Nampo4 triphylite and olivine phases

In order to explore the effects of synthetic conditions on the relative phase stabilities, temperature- and pressure-dependent free energies of olivine and maricite NaMPO4 are calculated.

A full range of solid solution behavior was observed for olivine Na 1-x Mn 0.5 Fe 0.5 PO 4, in contrast to that of LiMPO 4 (M = Fe, Mn) olivine materials, and is ascribed to ion size effects. The ...

NaFePO 4 exists as two distinct polymorphs, triphylite (i. e., ...

NaFePO 4 exists as two distinct polymorphs, triphylite (i. e., olivine) and maricite. 16 To date, the triphylite phase was not reported by direct synthesis at neither high nor moderate ...

ions within the olivine phosphates cannot be fully described using only single-particle calculations. This method provides a means to analyse the collective dynamics of many particles and connect ...

In this study, we investigate the structural, thermodynamic, electronic and mechanical properties for the olivine NaMPO4 (M=Fe, Co, Mn) structures to determine their stability and competences...

These materials have been extensively studied in their most common olivine structures: maricite and triphylite.

Nampo4 triphylite and olivine phases ... The shooter method is a modification of the shooter algorithm used in transition path sampling, which is employed here to systematically perturbate points in phase ...

Amongst this family of compounds, triphylite NaFePO 4 emerged as the most promising material owing to its high theoretical capacity (154 mAh g -1). Unlike LiFePO 4, NaFePO 4 exists in ...

The impact of Na atom deintercalation on olivine NaMnPO4 was investigated in a first-principle study for prospective use as cathode materials in Na-ion batteries.

Compared to their lithium analogues, NaMPO4 materials exist in two structures, maricite and olivine. Their implementation calls for an in-depth investigation of diffusion/conduction ...

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