Electronic band structure and magnetic properties of La$_{2/3}$Pb$_{1/3}$MnO$_3$

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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 $d_{zx}$ and $d_{yz}$ states have two times larger contribution than $d_{x^2-y^2}$ and $d_{z^2}$ states. We attribute this to Mn-06 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 $\mu_B$. There is some discrepancy between this value and the measured magnetic moment 3.48 $\mu_B$/fu [3].


[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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