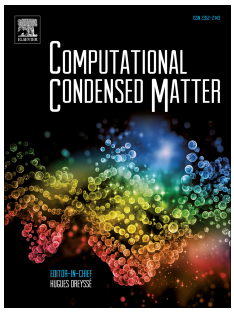
Accepted Manuscript



First-principles study of the electronic structure, magnetism, and phonon dispersions for CaX (X = C, N) compounds

L. Beldi, H. Bendaoud, K.O. Obodo, B. Bouhafs, S. Méçabih, B. Abbar

PII: S2352-2143(18)30208-9

DOI: 10.1016/j.cocom.2018.e00336

Article Number: e00336

Reference: COCOM 336

To appear in: *Computational Condensed Matter*

Received Date: 4 July 2018

Revised Date: 22 September 2018

Accepted Date: 23 September 2018

Please cite this article as: L. Beldi, H. Bendaoud, K.O. Obodo, B. Bouhafs, S. Méçabih, B. Abbar, First-principles study of the electronic structure, magnetism, and phonon dispersions for CaX (X = C, N) compounds, *Computational Condensed Matter* (2018), doi: https://doi.org/10.1016/j.cocom.2018.e00336.

First-principles study of the electronic structure, magnetism, and phonon dispersions for CaX (X = C, N) compounds

L. Beldi [1], H. Bendaoud[1], K. O. Obodo[2], B. Bouhafs[1], S. Méçabih[1], and B. Abbar [1,*]
[1]Laboratoire de Modélisation et Simulation en Sciences des Matériaux, Université Djillali Liabès de Sidi Bel-Abbès, Sidi Bel-Abbès, 22000, Algeria
[2]Physics Department, University of South Africa, Pretoria, P O Box 392, 0003, South Africa

*Corresponding author: (B. Abbar) E-mail: abbarb@yahoo.fr

Abstract:

The structural, vibrational, elastic, electronic, and magnetic properties of CaX (X = C, N) compounds in different phases are studied using first principles calculations based on spin polarized density functional theory within the generalized gradient approximation (GGA-PBEsol) and the modified Becke-Johnson approach (mBJ-GGA-PBEsol) for the exchange-correlation energy and potential. From the various phases of CaC and CaN compounds considered, which are rock-salt (NaCl), CsCl, zinc blende (ZB), NiAs- and WZ-type hexagonal, tetragonal (*P*4/*nmm*), and orthorombic (*Pnma*) phases, we obtained that NaCl and CsCl phases are the lowest energies as a function of volume for CaN and CaC compounds, respectively. The ferromagnetic phase is energetically favored with respect to the non-magnetic phase in CaN and CaC compounds, except for the CsCl and tetragonal phases in the CaC compound. The calculated elastic properties for the NaCl, ZB and WZ phases show that they are elastically stable. Considering the phonon dynamics of CaN and CaC compounds in the NaCl, ZB and WZ phases, we observed that CaC compound in the NaCl and ZB phases is dynamically stable due to the absence of imaginary modes in phonon dispersion. However, CaN compound is dynamically unstable in all considered phases. From electronic band structure and density of states, CaN and CaC compounds show half-metallic behaviour in NaCl and ZB phases. The half-metallic and magnetic character found in CaN and CaC compounds is attributed to the presence of spin polarized 2*p* orbitals of the nitrogen and carbon atoms, respectively. We found that CaN and CaC compounds are half-metallic ferromagnets with magnetic moment of 1 μ_B and 2 μ_B per formula unit, respectively. Using GGA-PBEsol (mBJ-GGA-PBEsol), our calculated half-metallic (HM) gaps for CaN and CaC compounds, are respectively, 0.003 eV (1.33 eV) and metallic (0.85 eV) in the NaCl phase, and 0.74 eV (1.94 eV) and 0.84 eV (1.95 eV) in the ZB phase.

Keywords: Density functional theory; Phase stability; Phonon; Half-metallic