Electronic band structure of \( \text{La}_{2/3}\text{Pb}_{1/3}\text{Mn}_{2/3}(\text{Co,Fe,Ni})_{1/3}\text{O}_3 \)

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We present calculations of the band structure of half-metallic \( \text{La}_{2/3}\text{Pb}_{1/3}\text{Mn}_{2/3}(\text{Co,Fe,Ni})_{1/3}\text{O}_3 \) 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 \( \mu_B \) respectively for Ni, Co and Fe doping are in good agreement with experiment \([2, 3]\).

References: