Poster

Electron diffraction boosts research on molecule-based magnets

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Development molecule-based magnetic materials built of metal-organic coordination frameworks requires their structural characterization [1]. However, large enough single crystal suitable for X-ray diffraction are notoriously difficult to grow hampering structure determination and discouraging research in the field.

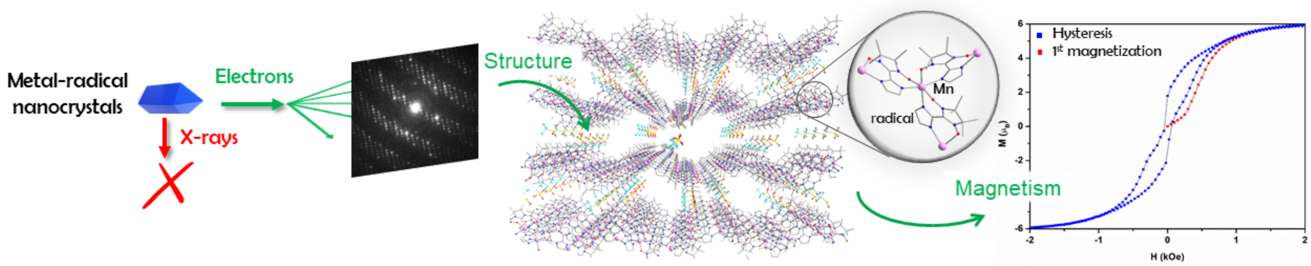

Figure 1. Electron crystallography of 2D metal-radical coordination frameworks with metamagnetic properties

To address this obstacle we show here that the structure of two novel compounds based on 2D manganese(II)-radical coordination polymers could be successfully determined from nanocrystals by combining recent developments in TEM [2,3] with electron crystallography data processing methods designed for protein crystals [4] . Diffraction data were collected using a low-dose technique on a Tecnai F20 TEM operated at 200 kV. Samples were continuously rotated while recording diffraction patterns with a Medipix3RX hybrid pixel detector (Figure 2). Crystal structure solution was achieved by molecular replacement [5] . Magnetic measurements show a ferrimagnetic behavior within the 2D metal-radical sheets due to alternating antiferromagnetically coupled spins ($S_{Mn^{2+}}$ = 5/2 and $S_{radical}$ = 1/2). Both compounds exhibit a long-range 3D ordering of weak ferromagnetic nature with Curie temperatures T_c = 45 K (for **1**) and 40 K (for **2**) associated with spin canting and a field-induced metamagnetic transition from antiferromagnetic to ferromagnetic coupling of 2D metal-radical sheets is observed.

This results are novel evidence electron crystallography is a unique tool to solve structures of metal-organic nanocrystals even with components too sensitive to standard electron doses. This open new prospects for development of molecule-based for which structural knowledge is a prerequisite for establishing magnetic-structural correlations and new advances in their design.

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