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Electronic band structure of $La_{2/3}Pb_{1/3}Mn_{2/3}(Co,Fe,Ni)_{1/3}O_3$

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We have investigated the theoretical valence band structure of half-metallic $La_{2/3}Pb_{1/3}Mn_{2/3}(Co,Fe,Ni)_{1/3}O_3$ Colossal magnetoresistance (CMR) manganites. The calculations were done based on first-principles Density Functional Theory (DFT) with General Gradient Approximation GGA+U using Wien2K package [1]. Density of state (DOS) was calculated using the modified tetrahedron method.

The calculated photoemission spectra for all three substitutions are similar in shape. The main effect of the substitution of an Mn atom by a transition metal such as Fe, Co or Ni, is a progressive decrease of width of an insulating gap. This effect should be seen in the UPS or XPS valence band spectra.

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The influence of NP's with Fe_3O_4 core on biomembrane modelsystems - the ATR-FTIR studies

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Keywords: nanoparticles, phospholipids, DMPC, ATF-FTIR spectroscopy

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Studies were performed to investigate the influence of nanoparticles with magnetic core - Fe_3O_4 on biomembrane model systems, based on DMPC. NP's were synthetized using standard methods [1,2] and characterized by TEM, magnetic (SQUID) and Raman spectroscopies. Samples with 10% DMPC and different concentrations of NP's were examined by ATF-FTIR to establish the impact of NP's on phase behavior of model phospholipids systems. NP's with magnetic core have attractive properties which can be used in biomedical application (for example MRI), so also were done measurements to define the nanotoxicity on model systems at physiological temperature of human body.

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