

DIRECTION DES SCIENCES DE LA MATIÈRE,
INSTITUT RAYONNEMENT MATIÈRE DE SACLAY
SERVICE DE PHYSIQUE ET DE CHIMIE DES SURFACES ET DES INTERFACES

SEMINAIRE

Jeudi 18 octobre 2012 à 11h00[†]

Bâtiment 466, salle 111 - CEA Saclay, 91191, Gif sur Yvette

Frustration and magnetic order in α - CoV_2O_6 Andres Saul¹, Damir Vodenicarevic¹, and Guillaume Radtke²

¹CINaM, CNRS and Université d'Aix-Marseille

²IM2NP, CNRS and Université d'Aix-Marseille

(invité par Cyrille Barreteau)

CoV_2O_6 is currently at the center of an intense research activity due to its peculiar magnetic properties. It shows a very strong magnetocrystalline anisotropy accompanied by a huge orbital contribution to its total magnetic moment (4.6 μB /Co ion instead of 3.0 μB 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.

These calculations reveal a strong magnetocrystalline 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)).

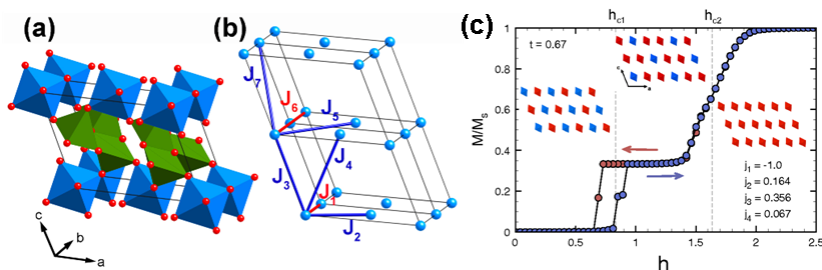


Figure 1) (a) Atomic structure of α - CoV_2O_6 : Red balls denote oxygen ions, CoO_6 octahedra are shown in blue and VO_5 square pyramids in green. (b) Magnetic couplings in α - CoV_2O_6 : Intrachain couplings are shown in red and interchain couplings are shown in blue. (c) Magnetization curve obtained 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.

†Attention: Date Inhabituelle

Formalités d'entrée: Contacter le secrétariat pour l'établissement de votre autorisation d'entrée sur le centre de Saclay. Tel : 01.69.08.65.32 ou 01.69.08.40.12; Fax : 01.69.08.40.44 ; e-mail : catherine.julien@cea.fr. Le délai minimum est de 24 heures pour les visiteurs ressortissants des pays de l'Union Européenne, et de huit jours pour les autres. Sans autorisation, vous ne pourrez entrer sur le centre de Saclay. Dans tous les cas, se munir d'une pièce d'identité.