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Density functional calculation of the electronic and magnetic properties of α-CoV_2O_6 ANDRES SAUL, CINaM/CNRS, GUILLAUME RADTKE, IM2NP — In this work, the magnetic properties of the low dimensional α-CoV_2O_6 system have been investigated using density-functional calculations. This system is constituted of CoO_6 octahedra connected by the edges and forming one dimensional linear chains. The experimental magnetization curves recorded at very low temperature show a surprising magnetization plateau at one-third of the saturation magnetization and a strong anisotropy. The estimated Co magnetic moment is large reaching a value of 4.5 μ_B suggesting a large orbital contribution. Our calculations show that three different magnetic configurations for the Co are possible, the lowest energy one being a high spin configuration in agreement with the S=3/2 character of the Co^{+2} ion observed in this compound. Spin-orbit interactions have been included in order to calculate the magnetic anisotropy and the orbital contribution to the magnetic moment. The results are discussed in terms of crystal field splitting of the $3d$ orbital and a tight-binding Hamiltonian. Using a broken-symmetry formalism we have evaluated the effective exchange interactions of the Heisenberg Hamiltonian. They allow us to propose the magnetic structures corresponding to the ground state and to the observed magnetization plateaus.

Andres Saul
CINaM/CNRS

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