Abstract

Using the plane wave pseudopotential approach to density functional theory within the generalized gradient and local density approximations, we investigated the structural, electronic, magnetic, lattice-dynamics, and thermodynamic properties of rocksalt alkaline earth metal carbides CaC, SrC, and BaC. The phonon dispersion spectra were investigated by using the linear response to density functional theory within generalized gradient approximation. The quasiharmonic approximation allowed us to calculate the evolution with temperature of some fundamental thermodynamic properties such as heat capacity, vibrational entropy, internal energy, free energy of vibration, mean squared displacement, and thermal expansion coefficient.