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# Review

A review on First principles based studies for improvement of cathode material of lithium ion batteries

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## Abstract

Lithium ion batteries (LIBs) are currently best energy storage devices providing rechargeable electrical storage to wide variety of applications — from portable electronics to automobiles. Though, these batteries are fully adopted, widely used and commercialized, but researchers are still extensively working on their constituent materials and developing technology to improve the performance. A major part of related research activities is devoted to the electrode of the battery for improvement in its performance thereby addressing issues like safety, lifetime, specific capacity, energy density and most importantly abundance and cost. There are number of cathode materials that have been proposed and tested at laboratory scale and subsequently utilized in commercialized batteries ever since the appearance of LIBs. Owing to the availability of improved computational resources in the last decade, First principles calculation has become a reliable tool and played a vital role to predict the material properties of electrodes prior to their experimental analysis. This review gives a comprehensive insight and thorough analysis of the global research efforts related to the cathode materials based on First principles framework, sheds light on current status of knowledge and explores the ways forward.

**Keywords:** Lithium ion batteries; Electrodes; First principles methods

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