First principles calculations of atomic structure and physical properties of calcium apatites

O. D. Feya, V. L. Karbovskii, A. P. Soroka

G.V. Kurdyumov Institute of Metal Physics of NASU, Kiev, Ukraine

Electronic structure of calcium apatites $Ca_{10}(ZO_4)_6X_2$, where Z=P, As, V; X=OH, F, Cl was investigated by quantum-mechanical modelling methods in the density functional theory (DFT) in the generalized gradient approximation (GGA) and LMTO-approximation using the ABINIT package. It was shown that $Ca_{10}(PO_4)_6Cl_2$ and $Ca_{10}(PO_4)_6F_2$ organizes in space group $P6_3/m$, but not in $P6_3$. Small deviations of the total energy per unit cell indicate that the anions F-and Cl-stored relative lability position on the axes of the sixth order. Phonon density of states for all series apatite $Ca_{10}(PO_4)_6X_2$, where X = F, Cl, OH, have a distinct band character with different length of the individual sub-bands. The first band contains most vibrational states and is localized in the range of wave vectors from 0 to 370 cm^{-1}, the second band – from 380 to 500 cm^{-1}, the third band is localized in 600-800 cm^{-1}, and the fourth – 800-1150 cm^{-1}.The first, second and third bands correspond to the vibrations of the PO_4 tetrahedra in the apatite, the frequencies of which are in good agreement with the experimental phonon frequencies of isolated PO_4 tetrahedron. Also, the dielectric tensor and the elastic constants of calcium apatite are calculated.