Scientists use supercomputers to search for innovative answers to rare-earth supply needs

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Our lives depend on our electronics – our cellphones and computers. In turn, our electronics depend on a special class of elements known as rare-earths. Computers, cellphones, electric vehicles, televisions, and more are built using these materials. Their value lies in their unique properties; some are strongly magnetic; others create vivid colors for optical uses.

For example, an average laptop employs a magnet of rare-earth in its hard drive spindle that weighs 1.8 to 2.5 grams, a tiny fraction of the laptop's weight. And although their physical size and processing speeds differ by magnitudes, U.S. Department of Energy (DOE) supercomputers such as Titan at the Oak Ridge National Laboratory and Icestorm at the Idaho National Laboratory also use rare-earth materials - in their semiconductor components, power supplies, and data storage systems.

Daily, new inventions are increasing the uses for rare-earths, but the mined and processed totals are falling short. Green energy technology needs rare earth materials for wind turbines, rechargeable batteries, and batteries for electric and hybrid vehicles. Although these elements are found throughout the world, as recently as 2012 the United States produced only 800 metric tons of the global production of 110,000 tons. This amount - far short of its needs - means the United States is relying on uncertain and costly imports for manufacturing and energy output. Researchers in the Critical Materials Institute (CMI) at the DOE's Ames Laboratory are looking for innovative answers to rare-earth supply problems. As an Energy Innovation Hub funded out of the Advanced

Manufacturing Office in the Office of Energy Efficiency and Renewable Energy, the CMI mission is to diversify the global supply, discover substitutes, and invent new ways to re-use and recycle the rare-earths.

Extracting Answers

Rare-earths are not particularly rare; rather they are costly and scarce because the current mining and extraction processes are complex, often toxic, and expensive in time and money. Because they are chemically very similar, rare-earth elements are difficult to separate from each other. Each extraction step depends on varying factors: the suitable acidic or base stripping solution, contact times and appropriate ratios of different reagents, reagent concentrations, and chelating solutions. A team headed by CMI lead researcher Theresa Windus is tackling the processing problem to find a new generation of extraction agents.

Using data produced during 5 million core hours of research generated by CMI associate Nuwan De Silva on the supercomputer Titan, Windus' team will design ligands – molecules that attach with a specific rare-earth – that allow metallurgists to extract elements with minimal contamination from surrounding minerals. Through this simplified processing, savings in time and labor will increase the availability of these vital rare-earths.

Producing New Solutions

Critical Materials Institute teams are also exploring chemical substitutions to reduce the amount of rare-earth elements needed to make permanent magnets – magnets that have a stable magnetic field without the use of an electric current. These permanent magnets are needed for vehicles, wind turbines, speakers in cellphones and headphones, cordless tools, and much more.

A team led by Ames Laboratory senior scientist Bruce Harmon - who recently retired - has been given up to 45 million core hours on Titan to look at multi-element materials. With its 27 petaflops (27,000 trillion calculations per second) processing power, Titan is able to examine the interactions of hundreds of thousands of atoms in three- and even four-element compounds.

"We finally have the computing capability to explore greater complexities using quantum mechanics – greater numbers of atoms, the possible crystal structures, and their properties," said Harmon. With the data from Titan's calculations, Harmon's team will select promising compositions as new magnetic materials to test. As Bill McCallum, also a senior scientist at the Ames Laboratory's CMI, puts it, "A refrigerator magnet is the lowest of the permanent magnets, used to hold your child's drawing to the front of the fridge. We want to make a refrigerator magnet that will hold the Manhattan phone book to the fridge door."

If anyone can "hit pay dirt" in rare-earth challenges, it is the researchers using the DOE's supercomputing power.

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