GCEP

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A High Energy Density Lithium-Ion Battery with Self-Healing Polymers

Investigators

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Objective

The goal of this work is to develop high-energy, durable lithium-ion batteries for electric vehicles by improving the cycle life of the electrodes using self-healing polymers. The ideal polymer has three characteristics: 1) exhibits the self-healing capability at room temperature; 2) interactions strongly with the active electrode materials; and 3) can stretch to accommodate large volume changes associated with charge and discharge.

Background

To improve batteries for the transportation market, new materials for battery electrodes are needed. A typical lithium-ion battery has a phosphate cathode or a carbon anode made with a lithium-metal oxide. Using silicon-based anodes in place of graphite (carbon) results in a 10-fold increase in the theoretical specific charge capacity. One drawback, however, is that the active material experiences extreme expansion and contraction during the lithiation and delithiation process. These volumetric changes rapidly deteriorate the electrode materials producing cracks, electrical isolation or pulverization. By limiting its ability to endure several charge-discharge cycles, this results in a reduced battery life. Researchers have tried to address these challenges using nanostructured active materials and nanoparticles. But synthesizing these materials is costly, impairs the electronic connections between the nanoparticles and may lead to more side reactions with the electrolyte. Other research efforts on polymeric binders and metal alloys have yet to produce stable operation of the battery.

Approach

The researchers will create self-healing electrodes by coating high-capacity active materials with a layer of soft, self-healing polymers. The coating maintains the structural integrity of the electrode and accommodates volume expansion, as illustrated in Figure 1. Cracks may form when lithium enters the electrode, but in contrast to conventional polymer binders, these cracks can be closed through reversible non-covalent bonds or dynamic covalent bonds. This concept leads to stable electrical connections among the active particles and can be applied to other high-capacity electrode uses, such as fuel cells.

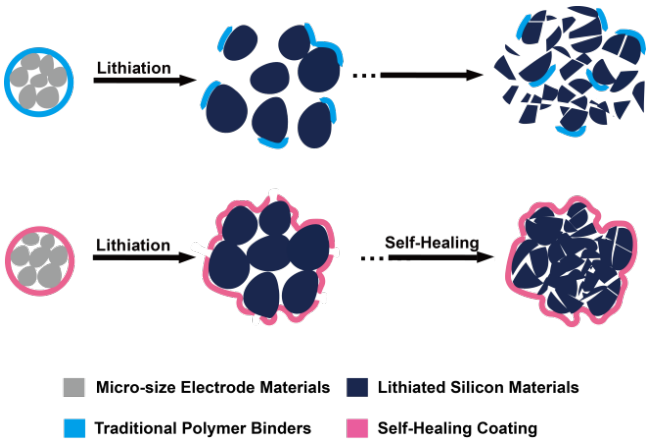

Figure 1: Schematic illustration of the self-healing concept applied to electrodes for a lithium-ion battery.

Design and synthesis of self-healing polymers for a lithium-ion battery

Hydrogen bonding-based supramolecular polymers appear to be the best candidates for the self-healing material. The general design is composed of a polymer backbone, hydrogen bonding sites and covalent cross-linking sites. The weak hydrogen bonds are expected to preferentially break during a mechanical event but then dynamically rearrange, intermix and associate. The covalent cross-linking sites further tune the mechanical properties of the polymer to different strengths and properties to obtain the optimum correlation between polymer design and battery performance.

Fabrication of self-healing electrodes for a lithium-ion battery

Conventional lithium-ion batteries consist of a graphite anode and a lithium-cobalt oxide ($LiCoO_2$) cathode. Researchers will investigate other electrode materials (such as silicon, germanium, tin and sulfur) with theoretically higher storage capacity. Figure 2 compares the capacity of these materials. For each material type, polymer structures will be tailored to electrode performance to achieve the best conductivity, chemical interaction and mechanical integrity. Standard characterizations, such as cycle life, rate and voltage profile, will also be performed.

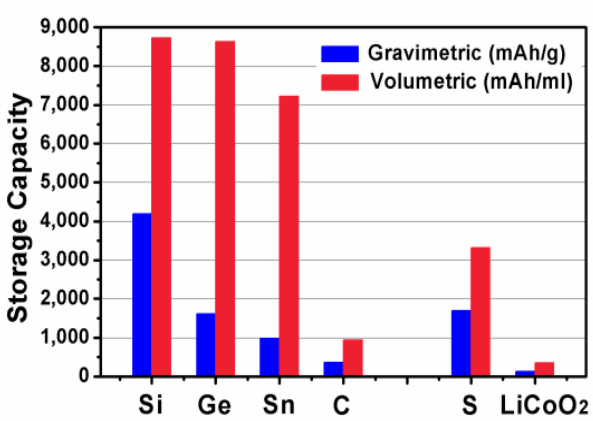

Figure 2: Theoretical gravimetric and volumetric capacities for electrode elements

Understanding the self-healing effect in the battery

It is important to understand what happens to the assembled electrodes during electrochemical cycling. To monitor size, morphology and composite changes during cycling, electron and X-ray based techniques will be used. For example, scanning electron microscopy will help elucidate morphological change in the materials and how self-healing polymers accommodate volumetric variations. *Ex-situ* X-ray diffraction will help determine structural changes of the materials, and X-ray absorption spectroscopy will reveal the time evolution of the oxidation state in both the active materials and the local environment.