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Ab initio thermodynamics of LaB_6 and CeB_6 TANJU GUREL, RESUL ERYIGIT, Abant Izzet Baysal University — We have investigated the phonon and thermodynamical properties of rare-earth hexaborides RB_6 (R=La and Ce) on the basis of first-principles pseudopotential plane wave method together with the quasiharmonic phonon calculations. The phonon dispersion relations which are calculated in the linear response framework and the temperature dependent lattice constant, bulk modulus and the volume expansion coefficients which are calculated in the quasiharmonic approximation are in good agreement with the experimental data. We calculate the low temperature constant volume specific heat due to phonon and electronic degrees of freedom and extract the Kondo contribution to specific heat of CeB_6.

Tanju Gurel
Abant Izzet Baysal University

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