Centre Interdisciplinaire de Nanoscience de Marseille

Sous la cotutelle de

Frustration and magnetic order in α-CoV_2O_6

Andres Saul[1], Damir Vodenicarevic[1], and Guillaume Radtke[2]
[1]CINaM, CNRS and Université d'Aix-Marseille
[2]IM2NP, CNRS and Université d'Aix Marseille

CoV_2O_6 is currently at the center of an intense research activity due to its peculiar magnetic properties. It shows a very strong magnetocristalline anisotropy accompanied by a huge orbital contribution to its total magnetic moment (4.6 μ_B /Co ion instead of 3.0 μ_B for the spin S=3/2 only value). More interestingly, it exhibits a metamagnetic behaviour characterized by two steps in its magnetization curve for finite external fields, delimiting a plateau at 1/3 of the saturation magnetization in the absence of obvious triangular or kagome type lattice (Fig. 1(a)).

In this work, the electronic structure and magnetic properties of α-CoV_2O_6 are investigated using density functional theory calculations including spin-orbit coupling and orbital polarization effects.

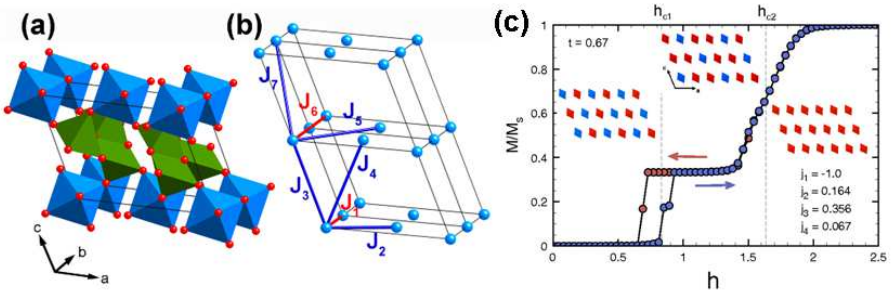

Figure 1) (a) Atomic structure of α-CoV_2O_6 : Red balls denote oxygen ions, CoO_6 octahedra are shown in blue and VO_5 square pyramids in green. (b) Magnetic couplings in α-CoV_2O_6 : Intrachain couplings are shown in red and interchain couplings are shown in blue. (c) Magnetization curve obtained by Metropolis Monte Carlo calculations. The crystal is observed along the chain direction and red (resp. blue) octahedra represent spin-up (resp. spin-down) magnetic moments.

These calculations reveal a strong magnetocristalline anisotropy with a magnetization easy axis close the **c** axis. Moreover, the evaluation of magnetic couplings (Fig. 1(b)) on the basis of broken-symmetry formalism suggests the occurrence of an antiferromagnetic ground-state order where ferromagnetic chains running along **b** are coupled antiferromagnetically to their nearest-neighbors along **a** and **c**.

Monte Carlo simulations are finally employed to explore the origins of the 1/3 plateau observed in the magnetization curves of this compound and to propose a structure for the corresponding state (Fig. 1(c)).