MAR13-2012-020185

Abstract for an Invited Paper
for the MAR13 Meeting of
the American Physical Society

Materials for Electrochemical Energy Storage

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Electrochemical energy storage is a primary concern of both the consumer and public energy sectors. Energy, once generated, must be stored, transported and retrieved efficiently. This is commonly done through the use of various kinds of batteries and recently through the use of capacitors. Optimal energy storage involves the complete electrochemical system, but many of the performance properties can be understood in terms of the constituent materials that make up the anode, cathode and electrolyte. In this talk will give a brief overview of electrochemical energy storage systems and the role of materials in improving them. Using computational methods as a framework, I will discuss how discuss how macroscopic properties, such as capacity, conductivity, voltage, and stability are determined by fundamental materials properties at the quantum mechanical level. Using the knowledge gained from understanding the underlying processes, I will discuss some common battery materials, such as $LiFePO_4$, layered transition metal oxides, and oxide electrolyte materials. I will show how predictions for better materials can be made using computational tools to save time and money by circumventing expensive screening in the laboratory. I will also discuss how tailoring the morphology of materials, for example by synthesizing at the nanoscale, can have extreme benefits for battery materials performance.