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# Ab initio simulation study of spinel LiMn<sub>2</sub> O<sub>4</sub> and nickel doped LiMn<sub>2</sub> O<sub>4</sub>

*Wednesday, 10 July 2013 15:40 (20 minutes)*

## Abstract content <br>   (Max 300 words)

Lithium ion batteries have been successful in portable electronics market due to their high energy density. However, increasing interest in lithium ion batteries for electric and hybrid electric vehicle applications require alternative cathode materials due to the high cost, toxicity, and limited power capability of the layered LiCoO<sub>2</sub> cathode. Doping in batteries improves the efficiency in maintaining electrochemical capacity over a large number of cycles without sacrificing initial reversible capacity at room temperature. Density functional theory employing the pseudo-potential plane-wave method within the generalized gradient approximation was used to investigate structural properties, density of states and elastic constants. The lattice parameters are in agreement with the available experimental results. Analysis of calculated elastic properties of LiMn<sub>2</sub>O<sub>4</sub> system predicts mechanical stability when the system is subjected to various strains.

## Apply to be<br> considered for a student <br>   award (Yes / No)?

No

## Level for award<br> (Hons, MSc, <br>   PhD)?

No

## Main supervisor (name and email)<br>and his / her institution

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## Would you like to <br> submit a short paper <br> for the Conference <br> Proceedings (Yes / No)?

No

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