

Room-temperature multiferroic behavior in layer-structured Aurivillius phase ceramics

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Zheng Li, Vladimir Koval , Amit Mahajan, Zhipeng Gao, Carlo Vecchini, Mark Stewart, Markys G. Cain , Kun Tao, Chenglong Jia , Giuseppe Viola, and Haixue Yan 



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Zheng Li,¹ Vladimir Koval,² Amit Mahajan,³ Zhipeng Gao,⁴ Carlo Vecchini,⁵ Mark Stewart,⁵ Markys G. Cain,⁶ Kun Tao,⁷ Chenglong Jia,^{7,a)} Giuseppe Viola,³ and Haixue Yan^{3,b)}

AFFILIATIONS

¹Guangxi Institute of Materials, Guangxi University, Nanning 530004, China
²Department of Materials Science and Engineering, Tsinghua University, Beijing 100084, China
³Department of Physics, University of Calabria, I-87030 Arcavacata, Italy
⁴National Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, Beijing 100190, China
⁵Department of Physics, University of Calabria, I-87030 Arcavacata, Italy
⁶Department of Physics, University of California, Los Angeles, California 90095, USA
⁷Department of Materials Science and Engineering, Tsinghua University, Beijing 100084, China

a)Email: chengljia@tsinghua.edu.cn
 b)Author to whom correspondence should be addressed: yanhx@semi.ac.cn

ABSTRACT

Multiferroic Aurivillius phase ceramics (APCs) are a class of layered perovskite materials with a unique structure. In this work, we report the synthesis and characterization of a series of APCs with the general formula $B_{5-2x}L_{0.75}F_xC_{1-x}O_{18}$ (where $B = Bi, Pb, Ba, Sr, Ca, Sr, Ba, Sr, Ca$ and $L = La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Y, Yb, Lu$). The structure of these materials is characterized by the presence of a central layer of AB_2O_4 units, which is sandwiched between two layers of AB_2O_4 units. The structure of these materials is characterized by the presence of a central layer of AB_2O_4 units, which is sandwiched between two layers of AB_2O_4 units. The structure of these materials is characterized by the presence of a central layer of AB_2O_4 units, which is sandwiched between two layers of AB_2O_4 units. The structure of these materials is characterized by the presence of a central layer of AB_2O_4 units, which is sandwiched between two layers of AB_2O_4 units.

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~ 494 K
 $M/$),
 $B_6F C_3O_{18}$ (526 K).²³
 BLFC
 $F^{3+} O F^{3+}, C^{3+} O C^{3+}, F^{3+} O C^{3+}$ (.
 ED
 FC $2 \sim 353$ K
 $C_2F O_4$ 2 $16,25$
 $C_2F O_4$ (460 K)
 (M) $C_2F O_4$ 1.4 . %
 16 23.5 / .²⁵ , 0.22 0.32 / ,
 $C_{2-} F O_4$ BLFC
 $M = 1.85$ / , $F . 2() . I$
 $M H$
 $2 (F . 3)$ 1
 425 K 1.58 / . 0.27 / ,
 ED
 BLFC
 F 3 A
 $F^{3+} O C^{3+}$
 (DF) *ab initio*
 (A P)
 $U_F = 2$ $U_C = 3$ F C ,
 (GGA) U . I
 BLFC
 $F . 3()$, F^{3+} C^{3+} (3.1 $2.1 \mu_B/$,) ,
 O
 ($0.1 \mu_B/$) .
 F O_6 $C O_6$ F / C -
 F O - / $F . 3()$.
 F^{3+} C^{3+} ,
 (. ,) (. ,)
 $E_{FM} - E_{AFM}$
 $= -144.1$.
 H , (FM)
 43.5 (. , 504.6 K),
 1 FC/FC $F . 2()$.
 $a b$
 010 .
 BLFC F 4 . I
 PFM BLFC , 399 O .
 $5() . A$ F .
 P F M
 F -

