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AFFILIATIONS

[1]G _ I ᴜ , C f G f , ᴜ 430074, C
[2]I ᴜ f M , _ A _ f _ 47, K 04001, _
[3] f E f M , ᴜ M , _ f L , L E1 4N , K f _
[4]N K L _ D I ᴜ F ᴜ , C A _ f E , M 621900, C
[5]N L , H _ , 11 0L , K _
[6]E L , F _ , ᴜ G 9 9 , K _
[7] f , L ᴜ _ , L ᴜ 730000, C

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ABSTRACT

M . H , A . H , A $B_{5.25}L_{0.75}FC_3O_{18}$ P A *in situ* F $^{3+}$ O F $^{3+}$, C $^{3+}$ O C $^{3+}$, F $^{3+}$ O C $^{3+}$ A , C /F -

M (FM) (FE) A $B_5F_3O_{15}$ (=4) $B_6F_2O_{18}$ (=5), B_4O_{12} BFO_3, FE FM .[12,13] B C F B- , $B_5F_{0.5}C_{0.5}O_{15}$ (=4) B_6FCO_{18} (=5) .[1–4] H , .[5] A $(B_2O_2)^{2+}(A_{-1}B\ O_{3\ a+1})^{2-}$ (A , 12- , B).[6] B- BFO_3 .[7–11] .[14,15] H , D .[16] , A

I , A B 5.25L 0.75F C 3O18 (BLFC) P (P). P L P C , F , [14,17] D A BLFC *a b* , P *a b* A . A , [18] A , *in situ* I H I I N , AL, D O , K. F ( ). , A BLFC P . BLFC P . , . F 1 (D) BLFC . A *B2cb* A *A2*$_1$, A . [19,20] *B2cb* *a* = 5.4530(2) A, *b* = 5.4427(1) A, *c* = 50.670(2) A *A2*$_1$*am* *a* = 5.4651(6) A, *b* = 5.3943(6) A, *c* = 41.487(2) A F P (:// . .).

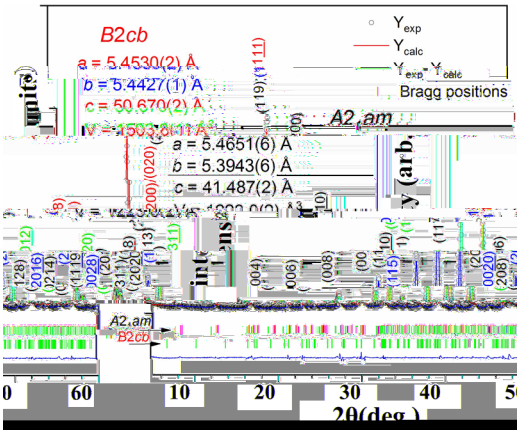

FIG. 1. - B .

BLFC - A = 4 = 5 . N D' . F 1 EM BLFC . - (*a–b*) . M , F . 1 1.4 . %, D. ED (F . 2 1) F , C , O, . , C 2F O4 - A B 5F 0.5C 0.5 3O15.[16] F 2( ) BLFC P (50, 70 100, 300, 500 H). 1060 K FE *T* BLFC . H BLFC B 6 3F 2O18 (973 K).[13] F 2( ) *P–E* *I–E* BLFC P . *I–E* [21,22] BLFC 10 μC/ 2. F 2( ) (FC) - (FC) 200 O BLFC . BLFC

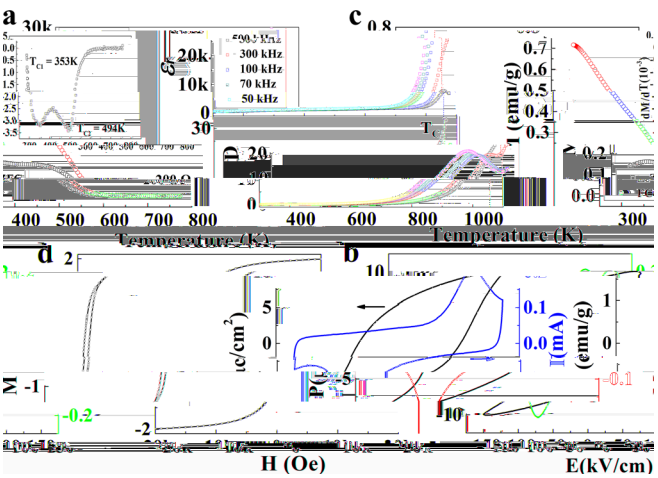

FIG. 2. ( ) ( ) B ⊥ P . ( ) P B P . ( ) B ⊥ / = 200 . - M/ . ( ) - 300 B .

