Louisiana EPSCoR
EXPERIMENTAL PROGRAM TO STIMULATE COMPETITIVE RESEARCH VOL.10 NO.8

Materials Research Driving Next Generation of High Capacity Batteries

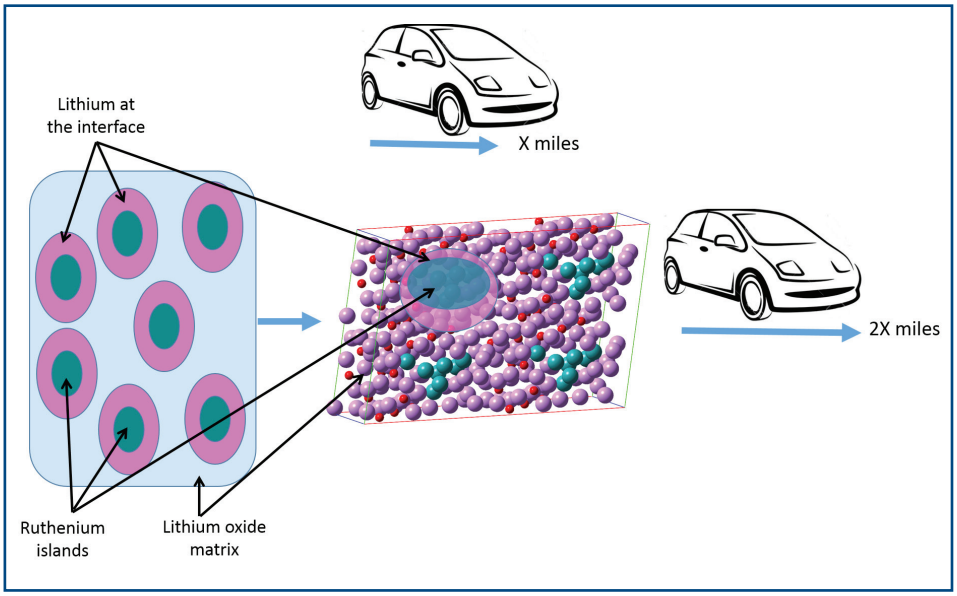
Back in 1983, Motorola revealed the world's first mobile phone, nicknamed "the brick," because the size was reminiscent of a brick and it weighed almost three pounds. Over the last 30 years, mobile phones have consistently shaved off weight and thickness, and today's mobile phones weigh less than 5 ounces, due to advances in lithium-ion battery technology. Lithium-ion batteries are extremely popular in mobile devices because they are lightweight, hold their charge over time, and can be discharged and recharged hundreds of times.

While great for small devices, lithium-ion battery technology is having difficulty making the transition to powering electric and hybrid vehicles. Current car lithium-ion batteries are not strong enough, recharge slowly, and don't last very long — all important criteria when driving a vehicle. A two to five fold increase in energy density is needed for this application, so this will require a major change in the technology.

Researchers worldwide are experimenting with different materials that show promise for the next generation of lithium-ion batteries.

One such material, an oxide of a metal called ruthenium, shows promise when used in the electrode part of a lithium-ion battery that stores the ions.

Experiments conducted by Dr. Lamartine Meda, Associate Professor of Chemistry at Xavier University, and researcher in the NSF-funded Louisiana Alliance for Simulation-Guided Materials Applications consortium (LA-SiGMA), demonstrated that ruthenium oxide stored twice the capacity of lithium than was theoretically predicted.



While investigating new materials for the next generation of lithium-ion batteries, LA-SiGMA researchers discovered that ruthenium atoms group into nanometer sized "islands," creating twice the storage capacity than theoretically predicted.

Dr. Lamartine Meda

Inspired by Dr. Meda's results, three LA-SiGMA chemistry researchers at Louisiana Tech University's College of Engineering and Science, Dr. Ayorinde Hassan, Dr. Collin Wick, and Dr. B. Ramu Ramachandran, set out to determine the cause of this interesting phenomenon.

Understanding how this observed increased capacity happens on the atomic level will help in the discovery of better materials for the next generation of lithium-ion batteries.

Using world class computational tools, the research team extensively tested different theories of the source of this extra capacity, determining how the atoms were interacting and predicting how different atomic configurations influenced their properties.

The results are in: They were able to computationally explain the mechanism for this observed extra capacity for ruthenium oxide.

When the ruthenium oxide reacts with the lithium, forces of physics change the alignment and behavior of the molecules. They found that the ruthenium atoms group into nanometer sized "islands", while the

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lithium and oxygen group together in a "sea" outside these islands (illustrated on page 1).

And keeping with the tropical analogy, extra space to store more lithium ions is created at the interface, or the "beach" of the islands.

The computational research was conducted on supercomputers through the Louisiana Optical Network Initiative (LONI), a high-speed, fiber-optic network that connects supercomputers at eight of Louisiana's premier universities.

Computational research has tremendous advantages for discovery because the experiments can be conducted "virtually" without a physical laboratory, greatly speeding up discovery time and testing of novel materials.

"One of the goals of the 2011 White House Materials Genome Initiative is to develop computational methods that can help us explore the properties of novel materials cheaper, faster, and safer than is possible by experimentation alone," said Dr. B. Ramu Ramachandran, Hazel Stewart Garner Professor of Chemistry and Executive Associate Dean for Research at Louisiana Tech University.

"This is also a goal we articulated back in 2009, in the NSF EPSCoR proposal that led to establishing LA-SiGMA. I believe our work on ruthenium oxide is an example of achieving that national goal. The computations reproduce the qualitative features of the cell voltage variations observed in the lab, and so we have some confidence that we are also getting qualitatively correct insights into the behavior of the material at the atomic scale."

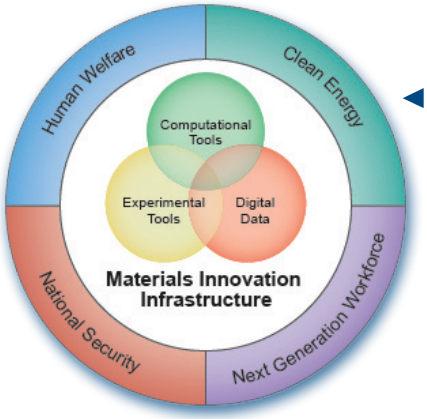
"This has opened the door to screening a wide range of potential anode materials computationally, which is exactly what we have done over the past two years, along with our LA-SiGMA graduate students and summer REU students."

This kind of insight from computational research could drastically improve the design, engineering and production of better, cheaper, and more durable lithium-ion batteries for large scale applications.

Dr. Ayorinde Hassan

Dr. Collin Wick

Dr. B. Ramu Ramachandran



"The vast spans of length and time scales covered by materials research create unique challenges for delivering quantitative and predictive scientific and engineering tools. Important components of the Materials Innovation Infrastructure will be the development of advanced simulation tools that are validated through experimental data, networks to share useful modeling and analysis code, and access to quantitative synthesis and characterization tools."

- Materials Genome Initiative Strategic Plan, U.S. Office of Science and Technology Policy, https://www.whitehouse.gov/mgi

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