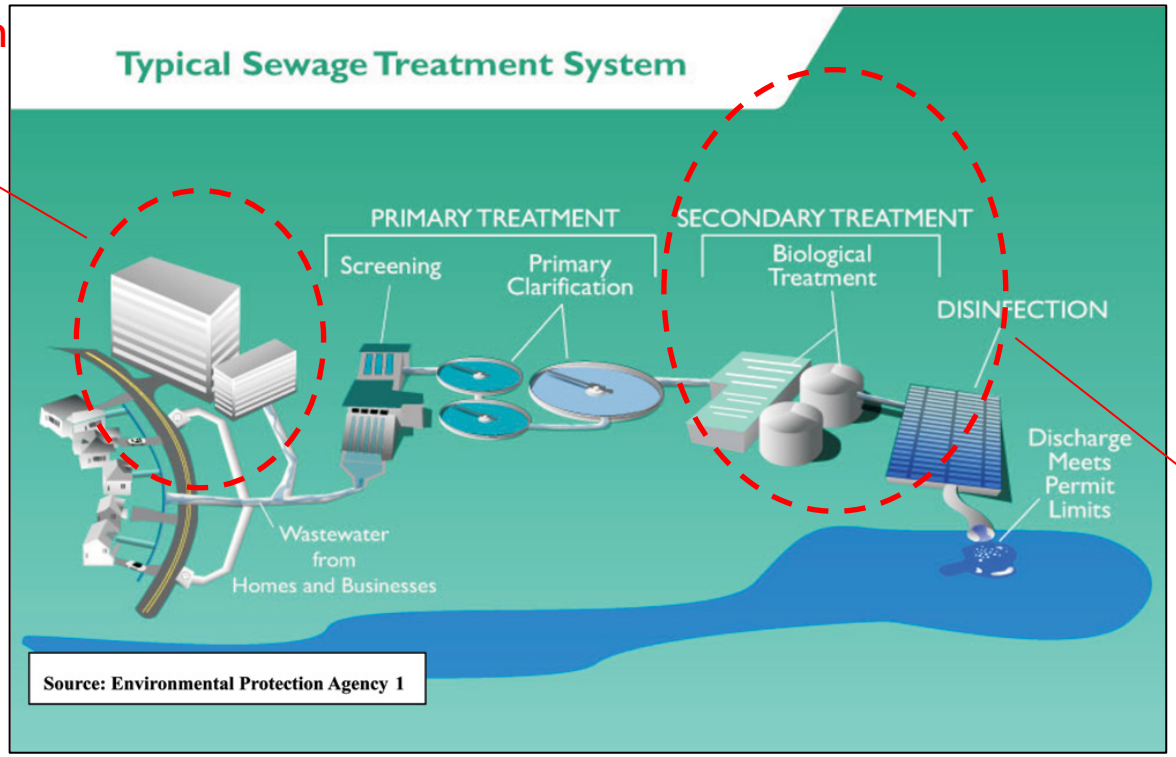
Identify compositions of interest

Methodology is still lacking

- **Need synthesis techniques for libraries on both micro- and bulk-scale**
- **Develop rapid characterization techniques in parallel**
- **Synthesis and characterization informed by theory**

Rare Earth Effects on Biological Wastewater Treatment Systems

Industries often release pretreated wastes to publicly owned treatment works (POTWs)



Impairment of treatment function could cause failure to meet discharge criteria

- REE processing/recycling technologies will produce wastewaters containing residual REEs and associated constituents; currently no pretreatment standards for REEs.

