Louisiana researchers discover additional mechanisms for extra storage in battery electrode materials

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RII: Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA)
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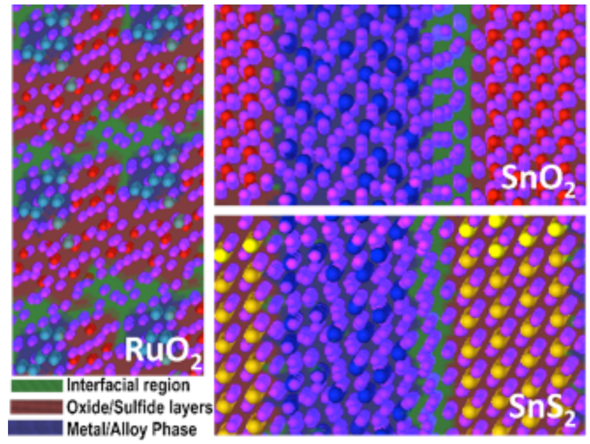

Three examples of how atoms arrange within oxide and sulfide electrode materials where the lithium is stored. The creation of the interfacial regions (green) during battery operation and the storage of the lithium (purple) in these green areas is one of the ways in which researchers discovered how these materials are able to achieve extra lithium storage capacities beyond expected limits.

Credit: Collin D. Wick, Louisiana Tech University.

Outcome: When comparing the capacity of different lithium battery electrode materials, experiments have shown a higher storage capacity than what was predicted based on the chemistry of the components. Louisiana computational researchers were successful in finding the mechanism driving the interactions between atoms that create this extra storage capacity in tin-based battery electrodes.

Impacts/Benefits: Understanding the underlying mechanisms at the atomic level that are responsible for the observed extra capacity will help speed up the discovery of new electrode materials and configurations for the next generation of lithium-ion batteries in cell phones, laptops and electric vehicles. Computational research has tremendous advantages for discovery because the experiments are conducted virtually without a physical laboratory, greatly speeding up discovery and testing times.

Background: In 2015, a Louisiana Tech University research team used world-class computational tools to extensively test different hypotheses for the source of the extra capacity observed in ruthenium oxide electrodes, and discovered that the ruthenium atoms group into “islands” creating extra space to store more lithium ions at the interface, or the “beach” of the islands (left illustration). At the end of 2015, this computational discovery was confirmed in lab experiments by a South Korean research team.

In 2016, the Louisiana researchers focused their computational research on more economical battery electrode materials, like tin oxide. They discovered that tin-based electrodes also held additional storage capacity like ruthenium oxide did, but with a different two-step mechanism (top right and bottom right illustrations).