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(Research Article)

Ab-initio study of the structural and phononic properties sodium hydroxide

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Abstract

In this work the structural phase stability and phononic properties of sodium hydroxide compound have been reported. The calculations have been performed using the pseudo potential method with plane wave based on density functional theory (DFT). Local density approximation (LDA) and generalized gradient approximation (GGA) have been used for modeling the exchange-correlation potential. Negative frequencies have been observed to indicate system instability. The calculated results are in good accordance with existing theoretical and experimental data.

Keywords: Density Function Theory, NaOH, Orthorhombic phase, Structural stability, Phononic properties.

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