2nd World Congress and Expo on
Nanotechnology and Material Science
April 04-06, 2016 at Dubai, UAE

First-principle calculations of structural, elastic, vibrational and thermodynamic properties of BaHfO3 under hydrostatic pressure

H.Krarcha, B. Bennecer
LPG laboratory University 08 Mai 1945,Guelma, Algeria

The influence of pressure on the structural, elastic, vibrational and thermal properties of cubic Perovskite BaHfO3 is studied by employing the density –functional theory within the local density approximation (LDA) in conjunction with the quasiharmonic approximation. The results are compared with previous calculations and experimental data. Through the quasi-harmonic Debye model, in which the phononic effects are considered, the temperature effect on the lattice constant, bulk modulus, thermal expension coefficient, heat capacity and Debye temperature is calculated.