Project 2: Engineering, Synthesis Scale-up, and Characterization of Sulfur-Infused Microporous Carbons (1 student)[#] - Lynden Archer

Electrochemical storage technologies that offer higher specific capacity, improved safety and extended performance lifetimes have received intensive consideration during the past decade to meet rising standards for portable electronic devices, electric vehicles, and

high-performance autonomous aircraft and robotics. Rechargeable electrochemical cells that use earth-abundant and low-cost materials are understood to be particularly good candidates to achieve many of these performance goals and may also offer other attractive attributes, such as environmental benignity and scalability. Among all solid-state cathodes, elemental sulfur offers the greatest promise for reversibly storing large amounts of electrical energy, up to 2.5 kWh/kg or 2.8 kWh/L, at moderate cost. Unlike currently used lithium-ion (Li-ion) batteries, which are based on intercalation chemistries in the cathode that yield one or fewer than one electron per transition-metal ion, a lithium-sulfur (Li-S) cell takes advantage of the spontaneous and reversible conversion reaction of sulfur with lithium ions in the cathode to ideally form lithium sulfide (Li_2S). The high energy of these cells derives from the fact that the conversion reaction yields up to two electrons per sulfur atom (1675 mAh/g) at a potential of around 2.1 V [5].

The superficial simplicity of the electrochemistry in the Li-S cell belie multiple challenges stemming from the complicated solution phase thermodynamics of sulfur and its reduction products in the cathode, and the resultant poor transport of electrons and ions in the Li-S battery electrodes and electrolyte. The insulating nature of sulfur and sulfides, for instance, limit electron transport in the cathode and leads to low active material utilization. Sulfur electrodes also have low stability due to the formation of soluble lithium polysulfides (LiPS) during the reduction of sulfur with lithium. In particular, the high solubility of intermediate LiPS species in commonly used electrolytes and its reactivity with others, causes loss of active material. Dissolved LiPS may also diffuse in the electrolyte, which increases its viscosity, lowers ionic conductivity, may clog the separator membrane, and may react with the metallic lithium anode in a parasitic, cyclic process termed shuttling, which not only leads to Li-S cell performance well below expectations for this chemistry, but also leads to degradation in performance over time. Thus, unlike the traditional Li-ion batteries, where cell-level performance usually approach 90% of theoretical capacities set by the chemistry of the anode and cathode, the best performing Li-S cells rarely deliver storage capacities above 60% of theoretical value.

Previous research in the Archer group has shown that infusing elemental sulfur in the vapor phase deep into the pores of a carbon host facilitates creation of Li-S batteries that overcome some of the aforementioned performance constraints on the cathode of a Li-S cell [6-7]. Preliminary results show that if the carbon host is engineered with a microporous, tortuous structure, these beneficial effects may be amplified. The proposed project will investigate scale-up of synthesis of these microporous carbons using two approaches. The project will also investigate creation of S@C composites in which elemental sulfur is infused in the vapor phase into the carbon hosts. Finally, the project will utilize electrochemical and physical characterization tools to evaluate the materials as cathodes in Li-S@C electrochemical cells.

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Interested M.S. and M.Eng. students should contact Prof. Lynden A. Archer, laa25@cornell.edu for additional information