Really first principles calculations for CoF_3

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We have performed calculations of the low-energy electronic structure of CoF_3 from first principles, assuming the atomistic construction of matter and the electrostatic origin of the crystal-field splitting. CoF_3 is one of compounds with the trivalent Co ions but in contrary to nonmagnetic $LaCoO_3$ (Phys. Rev. B **67** (2003) 172401) exhibits antiferromagnetism below $T_N = 460$ K. In our atomic-like approach QUASST the d electrons of the Co^{3+} ion in CoF_3 form the highly-correlated atomic-like system $3d^6$ in the high-spin state resulting from the octahedral subterm $^5T_{2g}$ (^5D term) ground state. We have derived the low-energy electronic structure taking into account the trigonal distortion and the relativistic spin-orbit interaction. With the discrete electronic structure for $3d$ electron we have described the magnetic properties (the value of the magnetic moment and its direction) and temperature dependence of the specific heat together with the λ-type peak at T_N. We evaluated the orbital moment and the strength of spin interactions responsible for the formation of the magnetic state.