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Stabilities of low and high pressure structures of CoPO_4 and MnPO_4

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Crystals of LiFePO_4 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 LiCoPO_4 , 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 LiMPO_4 (M=Mn and Co), it will be important to commence with ternaries (CoPO_4 and MnPO_4), since ternaries are less complex. Hence we investigate the mechanical, optical and structural stabilities of the different polymorphs of CoPO_4 and MnPO_4 , before atomistic simulations, by employing the pseudo-potential planewave calculations within the Local Density Approximation (LDA) and Perdew-Wang Generalized Gradient Approximation (GGA).

Level (Hons, MSc, PhD, other)?

MSc

Consider for a student award (Yes / No)?

Yes

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

No

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