FLAIR Colloquium

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Relation between local structure and magnetic exchange interactions in $RE_2Mo_{2-y}Mn_yO_7$ pyrochlores

Prof. Dr. Carlo Castellano

Dipartimento di Chimica, Università degli Studi di Milano, Italy

Abstract

Pyrochlores are complex and multifunctional oxides having general formula $RE_2^{3+}B_2^{4+}O_7$, where *RE* is a trivalent rare earth and *B* is a tetravalent transition metal ion. Due to their several possible compositions and highly versatile nature, they offer a wide range of challenging physical properties and potential technological applications. Pyrochlores can be employed as insulators, ion and electron conductors, superconductors, catalysts, ion exchangers, nuclear waste matrices, phosphors and solid-oxide fuel cells cathodes.

The *RE* and *B* cationic sites form a network of corner-sharing tetrahedra in presence of competing magnetic interactions and of short-range ordered geometrically frustrated phases at low temperature, such as spin glasses, spin ices and spin liquids. Indeed, the everlasting order/disorder competition observed in these strongly correlated electron oxides, permanently coupled with different magnetic exchange couplings, plays a pivotal role in tuning their physico-chemical properties.

In this contribution an EXAFS study at the Mo K-edge of novel $RE_2Mo_{2-y}Mn_yO_7$ pyrochlores (*RE* = Gd and Ho; y = 0.00, 0.10 and 0.20) performed as a function of temperature and coupled to magnetic susceptibility measurements is presented, to check the relation between local structure parameters and nearest-neighbor magnetic interactions. The $RE_2Mo_2O_7$ undoped compounds display a transition from a spin-glass (SG) to a long-range ferromagnetic (FM) phase on increasing the rare earth average ionic radius on site *RE* and the related Mo-O-Mo bond angle. Evidence of an anomalous local lattice disorder below 225 K was found in the first Mo-O shell of the low-temperature FM $Gd_2Mo_2O_7$ related to the location of this composition on the border

between the SG and FM regimes. Otherwise, a local order compatible with a lattice frustration was observed in the SG $Ho_2Mo_2O_7$ [1]. After Mn-doping, a competition between double-exchange (undoped case) and superexchange magnetic couplings is established. $Ho_2Mo_{2-y}Mn_yO_7$ (y = 0.10 e 0.20) remain SG while the two $Gd_2Mo_{2-y}Mn_yO_7$ compositions show the appearance on a local scale of a new SG transition mirrored by a quite high structure disorder and by a distortion coherent with a lattice frustration after Mn-doping [2]. As in the undoped system, we confirm the presence on a local scale of a MoO_6 octahedra distortion for all the compounds. Therefore, the Gd and Ho Mn-doped samples display a similar structure and magnetic frustrated behavior, differently from the corresponding undoped compositions.

[1] C. Castellano *et al.*, J. All. and Compd. **723**, 327 (2017)

[2] C. Castellano *et al.*, J. All. and Compd. **865**, 158958 (2021)