World Academy of Science, Engineering and Technology
International Journal of Physical and Mathematical Sciences
Vol:9, No:06, 2015

First Principles Study of Structural and Elastic Properties of BaWO4 Scheelite Phase Structure under Pressure

Authors : Abdennour Benmakhlouf, Abdelouahab Bentabet

Abstract : In this paper, we investigated the athermal pressure behavior of the structural and elastic properties of scheelite BaWO4 phase up to 7 GPa using the ab initio pseudo-potential method. The calculated lattice parameters pressure relation have been compared with the experimental values and found to be in good agreement with these results. Moreover, we present for the first time the investigation of the elastic properties of this compound using the density functional perturbation theory (DFPT). It is shown that this phase is mechanically stable up to 7 GPa after analyzing the calculated elastic constants. Other relevant quantities such as bulk modulus, pressure derivative of bulk modulus, shear modulus; Young's modulus, Poisson's ratio, anisotropy factors, Debye temperature and sound velocity have been calculated. The obtained results, which are reported for the first time to the best of the author's knowledge, can facilitate assessment of possible applications of the title material.

Keywords : pseudo-potential method, pressure, structural and elastic properties, scheelite BaWO4 phase
Conference Title : ICPM 2015 : International Conference on Physics and Mathematics
Conference Location : Paris, France
Conference Dates : June 25-26, 2015