Testing REE wastewater impacts on microbial function and community structure

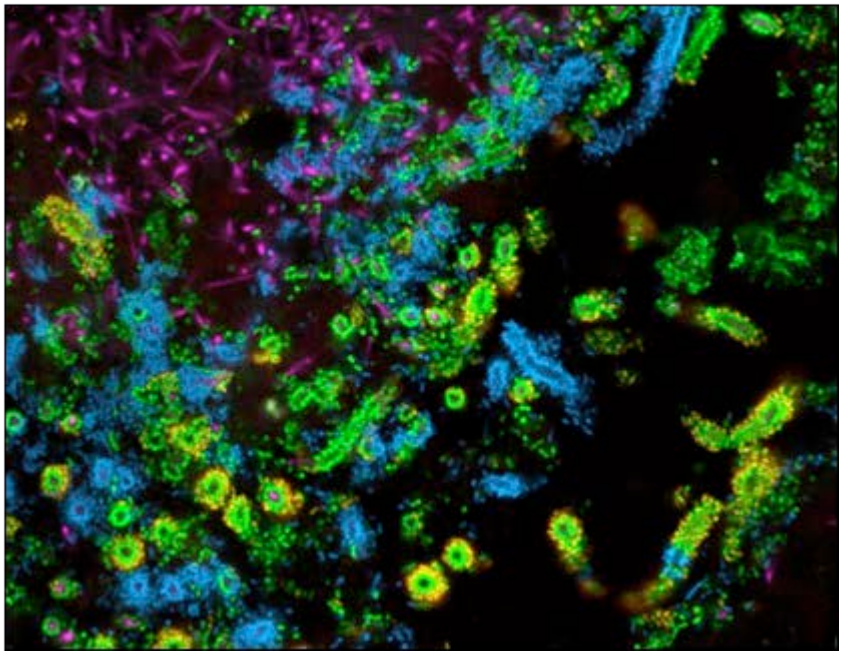


Image of mixed microbial community; from MBL.edu

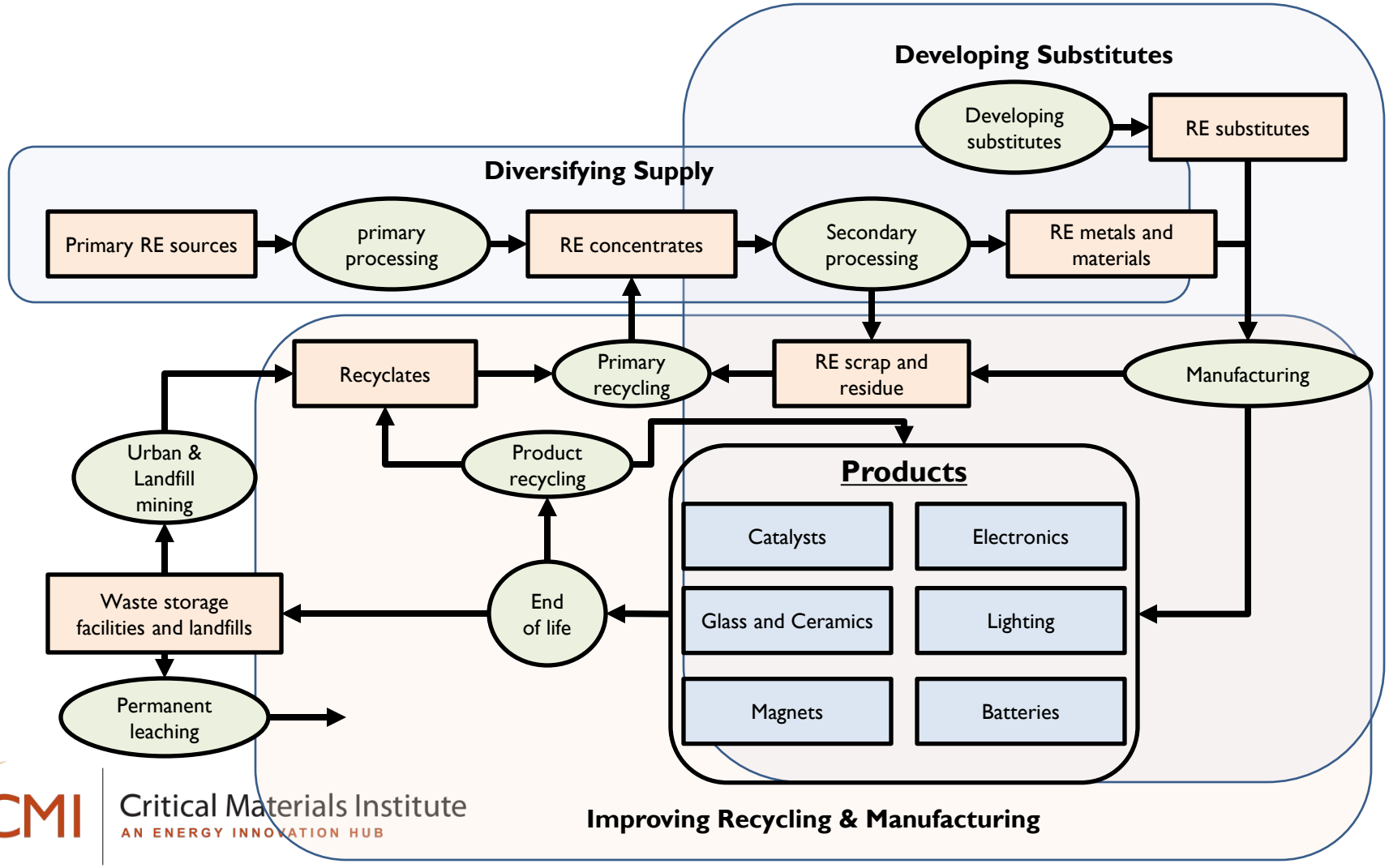
- Using wastewater selected in consultation with partner project(s) in FA1 – FA3, will measure impacts on growth and function (*i.e.*, ability to degrade pollutants) of model organisms and microbial communities obtained from POTWs.
- Results can influence processing technology development.

