

ELECTRONIC STRUCTURE PECULIARITIES OF DISORDERED DIPHOSPHATES of Mn and Co

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Disordered diphosphates are of scientific interest in terms of modifying their operational properties by varying the nature of the cations and their content in the structure.

In these work the electronic structure peculiarities of disordered diphosphate - $\text{Mn}_{2-x}\text{Co}_x\text{P}_2\text{O}_7 \cdot 5\text{H}_2\text{O}$, were $x=0, 0.6, 1.0, 1.9, 2.0$, have been studied out by the XPS and X-ray emission spectroscopy.

The data obtained suggest that the substitution of manganese by cobalt is accompanied by both a redistribution of the electron density between the atoms of the metal sublattice, proceeding according to their electronegativity values, and the change in the chemical bond nature between the metal atoms and the surrounding oxygen.

The increase of cobalt content leads to an increase in the covalent component of the chemical bond in the overall charge balance.

Substitution of cobalt by manganese is accompanied by an essential increase in the electron density on the oxygen atoms involved in formation of the chemical bond with metal atoms, which leads to the formation of states laying in the upper part of the valence band of the investigated samples.