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Vibrational and thermodynamic properties of monazite-type LnPO4 (Ln=La, Ce): A first Principles study

Monazite is an ore mineral consisting of various rare earth elements (REEs), thorium (Th), and uranium (U). These components are utilized in numerous modern areas of technology, including metallurgy, catalysis, and magnetic fields. This monazite mineral has a notoriously stable structural conformation, making the conventional cracking process extremely inefficient. However, new innovative technologies (e.g., thermal cracking) have been proposed for improving the extraction of REEs (such as La,Ce and Nd), Th and U. In this study, we evaluate theoretical considerations relating to these thermal processes on the inherent monazite structure. First-principles calculation based on density functional theory was used to investigate vibrational and thermodynamic properties of monazite systems. It was found that the lattice parameters of LaPO4 and CePO4 monazite correlate well with experimental values to within 5% error. The heats of formation value for LaPO4 (-0.766 eV/atom) is more negative than for CePO4 (-0.729 eV/atom), suggesting the most stable structure. The vibrational instability of LaPO4 and CePO4 systems emanates from the observed soft mode by the phonon dispersion curves. Furthermore, monazite systems were found to exhibit electron excitation at a temperature of about 500 K. The findings assisted in understanding the physical movement of atoms, crystal packing and thermodynamic structure of monazite at evaluated temperatures.

Keywords: Monazite, Density functional theory, Thermodynamics properties

Apply to be considered for a student ; award (Yes / No)?

yes

Level for award;(Hons, MSc, PhD, N/A)?

Msc

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