Contribution ID: **287** Type: **Oral Presentation**

Stabilities of low and high pressure structures of CoPO₄ and MnPO₄

Wednesday, 13 July 2011 14:45 (15 minutes)

<p>Crystals of LiFePO₄ and related materials have recently received a lot of attention due to their promising use as cathodes in rechargeable lithium ion batteries. These compounds have been known for good stability and low cost. The Co based compound LiCoPO₄, has rapidly become of particular interest as recent measurements found a potential of 4.8 V, while the Mn based compound structure has an equilibrium voltage of 4.1 V, which is compatible with the electrolyte presently used in Li-ion batteries. Before the introduction of amorphisation recrystallisation methods to quaternary LiMPO₄ (M=Mn and Co), it will be important to commence with ternaries (CoPO₄ and MnPO₄), since ternaries are less complex. Hence we investigate the mechanical, optical and structural stabilities of the different polymorphs of CoPO₄ and MnPO₄, before atomistic simulations, by employing the pseudo-potential planewave calculations within the Local Density Approximation (LDA) and Pardew-Wang Generalized Gradient Approximation (GGA).

Level (Hons, MSc,
   PhD, other)?

MSc

Consider for a student
   award (Yes / No)?

Yes

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

No

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Session Classification: CMPMS2

Track Classification: Track A - Condensed Matter Physics and Material Science