

STUDY OF THE ATOMIC AND ELECTRONIC  
STRUCTURE OF THE  $\text{La}_{0.5}\text{Li}_{0.5}\text{TiO}_3$   
IONIC COMPOUND

*A.N. Timoshevskii, S.A. Kalkuta, L.V. Tymoshevska*

Institute of Magnetism, Nat. Acad. Sci. of Ukraine  
(36b, Academician Vernadsky Blvd.,  
Kyiv 03142, Ukraine)

S u m m a r y

We have studied the electronic structure of the  $\text{La}_{0.5}\text{Li}_{0.5}\text{TiO}_3$  ionic compound using the FLAPW first-principle method. We performed the total energy calculations for a number of ordered crystal structures having different La and Li atoms distributions which simulate this compound. It is shown that the ordered structure with alternating La and Li atomic layers is more favorable energetically. It is found that, in this structure, a La atom is placed at the center of the face of a cube built by Ti atoms contrary to the common view that it is placed at the center of the cube itself. This fact enables explaining the availability of ionic conductivity in the  $\text{La}_{0.5}\text{Li}_{0.5}\text{TiO}_3$  compound and allows one to describe ionic compounds by the common formulae  $\text{La}_{1/3(2-x)}\text{Li}_x\text{Ti}_{3-x}\text{O}_3$ . Using the method of X-ray Emission Spectroscopy, we have studied experimentally the electronic structure of the  $\text{La}_{0.5}\text{Li}_{0.5}\text{TiO}_3$  compound. A good correspondence between theoretical and experimental results is demonstrated.