Electronic band structure and magnetic properties of $La_{2/3}Pb_{1/3}Mn_{2/3}Fe_{1/3}O_3$

Marcin Kowalik[1,2], Waldemar Tokarz[1], Ryszard Zalecki[1], Andrzej Kołodziejczyk[1]

1. *AGH University of Science and Technology, Faculty of Physics and Applied Computer Science (AGH), Mickiewicza 30, Kraków 30-059, Poland* **2.** *Rzeszow University of Technology, Rzeszów, Poland*

e-mail: mkowalik@prz.edu.pl

We present theoretical study of some electric and magnetic properties in manganese perovskite $La_{2/3}Pb_{1/3}Mn_{2/3}Fe_{1/3}O_3$. The calculation was carried out based on first-principles density functional theory (DFT) with general gradient approximation GGA+U using Wien2K package. The P-3c1 crystal structure was taken from the detailed X-ray diffraction data for the perovskite [1]. For Mn and Fe *d* electrons exact exchange energy was utilized. Two different configurations of initial magnetic moment orientation (parallel *[Mn UP, Fe UP]* and antiparallel *[Mn UP, Fe DOWN]*) between Mn and Fe atoms was considered in self consistent calculation. Density of state (DOS) determined by modified tetrahedron method displays band gap for both spin initialization (fig.1 and 2). On the basis of previous work [2] we expect that this compound should show insulating ground state. In order to get consistent results we have started calculations in paramagnetic non-polarized spin magnetic ground state of the compound.

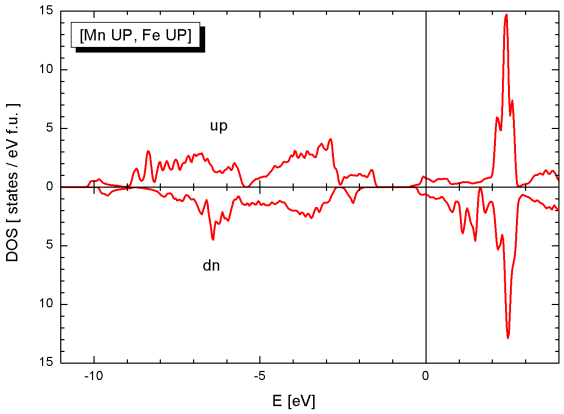

Fig. 1. Total DOS for spin up (up) and down (dn) for parallel magnetic moment orientation.

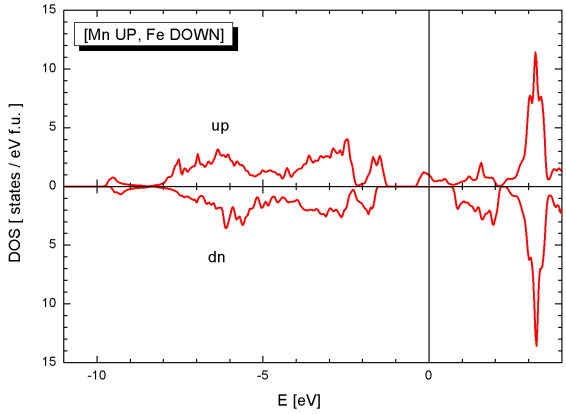

Fig. 2. Total DOS for spin up (up) and down (dn) for antiparallel magnetic moment orientation.

References:

[1] Gritzner, G., Koppe, M., Kellner, K., Przewoznik, 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] Przewoźnik, J., Kowalik, M., Kołodziejczyk, A., Gritzner, G., Kapusta, C., 2010. Magnetic and magnetotransport properties of the $(La_{0.67}Pb_{0.33})(Mn_{1-x}Fe_x)O_3$ ($0 \le x \le 0.1$) compounds. J. All. Comp. 497, 17–23

[3] 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