

Modeling Nanomaterials in Lithium Ion Battery with Experimental Validation

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A lithium-ion battery (Li-ion battery or LIB) is a rechargeable battery type in which lithium ions move from the negative electrode to the positive electrode during discharge and back when charging. Lithium systems are of considerable interest due to their high energy density and low toxicity compared to other rechargeable lithium battery chemistries. Conventional Lithium-ion battery materials typically start as 10-50 micron sized particles. In many of these new chemistries, having the materials in nanoparticle form or as a nanostructured particle or film is critical to achieving the desired performance. The goal of this study is to understand the mechanisms that govern the size-dependence of electrochemical properties and mechanical properties of nanomaterials in Lithium ion batteries using first principles method. We have been developing computational models of LiCoO₂ crystals. The specific objectives of the MURI project are to: (1) conduct first principles study of the electrochemical properties and mechanical properties of nanosize LiCoO₂; (2) investigate Li ion diffusion phenomena in the nanomaterial; and (3) experimentally validate the computational results.

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