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Computational studies of pressure dependence on Monazite-(Ce)

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Monazite-(Ce) is an orthophosphate mineral of the monazite group with the formula A[PO4], where A represents Ce and other light rare earth elements (LREE) in place of Ce. Studying the structural stability of monazite-(Ce) is of vital importance in the storage of radioactive waste application. A first-principle calculation based on density functional theory was used to study the structural, mechanical, and vibrational properties of Monazite-Ce under different pressure range from 10-50 GPa. The calculated structural parameters of monazite systems at zero pressure and temperature agree with the experimental data within 5 %. The Modulus (Bulk, Shear, Young's), and anisotropy increase with an increase in pressure. Furthermore, Pugh (B/G) and Poisson ratio show that monazite system is ductile and the ductility can be improved with an increase in pressure. The vibrational instability of the CePO4 system is observed which is caused by the soft mode detected from the phonon dispersion curve. However, the system becomes vibrationally stable when the pressure is increased. The insights gained from high-pressure studies are of interest for the applications of monazite.

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

yes

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

MSc

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