Accelerating Energy Innovations

Critical Materials Institute

AN ENERGY INNOVATION HUB

GRAND CHALLENGE PROBLEMS

Time is the biggest issue. *Materials typically become critical in a matter of months, but solutions take years or decades to develop and implement. Our first two grand challenges address this discrepancy.*

Anticipating Which Materials May Go Critical

In an ideal world, users of materials would anticipate supply-chain disruptions before they occur. They would undertake activities to manage the risks of disruption, including R&D to diversify and increase supplies or to reduce the need for materials subject to supply risks. In such a world, material users and their actions would reduce the likelihood of a disruption, as well as the impacts of a disruption, should it occur. In practice, however, many disruptions that might have been anticipated and managed are unexpected and become crises.

CMI is working with government agencies, the academic community and industry to develop an early-warning system for emerging criticality. The aim is to identify and prioritize areas for science and engineering research that will alleviate criticality before it occurs.

Increasing the Speed of Materials Discovery and Deployment

New technologies provide economic opportunities and improve the quality of our lives in areas spanning from housing to healthcare, transportation, communications and entertainment, but great ideas can fail for lack of the necessary materials. Energy security, national security, and economic leadership all depend on technologies which increasingly require specialized materials that work better, or are more available than the ones in current use. However, the timeframe to discover, develop, and deploy new materials currently stands at 10 to 20 years.

To reduce the time needed to discover and implement advanced materials for specific uses, and to close the gap on the timeframe on which materials criticality typically emerges, CMI will leverage the computational and database tools emerging from the Materials Genome Initiative into an integrated materials development and implementation framework. This will increase the effectiveness of materials discovery and deployment as a means of addressing shortages of materials needed for magnets, phosphors, catalysts, ligands, batteries, solar cells, and other commercial clean energy applications.

Rare earths are among the most difficult elements to process, and the hardest to do without. *Rare earth elements rank at the top of all lists of critical materials today, and the difficulty of working with them - or working around them - contributes significantly to this. Three technical grand challenges associated with rare earths are being addressed by CMI.*

Separating the Rare Earth Elements

Rare earths make vital contributions to a wide range of technologies but they have to be purified before they can be used. The most difficult aspect of purification is separating these elements from each other, which is costly and time consuming. Current processes are inefficient, need hundreds of repetitive process steps, and use potentially harmful acids and organic compounds in large quantities.

The development of new chemical separation methods with high efficiency, low cost, and low environmental impact will reduce costs and environmental impacts, allowing the materials to be processed more widely. This will advance the goals of diversifying the sources of these materials and increasing the amounts that are recovered through recycling.

Converting from Ore to Metal

Mines do not produce metals ready for use in clean energy technologies: they produce rocks that contain chemical compounds of the elements that we need. Ores are processed in successive stages known as (1) mineral processing, (2) separation, (3) metal making, and (4) end-use alloy production. Progress is being made in diversifying all of these stages of rare earth production, except metal making. Rare earth metal making capabilities are absent from North America, representing a significant strategic weakness in terms of both commerce and defense. This process step is carried out almost exclusively in China, even for ores that are mined in the U.S., representing a persistent chokehold on the supply-chain. Current processes for converting RE oxides into metal are environmentally hazardous, and difficult to establish wherever there are stringent licensing requirements.

Novel technologies for the conversion of oxide to metal that can be established in North America will play a significant role in assuring control of the complete REE supply-chain. These will need to be economical, have low energy requirements and low environmental risks, if they are to succeed.

Understanding the f-Electron

Rare earth elements make unique and valuable contributions in magnetism, lighting, catalysis and many other areas, and these all derive from the particular behavior of the electrons in their atomic structure. The elements from lanthanum to lutetium are related to each other by the successive addition of one electron to the 4f-shell of electron orbitals for each unit increase in the atomic number. The properties of these elements therefore depend particularly on the behavior of the 4f-electrons, which have highly localized electronic states, among other unusual properties, as compared to other electron orbitals. Understanding the interactions and behaviors of these electrons in realistic environments is one of today's fundamental challenges in condensed matter physics, and it directly affects our ability to understand how rare earth elements produce the specific desired properties of the materials that contain them. Current theoretical and simulation tools for describing these interactions and excitations are based on intellectual constructs in which each electron sees all of the other electrons only in an aggregated "cloud." This captures only the simplest aspects of the interactions between f-electrons, and greatly limits our ability to predict or control the properties that arise from them.

Better theoretical models for f-electrons, which account for more of the nuanced manner in which they interact which each other and with their environment, rigorously validated by experiment, will considerably accelerate the process of materials discovery and design. This will allow us to develop new chemical processes, substitute for, or more efficiently exploit the special properties of the rare earth elements.