Economic analysis of global critical material supply chains

- An integrative, cross-cutting viewpoint

Identifying global stocks and flows

Rectangles represent storage of critical-material-relevant commodities. Ovals represent processes that use one commodity to create another. The task is to determine a technical and market design for the entire system that improves long-term value. The model will track prices and volumes in each rectangle, and costs vs. characteristics in each oval.



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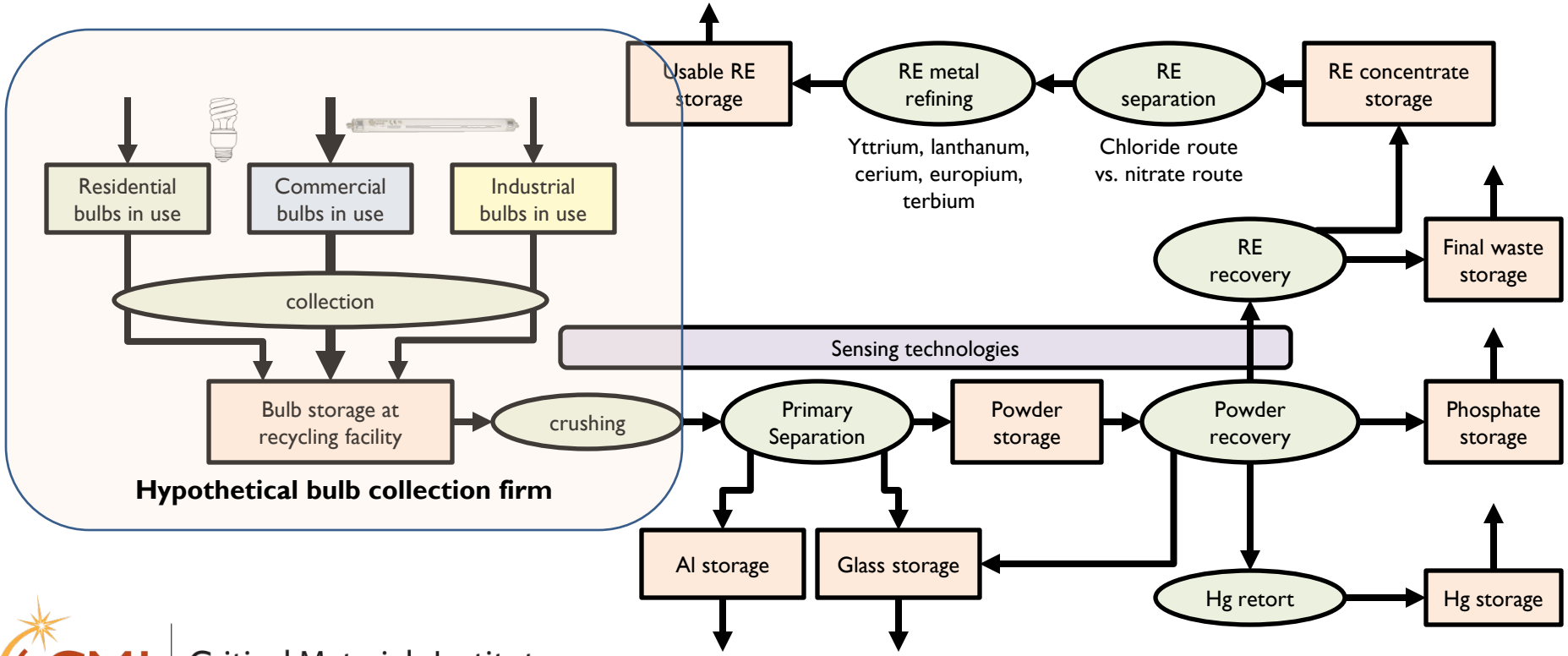
Modeling a firm within the supply chain

