Calculation of the lattice constant of hexagonal compounds with two dimensional search of equation of state and with semilocal functionals a new package (2D-optimize)

Abstract

A new package for calculating lattice constants and equation of state for hexagonal and tetragonal structure is released. We call it as 2D-optimize. The new package is compatible with the highly accurate all-electron full-potential (linearized) augmented plane-wave plus local orbital [FP-(L)APW+lo] method implemented in WIEN2k code. This package is available with WIEN2k code. We have performed a convenient volume and c/a structure optimization by using 2D-optimize package. First, we find the best value of c/a and therefore the energy for each volume, and then for those volumes and energies the equation of state (EOS) will obtained, and after that the value of c/a calculates within optimal volume. We have done 1D and 2D search of EOS for MnAs and Mg within PBE functional and compared the results with experimental data, the results of 2D search for EOS are better than 1D search of EOS. The cell parameters and the bulk modulus of 20 hexagonal structure compounds were calculated using the new package and compared with the experimental data.