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

S.G.Ovchinnikov[1,2], Yu.S.Orlov[1,2]

1) L.V.Kirensky Institute of Physics SBRAS, Krasnoyarsk, Russia

2) Siberian Federal University, Krasnoyarsk, Russia

Quasiparticle band structure of spin singlet Mott insulator LaCoO3 is calculated within the multielectron LDA+GTB approach. The low spin (LS) Co^{+3} ground term is separated by a small spin gap E_s ~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 Eg=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, Eg decreases up to zero at T_{IMT}=585. Smooth insulator –metal transition occurs around this temperature. The magnetic susceptibility has two maxima, the first at T~E_s, and the second at T_{IMT}. Strong magnetic field also decrease E_s and at T=0 the insulator –metal transition takes place at H>65T. For another ReCoO3 higher value of the spin gap shifts spin transition and insulator –metal transition to higher temperatures.