Each process in the global material supply chain will be modeled at a higher level of detail by identifying the storage and processing components that make up the overall process. This is a hypothetical example for phosphor recycling, beginning with products (bulbs) and ultimately closing the loop through the recycling chain. These logistics models will be coupled with the global economic models.



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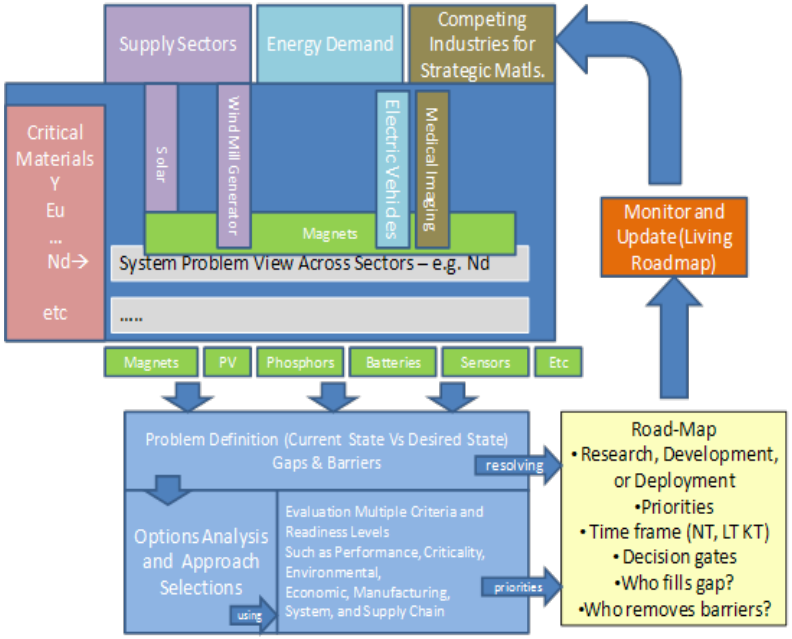
Energy Technologies Impacted by Limited Resources

- The supply of critical materials is limited for a number of reasons:
  - Rare earths are limited in supply and location
  - Demand in general for critical materials continues to increase
  - Critical gaps exist in the supply chain
- Current and clean energy technologies are dependent on a number of critical materials
- The lifecycle of critical materials will drive our energy future if short, mid and long-term solutions are not identified

Providing Direction

- Based on a better understanding the breadth of the critical materials problem across sectors and applications, a **National Technology Roadmap for Critical Materials** will:
  - Mitigate risks in pursuing new materials and energy technologies by taking a systems view, resulting in more-optimized solutions
  - Focus industry, laboratory, and university efforts on a common target while avoiding duplication
  - Greater options for innovation will be identified and evaluated to find superior direction for R&D