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Quantum mechanical calculations of the calcium apatites structure and properties

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Electronic and atomic structures as well as physical properties of the apatite series $Ca_{10}(PO_4)_6X_2$ (where X = F, Cl, Br, OH) were investigated by using quantum-mechanical methods within DFT (density functional theory): all-electron full-potential LAPW+LO (WIEN package), pseudopotential and PAW methods (Abinit package).

It was found that on account of energy expediency $Ca_{10}(PO_4)_6F_2$ and $Ca_{10}(PO_4)_6Cl_2$ formed group $P6_3/m$ instead of group $P6_3$, although small divergency of full energy for unit cell shows that anions F^- and Cl^- keep lability to their position on *c* axe. The shortest $O–O_{(adjacent\ tetrahedron)}$ bound of the investigated apatites is $O_{(1)}–O_{(1)c}$ bound, i.e. $O_{(1)}–O_{(1)}$ interactions make a main contribution into interactions between tetrahedron complexes.

Obtained X-ray emission bands O K_α of $Ca_{10}(PO_4)_6F_2$ and $Ca_{10}(PO_4)_6(OH)_2$, Ca K_β of $Ca_{10}(PO_4)_6(OH)_2$ were in good accordance with the experimental spectra. The accordance between theoretical and experimental curves of $L_{II,\ III}$-band of calcium in $Ca_{10}(PO_4)_6F_2$ was slightly worse, which indicates the need to consider relativistic corrections. Some discrepancy between theoretical and experimental forms of the bands P K_β of $Ca_{10}(PO_4)_6(OH)_2$ was caused by the small radius of MT-sphere of phosphorus and consequently by not taking into account the electron density of phosphorus located beyond it. The difference between the forms of curves of theoretical and experimental F K_α bands of $Ca_{10}(PO_4)_6F_2$ is caused by significant underestimation of the Ca—F bond covalent component by the calculation.

It was found that calcium phosphate chlor-, fluor- and hydroxyapatites have the elasticity constants C_{33} higher than C_{11}. Sound velocity along the sixth-order axis of calcium chlor-, fluor- and hydroxyapatites is higher than in the planes perpendicular to it.

Phonon spectra of calcium phosphate apatites were in good agreement with the IR-spectrometry data.