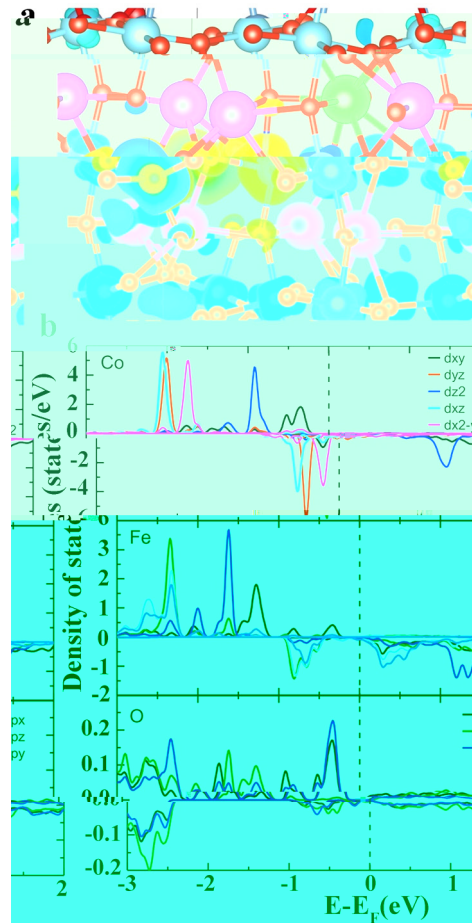


FIG. 3. (a) Crystal structure of BLFC. (b) Density of states (DOS) for Co, Fe, and O atoms. The DOS is calculated using the GGA+U method with $U_F = 2$ eV and $U_C = 3$ eV. The DOS is shown for the d_{xy} , d_{yz} , d_{z^2} , d_{xz} , and $d_{x^2-y^2}$ orbitals. The x-axis is $E - E_F$ (eV) and the y-axis is Density of states (stat/s/eV).

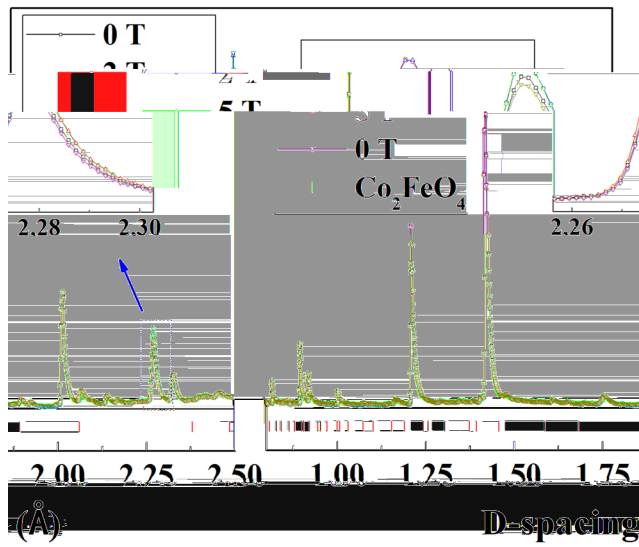


FIG. 4. XRD patterns of Co_2FeO_4 at various magnetic fields (0 T, 5 T) and temperatures. The inset shows a schematic of the experimental setup.

Co_2FeO_4 (P) (M) (G) 100 010
 +2000 O
 -2000 O
 F . 5 () .
 5 () .
 C₂F O₄

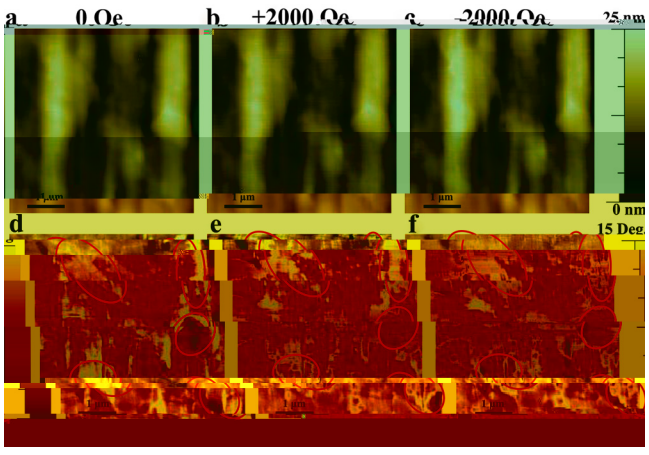


FIG. 5. MFM images of Co_2FeO_4 at different magnetic fields: (a) 0 Oe, (b) +2000 Oe, (c) -2000 Oe. The images show magnetic domains with a 25 nm scale bar. Below the MFM images are corresponding topographic images (d, e, f) with a 15 nm scale bar.

$T = P \times M$
 BLFC
 I , A BLFC
 F
 $\text{C}^{3+} \text{O} \text{C}^{3+}, \text{F}^{3+} \text{O} \text{C}^{3+}$ $\text{F}^{3+} \text{O} \text{F}^{3+}$
 A , C / F
 EM (ED) BLFC
 D . M , P D . K , D.
 D I H I I N , AL,
 D , O K.
 A E D F
 G A A (G N . 2/
 0038/20), C (G N . K2015-0602006), N FC (G
 N . 11474138 11834005). A
 E M P (EM P)
 P IND54 N EM P
 EM P E P AME E

DATA AVAILABILITY

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