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First principle stability study of FePO_4 and LiFePO_4 polymorphs

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Abstract content
 (Max 300 words)

Lithium iron phosphate, LiFePO_4 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/LiFePO_4 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 FePO_4 and LiFePO_4 employing the pseudo-potential plane-wave within the local density approximation. We also determine the effect of lithiation on FePO_4 polymorphs. Our results show that $\beta\text{-FePO}_4$ and HP- FePO_4 shows stability over $\alpha\text{-FePO}_4$, while lithiation stabilises FePO_4 polymorphs.

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