Electronic band structure and magnetic properties of $La_{2/3}Pb_{1/3}MnO_3$

W. Tokarz[a], M. Kowalik[a,b], R. Zalecki[a], A. Kołodziejczyk[a]

[a]Department of Solid State Physics, Faculty of Physics and Applied Computer Science, AGH Univ. of Science and Technology, 30, Mickiewicza Str, 30-059 Cracow, Poland

[b]Department of Physics, Rzeszów University of Technology, 6, Powstańów Warszawy Str, 35-959 Rzeszów, Poland

9.7 cm

We present a theoretical study of electric and magnetic properties in perovskite $La_{2/3}Pb_{1/3}MnO_3$. The calculation was carried out based on first-principles density functional theory (DFT) with general gradient approximation GGA+U using Wien2K package. The P3c1 crystal structure was taken from the detailed X-ray diffraction data for the perovskite [1]. For Mn d electrons exact exchange energy was utilized. Density of state (DOS) was determined by modified tetrahedron method. As a result we get a valance band shift for the spin up and down density of states with the top of the latter at 1.85 eV below the Fermi energy level (E_F). We noticed that conduction band is mainly dominated by d spin up manganese electrons, Mn d_{xz} and d_{yz} states have two times larger contribution than $d_{x^2y^2}+d_{xy}$. We attribute this to Mn-0_6 octahedral tilting. From the same reason d_{z^2} state has no contribution to the DOS at E_F. Comparison of total DOS with ultraviolet photoemission spectroscopy (UPS) measurements shows similar features [2] especially as far as the lead spectral intensity from the 6s electrons at about -9.5 eV is concerned. The calculated total magnetic moment per formula unit is 3.66 μ_B. There is some discrepancy between this value and the measured magnetic moment 3.48 μ_B/fu [3].

[1] Gritzner, G., Koppe, M., Kellner, K., Przewoźnik, J., Chmist, J., Kołodziejczyk, A., Krop, K., 2005. Preparation and properties of $La_{0.67}Pb_{0.33}(Mn_{1-x}Fe_x)O_3$ compounds. Appl. Phys. A 81, 1491-1495

[2] Kowalik, M., Zalecki, R., Kołodziejczyk, A., 2010. Electronic States of Collosal Magnetoresistive Manganites $La_{0.67}Pb_{0.33}Mn_{1-x}Fe_xO_3$ from Photoemission Spectroscopy. Acta Phys. Polon. A 117, 257-260

[3] Przewoźnik, J., Kowalik, M., Kołodziejczyk, A., Gritzner, G., Kapusta, C., 2010. Magnetic and magnetotransport properties of the $(La_{0.67}Pb_{0.33})(Mn_{1-x}Fe_x)O_3$ ($0 \leq x \leq 0.1$) compounds. J. All. Comp. 497, 1723

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Corresponding author :

W. Tokarz

Address for correspondence :

W. Tokarz
Department of Solid State Physics
Faculty of Physics and Applied Computer Science
AGH University of Science and Technology
30, Mickiewicza Str
30-059 Cracow, Poland

Email address :

tokarz@agh.edu.pl