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 present calculations of the 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 are based on first-principles Density Functional Theory (DFT) with General Gradient Approximation GGA+U using Wien2K package [1]. Density of states (DOS) are obtained by the modified tetrahedron method. The calculated DOS of all investigated compounds for the spin up electrons show a gap close to Fermi energy E_F. Doping of Fe and Co shifts this gap below E_F whilst Ni of above E_F. For the spin down electrons E_F lies in energy gap in all cases. The calculated magnetic moments per formula unit of 2.7, 2.3 and 2 μ_B respectively for Ni, Co and Fe doping are in good agreement with experiment [2, 3].

References:

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