

# Temperature and magnetic field dependent LDA+GTB band structure of LaCoO3

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Quasiparticle band structure of spin singlet Mott insulator LaCoO3 is calculated within the multielectron LDA+GTB approach. The low spin (LS)  $\text{Co}^{+3}$  ground term is separated by a small spin gap  $E_s \sim 10$  meV from the nearest excited high spin (HS) term. At  $T=0$  the top of the valence (bottom of conductivity) band is determined by the electron removal (addition) to the LS terms of  $d^5$  ( $d^7$ ) configuration. The large insulator gap is equal to  $E_g=1.5$  eV. At finite temperature the nonzero population of the HS  $d^6$  configuration results in the additional HS  $d^6$ -HS  $d^5$  electron removal excitation forming the in-gap band below the bottom of the valence band. The width of the in-gap increases with temperature,  $E_g$  decreases up to zero at  $T_{\text{IMT}}=585$ . Smooth insulator –metal transition occurs around this temperature. The magnetic susceptibility has two maxima, the first at  $T \sim E_s$ , and the second at  $T_{\text{IMT}}$ . Strong magnetic field also decrease  $E_s$  and at  $T=0$  the insulator –metal transition takes place at  $H>65$ T. For another ReCoO3 higher value of the spin gap shifts spin transition and insulator –metal transition to higher temperatures.