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Stabilities of low and high pressure structures of FePO4

On introducing amorphisation recrystallisation methods to LiFePO4, ternaries (FePO4), will be more amenable than the quaternary LiFePO4, since they are less complex. Hence we investigate the stabilities of the different polymorphs of FePO4, before atomistic simulations, by employing the pseudo-potential planewave calculations within the Local Density Approximation (LDA) and pardew-wang Generalized Gradient Approximation (GGA).

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