Contribution ID: **156** Type: **Oral Presentation**

First principle stability study of FePO₄ and LiFePO₄ polymorphs

Tuesday, 10 July 2012 14:30 (20 minutes)

Abstract content
   (Max 300 words)

Lithium iron phosphate, LiFePO₄ has been under intense study as a future cathode material for lithium ion batteries, due to its good thermal stability, competitive electrochemical properties, high safety, low cost, and long life cycle; and it has been recently commercialized in power tool applications. The electrochemical charge/discharge potential profile of Li/LiFePO₄ cells is very flat and located at 3.45V vs. Li/Li+, moreover, its theoretical capacity is relatively high (170 mAh/g). We use first principle calculations to investigate the structural, electronic and mechanical properties of FePO₄ and LiFePO₄ employing the pseudo-potential plane-wave within the local density approximation. We also determine the effect of lithiation on FePO₄ polymorphs. Our results show that β-FePO₄ and HP-FePO₄ shows stability over α-FePO₄, while lithiation stabilises FePO₄ polymorphs.

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Session Classification: DCMPM1

Track Classification: Track A - Division for Condensed Matter Physics and Materials