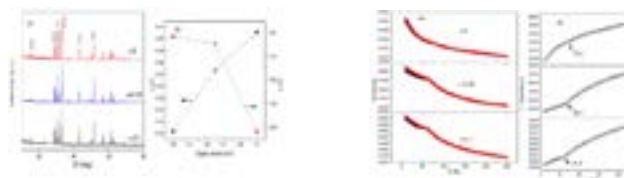


## Effect of Cu substitution on the magnetism and electronic structure of hexagonal $\text{YMnO}_3$

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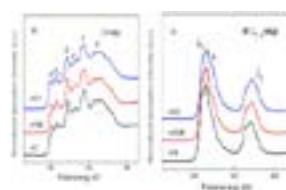
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$\text{YMnO}_3$ , a multiferroic, shows a low Neel temperature  $T_N$  of about 75 K which hinders its practical applications. Thus, we doped Cu into it to improve its magnetism. All the  $\text{YMn}_{1-x}\text{Cu}_x\text{O}_3$  samples crystallize into single phase of the hexagonal structure with P63 c m space group detected by XRD. The lattice parameter  $a$  increases while  $c$  decreases with increasing copper concentration, probably due to the difference in the ionic radii and the change of the hybridization between ions. The magnetic properties of  $\text{YMn}_{1-x}\text{Cu}_x\text{O}_3$  samples are enhanced after doping Cu due to the deformation of the Mn trimer magnetic frustration arrangement and the double-exchange interaction between  $\text{Mn}^{3+}$  and  $\text{Mn}^{4+}$ . The normalized O K-edge XAS spectra of  $\text{YMn}_{1-x}\text{Cu}_x\text{O}_3$  show the hybridizations of O1s with Mn 3d/Mn 4sp and Y 4d/Y 5sp orbitals. With increasing Cu ions concentration, the intensity of  $e_{2g\downarrow}$  peaks is enhanced indicating the enhancement of the orbital hybridization between Mn and  $\text{O}_p$ . The in-plane hybridization strength enhances, leading to the decreases of Mn-OP bond length, in accordance with the XRD results. The normalized Mn  $L_{3,2}$ -edge XAS spectra of the samples suggest the increase of the number of unoccupied Mn 3d states along the  $c$ -axis direction and the presence of  $\text{Mn}^{3+}$  and  $\text{Mn}^{4+}$  ions, causing double-exchange interactions and affecting the magnetic ordering of the frustrated  $\text{Mn}^{3+}$  spins.



**Figure 1:** (a) Room temperature XRD patterns of  $\text{YMn}_{1-x}\text{Cu}_x\text{O}_3$  samples ( $x=0, 0.05, 0.1$ ). (b) Cu-content dependence of lattice constants  $a$  and  $c$ .

**Figure 2:** Temperature dependence of the magnetization (a) and the in-verse susceptibility (b) for  $\text{YMn}_{1-x}\text{Cu}_x\text{O}_3$  ( $x=0, 0.05, 0.1$ ).



**Figure 3:** The X-ray absorption spectra (XAS) of O K-edge (a) and Mn  $L_{3,2}$ -edge (b) of the samples

### Biography

Qi Li has completed his PhD in 1997 from National Synchrotron Radiation Laboratory, University of Science and Technology of China, and Postdoctoral studies from Technical Physics Department, Peking University during Oct. 1997 to Aug. 1999, and from Physics Department, University of Leeds, United Kingdom, from Apr. 2001 to Apr. 2003. He has visited the Physics Department, University of Saskatchewan, Canada, from May 2007 to May 2008, as a Visiting Scholar. He is a Professor of Physics at Southeast University, China. He has published more than 40 papers in reputed journals and has been serving as a reviewer of several reputed journals.

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