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Finite temperature thermophysical properies of MgO

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In the present work, results of theoretical study of finite temperature thermophysical properties of MgO are reported. Ground state properties viz., total and cohesive energies are calculated using plane wave pseudopotential density functional theory within local density appproximation (LDA). Further, ionic contribution at finite temperature is taken into account using quasi-harmonic Debye model. Calculated free energies at elevated temperatures are minimized with respect to volume to obtain volume thermal expansion and thereby other thermophysical properties. The presently calculated results are compared with the experimental results as well as those due to Wang and Ahuja. It is found that the present results are in agreement with the experimental results in the whole temperature range. Results confirm the applicability of present appraoch in correctly determining the trends in thermophysical properties of lower earth mantle like MgO.

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