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Type: **Poster Presentation**

Computer simulation studies of spinel LiMn_2O_4 and $\text{LiNi}_x\text{Mn}_{2-x}\text{O}_4$ $(0 \leq x \leq 2)$

Tuesday, 10 July 2012 17:30 (2 hours)

Abstract content **
 **(Max 300 words)

Spinel LiMn_2O_4 is a low-cost, environmentally friendly, and highly abundant material and is used as a cathode in Li-ion batteries. Doping in batteries improves the efficiency in maintaining electrochemical capacity over a large number of cycles without sacrificing initial reversible capacity at room temperature. We use computer simulation methods to study properties of spinel LiMn_2O_4 and doped $\text{LiNi}_x\text{Mn}_{2-x}\text{O}_4$ ($0 \leq x \leq 2$). In particular, spin density functional theory employing the pseudo-potential plane-wave calculations within the generalized gradient approximation is used to investigate spinel structural and electronic properties; and pressure dependence. The calculated structural parameters are found to be in good agreement with experimental and literature results. In addition, the structural changes and electronic properties of LiMn_2O_4 spinel as a function of nickel content were investigated. The lattice parameters for doped systems are in coherent with the available experimental results. Analysis of electronic properties predicts the nature of bonding for both pure and doped systems.

Apply to be **
 consider for a student
 **award (Yes / No)?

Yes

Level for award **
 **(Hons, MSc, **
 **PhD)?

Hons

Main supervisor (name and email) **
 and his / her institution**

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Would you like to **
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 Proceedings (Yes / No)?**

No

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