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## ABSTRACT

Multiferroic Aurivillius phase ceramics (APCs) exhibit room-temperature multiferroic behavior. However, the origin of the multiferroicity in these materials remains unclear. In this work, we study the multiferroic behavior of  $B_{5.25}L_{0.75}F_2C_3O_{18}$  (Aurivillius phase) using *in situ* X-ray diffraction and neutron diffraction. The results show that the multiferroicity in  $B_{5.25}L_{0.75}F_2C_3O_{18}$  is due to the presence of  $F^{3+}$  and  $O^{3+}$  ions. The  $F^{3+}$  ions are located at the  $2c$  sites, and the  $O^{3+}$  ions are located at the  $4d$  sites. The presence of these ions leads to the formation of a magnetic structure with a net magnetic moment. This magnetic moment is coupled to the ferroelectric polarization, resulting in multiferroic behavior.

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$\sim 494$  K (M/),  
 $B_6FC_{3O_{18}}$  (526 K).<sup>23</sup>  
 BLFC  
 $F^{3+} O F^{3+}, C^{3+} O C^{3+}, F^{3+} O C^{3+}$  (.  
 ED  
 $\sim 353$  K  
 $C_2F_4O_4$  (460 K) (M)  $C_2F_4O_4$  .<sup>16,25</sup>  
 $16.235 / .$  ,  $0.22 0.32 /$  , BLFC  
 $C_2F_4O_4$  ,  $1.4 .\%$   
 $M = 1.85 / , F . 2( ) . I$   
 $M H$   
 $2 (F . 3) .$   $425$  K  $1.58 / .$   $0.27 /$  , ED  
 BLFC  
 $F_3$   $F^{3+} O C^{3+}$   
 (DF)  $ab initio$   
 (A P)  
 $F = 2$   $C = 3$   $F$   $C$  ,  
 (GGA)  $I$   
 BLFC  
 $F . 3(a)$  ,  $F^{3+}$   $C^{3+}$  ( $3.1$   $2.1 \mu_B/a$  , ) ,  
 $0.1 \mu_B/a$  ) .  
 $F O_6$   $C O_6$   $F/C$  -  $F . 3( )$  .  
 $F$   $O$  -  $F . 3( )$  .  
 $F^{3+}$   $C^{3+}$  ,  
 $( . , )$   $( . , )$  -  
 $E_{FM} - E_{AFM}$   
 $= -144.1$  .  
 $H$  , (FM)  $2 < H < 5$  ,  
 $43.5$  ( . , 504.6 K), FM  
 $1$  FC/FC  $F . 2( )$  .  
 $a b$   
 $010$  .  
 $F_4$   
 BLFC  $I$   $399 O$  .  
 $P F M$  BLFC ,  $F$  .  
 $5( ) . A$   $P F M$  BLFC ,  $F$  -

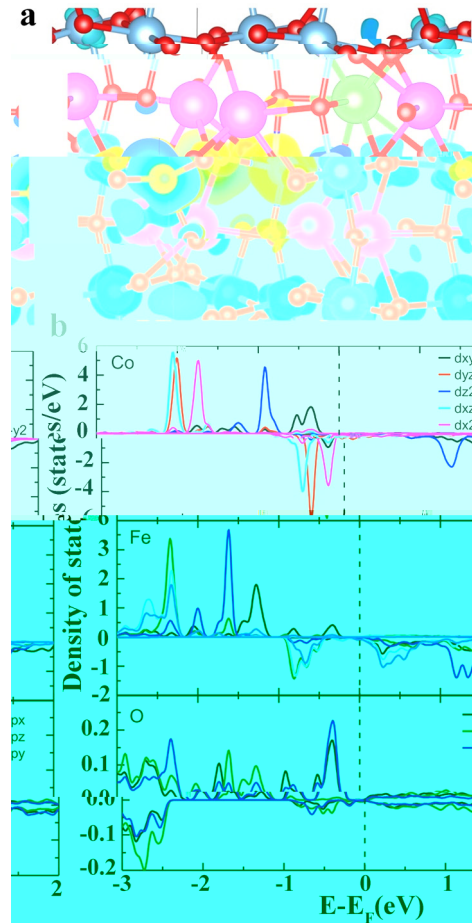


FIG. 3. (a) Crystal structure of BLFC. (b) Density of states (DOS) for Co, Fe, and O atoms. The DOS is calculated using the GGA+U method with  $U = 0.005$  eV. The x-axis is  $E - E_f$  (eV) and the y-axis is Density of states (states/eV).



- <sup>16</sup>M. P. ... P. C. ..., M. B. ..., A. P. B. ..., J. P. H. ..., K. ..., L. K. ..., M. P. ..., C. ..., H. K. ..., A. J. B. ..., *J. A. P.* **112**, 073919 (2012).
- <sup>17</sup>J. L. ..., H. ..., M. J. ..., K. ..., P. ..., *J. A. P.* **102**, 104107 (2007).
- <sup>18</sup>M. G. C. ..., *Characterisation of Ferroelectric Bulk Materials and Thin Films* (..., 2014), ...2.
- <sup>19</sup>...L., K. ..., J. M. ..., G. ..., K. ..., C. J. ..., G. ..., H. ..., A. M. ..., J. C. ..., M. C. ..., I. A. ..., C. N. ..., C. J. ..., H. ..., *J. M. C. C.* **6**, 2733 (2018).
- <sup>20</sup>...K. ..., I. ..., G. ..., M. ..., C. J. ..., H. ..., *J. P. C.* **122**, 15733 (2018).
- <sup>21</sup>L. J. ..., F. L. ..., ..., *J. A. C.* **97**, 1 (2014).
- <sup>22</sup>H. ..., F. I. ..., G. ..., H. N. ..., H. ..., J. ..., G. ..., M. J. ..., *J. A. D.* **1**, 107 (2011).
- <sup>23</sup>J. ..., L. ..., L. ..., ..., J. D. ..., ..., *A. P. L.* **101**, 012402 (2012).
- <sup>24</sup>B. ..., J. ..., J. C. ..., ..., L. ..., ..., J. D. ..., ..., *A. P. L.* **104**, 062413 (2014).
- <sup>25</sup>I. P. M. ..., ..., N. B. ..., ..., **11**, 719 (2009).