Improving Lithium-air batteries by correlated modeling and experiment

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Abstract

Li-ion battery technology has reached a point in which the energy density can only be increased incrementally and will not meet the needs of future electric vehicles, portable power and military applications. Metal/air batteries have the potential to yield much higher energy density due to the elimination of the cathode to make a lighter battery package and the unlimited availability of oxygen from the environment. In particular, lithium-air batteries are especially attractive due to a high theoretical energy density. However, there are numerous challenges that must be solved before these batteries can be used commercially. In particular, the performance of the battery is highly dependent on the transport of lithium and oxygen through the electrolyte. Here, we investigate the effect of carbonate based electrolyte chemistries on the transport properties by molecular dynamics simulations, which are further correlated with experimental results of overall battery performance. A comparison of modeled and experimentally obtained transport properties reveals that our simulations are valid for predicting electrolyte performance. Optimal electrolyte chemistry will be discussed as well as development of a high capacity cathode material.