

CHEMICAL ENGINEERING

DISTINGUISHED YOUNG SCHOLARS SERIES



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Understanding and Design of Polymer Materials for Stabilizing High Capacity Silicon and Lithium Metal Anodes

ABSTRACT: Lithium ion batteries have become the dominant form of energy storage used in consumer electronics and, recently, electric vehicles. However, high costs have prevented widespread deployment of lithium ion batteries for applications other than portable electronics, and the safety hazards of exothermic reactions associated with traditional materials remain to be addressed. In order to enable the greater utilization of electric vehicles, allow for grid scale energy storage, and meet the demands of new electronic applications, new materials for high energy density batteries must be developed. High capacity electrode materials like silicon and lithium (Li) metal can store 10x more charge than the graphite used in commercial electrodes, but significant hurdles must be overcome before these materials can be implemented in new technologies. Silicon, due to its brittle nature and large volume expansion during lithiation, has poor cycling stability, and lithium metal suffers from significant side reactions, poor quality deposition, and the potential to form hazardous dendrites which can short circuit the battery cell. Therefore, strategies to enhance the mechanical and chemical stability of these electrode materials are key to their successful application in commercial batteries.

In this presentation, I will discuss use of polymeric materials to address issues of stability in Li-ion batteries. The first portion of my talk will describe how varied crosslinking density in a supramolecular, hydrogen-bonding self-healing polymer affects the cycling stability of silicon anode materials. I have found that a balance of viscoelastic stress relaxation and stiffness is required to enable our self-healing electrode concept and maintain the mechanical integrity of the electrode. Following this study, I carefully developed a modified version of the polymer to be used as a coating that enabled the dendrite free deposition of Li metal anodes. With this new concept, improved Li deposition was obtained at current densities as high as 5 mA cm⁻², and we observed a

cycling Coulombic efficiency of over 97% for more than 180 cycles. This publication led to significant activity in the development of polymer coatings to protect the Li metal surface, yet many of these works were based on intuitive rather than rational design.

In the second part of my talk I will discuss further investigation toward general understanding of how polymer coatings affect lithium metal deposition and the identification of descriptors to be used for rational polymer design. I studied the effects of several carefully selected polymers with varied chemical and mechanical properties as coatings on the Li metal anode. By examining the early stages of lithium metal deposition, it was determined that while global morphology depends on the coating quality and mechanics, the local morphology of the lithium particles is strongly influenced by the chemistry of the polymer coating. Thermodynamic analysis of the Li nucleation process identified the polymer dielectric constant and surface energy as two key descriptors of the lithium deposit size.

High dielectric constant polymers increase the exchange current through improved Li⁺ ion solvation and promote larger lithium deposits, and low surface energy polymers have less interaction with the lithium surface and thus increase the interfacial energy, promoting larger deposits with smaller surface areas (Figure 1). Larger Li deposits are more desirable for higher efficiency cell operation. Overall, the work presented here contributes new materials to be used in electric vehicles, grid scale storage, and new electronic devices, and uses these materials to develop fundamental understanding about how materials properties affect the stability of lithium ion batteries in each application. This understanding provides direction for the design and synthesis of new polymer materials to better stabilize high capacity battery electrodes.

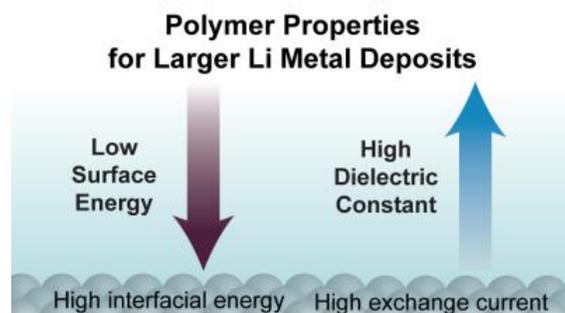


Figure 1 Schematic of the factors influencing Li metal deposition through a polymer coating

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BIOGRAPHY: Jeffrey Lopez earned his Ph.D. in 2018 from Stanford University under the supervision of Prof. Zhenan Bao. He was awarded a NSF Graduate Research Fellowship and a NDSEG Fellowship to fund his graduate work, which focused on developing new self-healing polymers and elastomers with novel mechanical properties for improving the stability of lithium ion batteries. Jeffrey is currently an Intelligence Community Postdoctoral Fellow at the Massachusetts Institute of Technology working with Prof. Yang Shao-Horn where he is studying mechanisms of electrochemical instability and ion transport in polymer electrolyte materials. Jeffrey has received multiple awards for his research including the ACS Eastman Chemical Student Award in Applied Polymer Science in 2018, the AIChE Excellence in Graduate Polymer Research Award 1st Prize in 2016. Jeffrey was involved with the Stanford Polymer Collective as President from 2013-2016 supporting the polymer research community on Stanford's campus, and has worked with various programs at Stanford and MIT to promote improved access to higher education among students from underrepresented minority groups.

LECTURE 4:00 - 5:00 (PAA) A118
Happy Hour in Benson Hall Lobby Following

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