Prediction study of the structural and elastic properties for the cubic skutterudites $LaFe_4A_{12}$ (A = P, As and Sb) under pressure effect

Abstract

We have performed accurate ab initio total energy calculations using the full-potential linear augmented plane wave plus local orbitals method with the local density approximation for the exchangecorrelation potential to investigate the systematic trends for structural and elastic properties of the cubic $LaFe_4A_{12}$ skutterudites' family depending on the type of A pnicogen atom (A stands for P, As and Sb). The calculated equilibrium lattice constants and internal free parameters are in good agreement with the experimental results. For the first time, the numerical estimates of the independent elastic constants and their pressure dependence are performed using the total energy variation as function of strain technique. Isotropic elastic parameters and related properties, namely bulk modulus, shear modulus, Young's modulus, Poisson's ratio, Lam's coefficients, average sound velocity and Debye temperature, are estimated in the framework of the VoigtReussHill approximation for ideal polycrystalline $LaFe_4A_{12}$ aggregates.