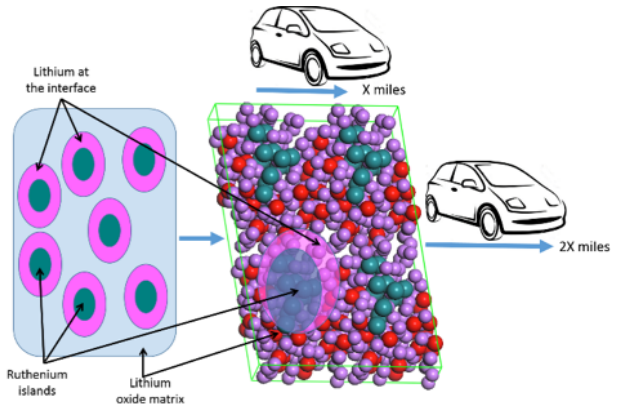
Materials Research Driving Next Generation of High Capacity Batteries

EPS - 1003897
RII: Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA) Louisiana **2010-2015**
PI: Dr. Michael Khonsari

What is the outcome or accomplishment?
While performing chemistry experiments with new materials for the next generation of lithium-ion high capacity batteries, Dr. Lamartine Meda, Associate Professor of Chemistry at Xavier University, demonstrated that ruthenium oxide stored more lithium than was theoretically predicted.



While investigating new materials for the next generation of lithium-ion batteries, LA-SiGMA researchers combined experiments and computations to shed new light on the mechanism by which one material, ruthenium oxide, is able to store far more lithium than predicted theoretically.

Credit: Dr. Collin Wick, Louisiana Tech University.

Inspired by Dr. Meda's results, three 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.

Using world-class computational tools, the research team extensively tested different theories for the source of this extra capacity, determining how different arrangements of the atoms influenced their properties. They were successful in finding the mechanism for this observed extra capacity: When the ruthenium oxide reacts with the lithium, ruthenium atoms group into nanometer sized "islands", while the lithium and oxygen group together in a "sea" outside these islands. Extra space to store more lithium ions is then created at the interface, or the "beach" of the islands, and this "interfacial storage" accounts for the extra capacity.

What is the impact?
Understanding the mechanisms responsible for the observed extra capacity at the atomic level will help in the discovery of better materials for the next generation of lithium-ion batteries.

What explanation/background does the lay reader need to understand the significance of this outcome?
While great for small devices like mobile phones and laptops, current generation 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 battery technology.