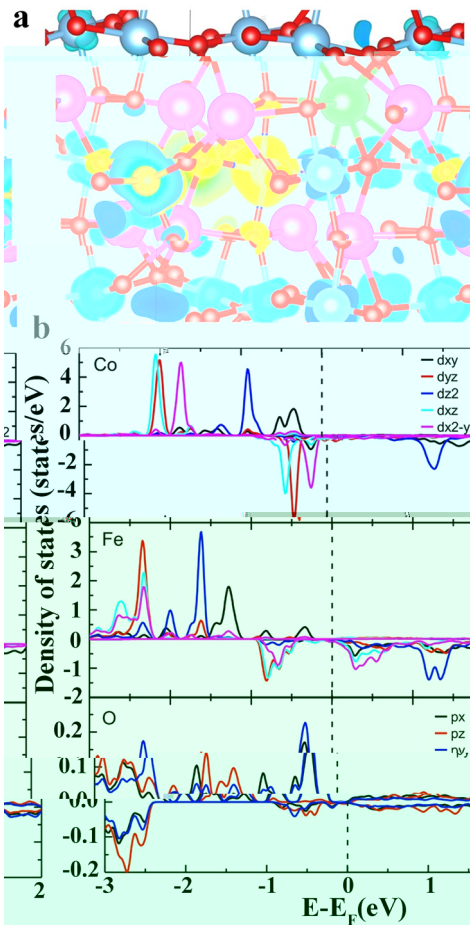

FIG. 3. ( ) (= 0.005) ( ), B ( ), ( ), ( ), ( ), ( ) . ( ) A 3+ 3+.

. N . I F . 4, A (0 1 20) , 2 . F (2 ≤ H < 5), 2 , M H F . 2( ) 3. F , F 5 BLFC P F M PFM BLFC , F . 5( ). A F -

(1 ∼ 494 K (M/), B 6F C 3O18 (526 K).[23] BLFC F 3+ O F 3+, C 3+ O C 3+, F 3+ O C 3+ (.).[24] ED A FC 2 ∼ 353 K C 2F O4. C 2F O4 (460 K) [16,25] (M) C 2F O4 16 23.5 / .[25] , 1.4 . % C 2– F O4 0.22 0.32 / , BLFC M = 1.85 / , F . 2( ) . I , M H 1 2 (F . 3). 425 K 1.58 / 0.27 / , ED BLFC A F 3 F 3+ O C 3+ *ab initio* (DF) (A P) . H F = 2 C = 3 F C , (GGA)+ . I BLFC F . 3( ), F 3+ C 3+ (3.1 2.1 μ_B/ ,), O (0.1 μ_B/). F O6 C O6 ( ) F /C F O / . F . 3( ). F F 3+ C 3+ (. .,) (. .,) , . $E_{FM} - E_{AFM}$ = −144.1 . H . (FM) 43.5 (. ., 504.6 K), FM 1 FC/FC . F . 2( ). *a b* . , 010 . F 4 BLFC I - , - ,

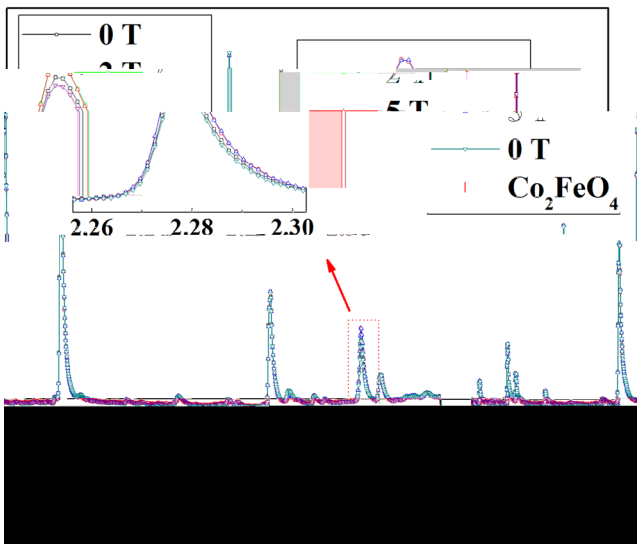

FIG. 4. - B (0, 2, 5 0).

C - ( ) +2000 O F . 5( ) . −2000 O F . 5( ) . (-) C 2F O4 - P A BLFC . G (P) 100 (M) 010 , (-

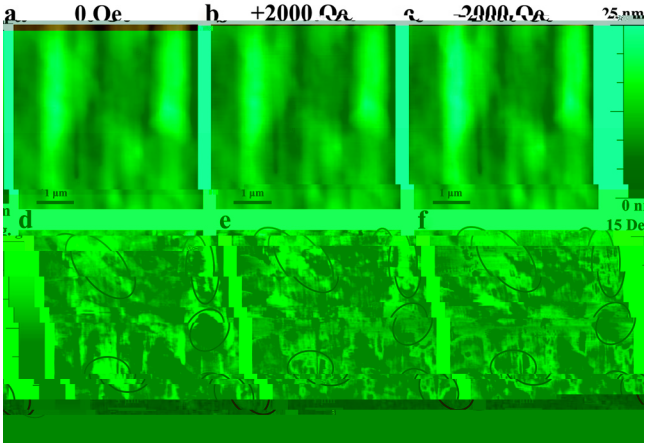

FIG. 5. B ( ). ( ) ( ) P M 0 ( ) ( ) P M +2000 ( ) ( ) P M −2000 .

) $T = P \times M$ BLFC . I , A BLFC . F F 3+ O F 3+, C 3+ O C 3+, F 3+ O C 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 AME E .

DATA AVAILABILITY

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